Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 03:35 am BST

PDB ID	:	6N77
Title	:	Structure of the human JAK1 kinase domain with compound 15
Authors	:	Lupardus, P.J.; Brown, D.
Deposited on	:	2018-11-27
Resolution	:	1.64 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
https://www.wwpdb.org/validation/2017/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:

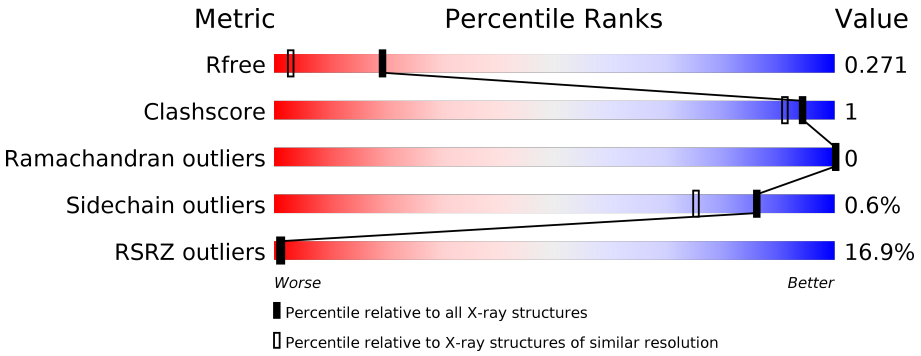
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.64 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}	130704	3122 (1.66-1.62)
Clashscore	141614	3268 (1.66-1.62)
Ramachandran outliers	138981	3215 (1.66-1.62)
Sidechain outliers	138945	3215 (1.66-1.62)
RSRZ outliers	127900	3079 (1.66-1.62)

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 respectively. 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 <=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	302	15% 89% • 7%
1	B	302	17% 90% • 8%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5016 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.

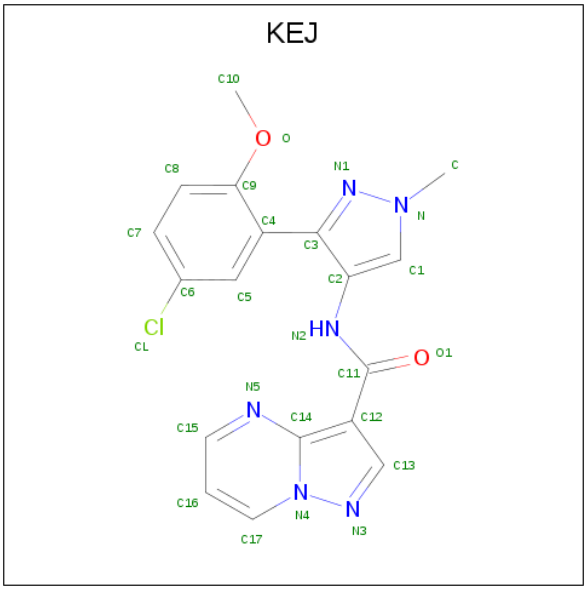
- Molecule 1 is a protein called Tyrosine-protein kinase JAK1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	280	Total	C	N	O	P	S	6	4	0
			2288	1462	388	421	2	15			
1	B	279	Total	C	N	O	P	S	0	2	0
			2271	1451	383	420	2	15			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	853	GLY	-	expression tag	UNP P23458
B	853	GLY	-	expression tag	UNP P23458

- Molecule 2 is N-[3-(5-chloro-2-methoxyphenyl)-1-methyl-1H-pyrazol-4-yl]pyrazolo[1,5-a]pyrimidine-3-carboxamide (three-letter code: KEJ) (formula: $C_{18}H_{15}ClN_6O_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Cl	N	O	0	0
			27	18	1	6	2		

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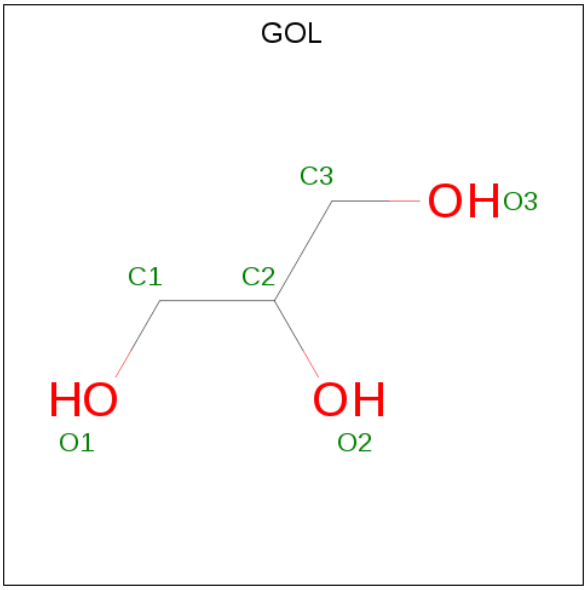
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	Cl	N	O	0	0
			27	18	1	6	2		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	O		0	0
			6	3	3			

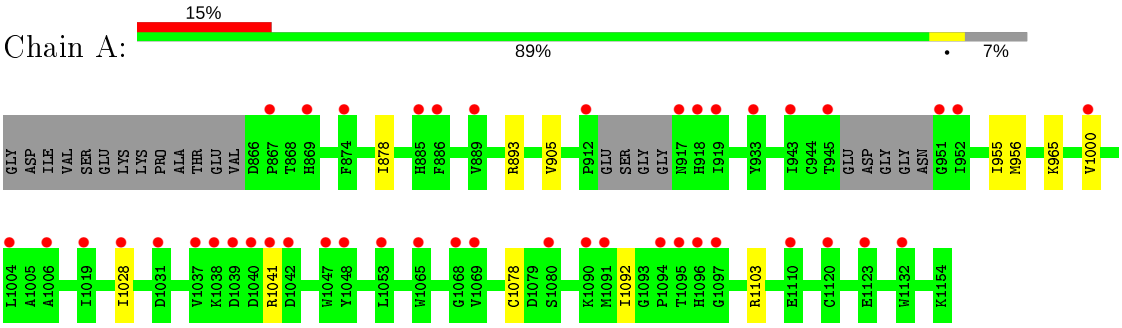
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	215	Total	O	0	0
			215	215		
4	B	182	Total	O	0	0
			182	182		

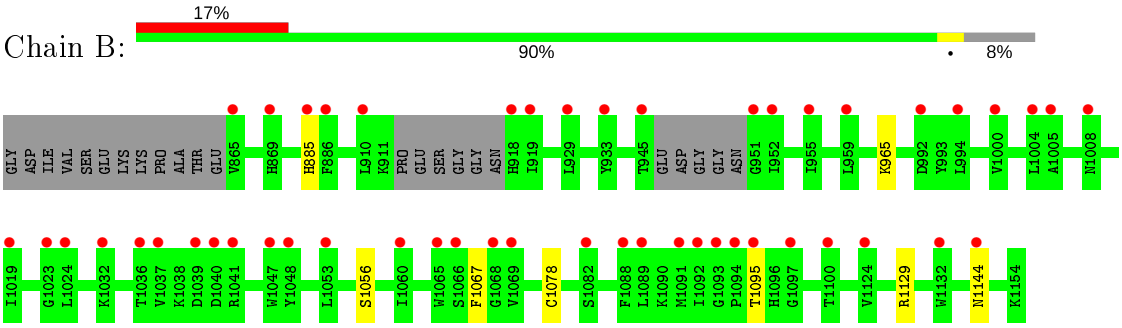
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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: Tyrosine-protein kinase JAK1



- Molecule 1: Tyrosine-protein kinase JAK1



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	43.12Å 175.54Å 45.68Å 90.00° 94.11° 90.00°	Depositor
Resolution (Å)	45.56 – 1.64 29.78 – 1.80	Depositor EDS
% Data completeness (in resolution range)	98.1 (45.56-1.64) 98.2 (29.78-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.48 (at 1.80Å)	Xtriage
Refinement program	BUSTER 2.11.7	Depositor
R, R_{free}	0.252 , 0.282 0.244 , 0.271	Depositor DCC
R_{free} test set	3117 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å^2)	18.5	Xtriage
Anisotropy	0.290	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 58.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	5016	wwPDB-VP
Average B, all atoms (Å^2)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.65% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: GOL, KEJ, 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	0/2312	0.61	0/3114
1	B	0.56	0/2295	0.60	0/3092
All	All	0.57	0/4607	0.60	0/6206

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	2288	0	2284	9	0
1	B	2271	0	2253	4	0
2	A	27	0	0	0	0
2	B	27	0	0	0	0
3	B	6	0	8	1	0
4	A	215	0	0	1	0
4	B	182	0	0	1	0
All	All	5016	0	4545	12	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 (12) 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:1092:ILE:HB	1:A:1103:ARG:HG3	1.88	0.56
1:B:1067:PHE:HD1	4:B:1462:HOH:O	1.90	0.53
1:A:1041:ARG:HD3	1:B:1095:THR:HB	1.90	0.52
1:A:905[B]:VAL:HG22	1:A:956:MET:O	2.12	0.50
1:A:1000[B]:VAL:HG21	1:A:1028:ILE:HD11	1.96	0.47
1:B:1129:ARG:HH21	3:B:1201:GOL:C1	2.28	0.47
1:A:1092:ILE:HB	1:A:1103:ARG:CG	2.44	0.47
1:A:878:ILE:HD11	1:A:893:ARG:HB2	1.98	0.45
1:A:956:MET:HE3	4:A:1490:HOH:O	2.16	0.44
1:B:965:LYS:HD2	1:B:1078:CYS:HB3	2.01	0.43
1:A:965:LYS:HD2	1:A:1078:CYS:HB3	1.99	0.43
1:A:905[B]:VAL:HG21	1:A:955:ILE:HG22	2.01	0.42

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	276/302 (91%)	270 (98%)	6 (2%)	0	100	100
1	B	274/302 (91%)	269 (98%)	5 (2%)	0	100	100
All	All	550/604 (91%)	539 (98%)	11 (2%)	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	251/267 (94%)	251 (100%)	0	100 100
1	B	248/267 (93%)	245 (99%)	3 (1%)	71 51
All	All	499/534 (93%)	496 (99%)	3 (1%)	86 75

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	885	HIS
1	B	1056	SER
1	B	1144	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

4 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	B	1034	1	15,16,17	0.51	0	19,22,24	0.88	2 (10%)
1	PTR	A	1034	1	15,16,17	0.50	0	19,22,24	0.51	0
1	PTR	B	1035	1	15,16,17	0.56	0	19,22,24	0.77	1 (5%)
1	PTR	A	1035	1	15,16,17	0.56	0	19,22,24	0.89	2 (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	PTR	B	1034	1	-	0/10/11/13	0/1/1/1
1	PTR	A	1034	1	-	0/10/11/13	0/1/1/1
1	PTR	B	1035	1	-	0/10/11/13	0/1/1/1
1	PTR	A	1035	1	-	0/10/11/13	0/1/1/1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	1035	PTR	O3P-P-OH	2.41	112.79	105.24
1	B	1034	PTR	CB-CA-C	-2.19	107.35	111.47
1	A	1035	PTR	CB-CA-C	-2.16	107.42	111.47
1	A	1035	PTR	P-OH-CZ	2.12	130.54	123.75
1	B	1034	PTR	O2P-P-OH	2.06	111.70	105.24

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)

3 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	$\#\|Z\|>2$
3	GOL	B	1201	-	5,5,5	0.09	0	5,5,5	0.26	0
2	KEJ	B	1202	-	22,30,30	0.69	0	25,43,43	0.58	0
2	KEJ	A	1201	-	22,30,30	0.72	0	25,43,43	0.65	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
3	GOL	B	1201	-	-	3/4/4/4	-
2	KEJ	B	1202	-	-	0/8/14/14	0/4/4/4
2	KEJ	A	1201	-	-	0/8/14/14	0/4/4/4

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	1201	GOL	O1-C1-C2-C3
3	B	1201	GOL	C1-C2-C3-O3
3	B	1201	GOL	O1-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1201	GOL	1	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^{th} 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	278/302 (92%)	1.27	44 (15%)	2	1	10, 19, 41, 60	0
1	B	277/302 (91%)	1.39	50 (18%)	1	1	12, 22, 40, 66	0
All	All	555/604 (91%)	1.33	94 (16%)	1	1	10, 20, 41, 66	0

All (94) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1095	THR	10.1
1	B	1095	THR	9.2
1	B	933[A]	TYR	8.5
1	B	886	PHE	7.9
1	B	1094	PRO	7.2
1	B	1040	ASP	7.0
1	A	1094	PRO	6.2
1	A	933	TYR	5.9
1	B	951	GLY	5.8
1	A	886	PHE	5.4
1	A	1040	ASP	5.1
1	A	917	ASN	5.1
1	B	885	HIS	5.0
1	B	865	VAL	4.9
1	A	885	HIS	4.7
1	B	918	HIS	4.2
1	A	951	GLY	4.2
1	B	1097	GLY	3.8
1	B	1041	ARG	3.7
1	A	1000[A]	VAL	3.7
1	A	919	ILE	3.6
1	B	919	ILE	3.4
1	A	1037	VAL	3.3
1	B	1024	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	1004	LEU	3.3
1	B	1004	LEU	3.3
1	A	945	THR	3.2
1	B	1093	GLY	3.2
1	B	945	THR	3.1
1	B	1005	ALA	3.1
1	B	1048	TYR	3.0
1	B	1082	SER	3.0
1	B	1066[A]	SER	3.0
1	A	1028	ILE	2.9
1	B	1000	VAL	2.8
1	A	918	HIS	2.8
1	B	1091	MET	2.8
1	A	1042	ASP	2.8
1	A	1039	ASP	2.7
1	B	1089	LEU	2.7
1	A	1120	CYS	2.7
1	B	1065	TRP	2.7
1	A	869	HIS	2.7
1	A	1048	TYR	2.7
1	B	959	LEU	2.6
1	A	912	PRO	2.6
1	A	1041	ARG	2.6
1	A	1065	TRP	2.6
1	A	1053	LEU	2.6
1	A	1038	LYS	2.5
1	A	1090	LYS	2.5
1	B	1088	PHE	2.5
1	A	1031	ASP	2.5
1	B	1092	ILE	2.5
1	B	1069	VAL	2.5
1	B	869	HIS	2.5
1	B	1060	ILE	2.5
1	A	1068	GLY	2.5
1	A	1091	MET	2.4
1	A	889	VAL	2.4
1	A	943	ILE	2.4
1	B	1068	GLY	2.4
1	B	1039	ASP	2.4
1	A	1069	VAL	2.4
1	A	1019	ILE	2.4
1	B	955	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	1036	THR	2.4
1	A	1132	TRP	2.4
1	B	992	ASP	2.3
1	B	994	LEU	2.3
1	A	874	PHE	2.2
1	A	867	PRO	2.2
1	A	1097	GLY	2.2
1	B	1008	ASN	2.2
1	A	1006	ALA	2.2
1	A	1047	TRP	2.2
1	B	1047	TRP	2.2
1	B	910	LEU	2.2
1	B	1053	LEU	2.1
1	B	952	ILE	2.1
1	B	1032	LYS	2.1
1	B	1019	ILE	2.1
1	B	1037	VAL	2.1
1	A	1123	GLU	2.1
1	B	929	LEU	2.1
1	A	952	ILE	2.1
1	B	1144	ASN	2.1
1	A	1110	GLU	2.1
1	A	1096	HIS	2.1
1	B	1100	THR	2.1
1	B	1124	VAL	2.1
1	B	1023	GLY	2.1
1	A	1080	SER	2.1
1	B	1132	TRP	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. The B-factors column lists the minimum, median, 95^{th} 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	B-factors(Å^2)	Q<0.9
1	PTR	B	1035	16/17	0.69	0.23	20,30,41,42	0
1	PTR	B	1034	16/17	0.73	0.26	21,27,39,40	0
1	PTR	A	1035	16/17	0.75	0.19	22,28,43,43	0
1	PTR	A	1034	16/17	0.86	0.18	19,26,41,42	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. The B-factors column lists the minimum, median, 95^{th} 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	B-factors(Å^2)	Q<0.9
3	GOL	B	1201	6/6	0.75	0.20	36,41,42,42	0
2	KEJ	A	1201	27/27	0.93	0.12	11,12,16,17	0
2	KEJ	B	1202	27/27	0.93	0.13	13,17,22,23	0

6.5 Other polymers (i)

There are no such residues in this entry.