



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 19, 2016 – 08:11 PM GMT

PDB ID : 4XV1
Title : B-Raf Kinase V600E oncogenic mutant in complex with PLX7904
Authors : Zhang, Y.; Zhang, C.
Deposited on : 2015-01-26
Resolution : 2.47 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026982
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) : rb-20026982

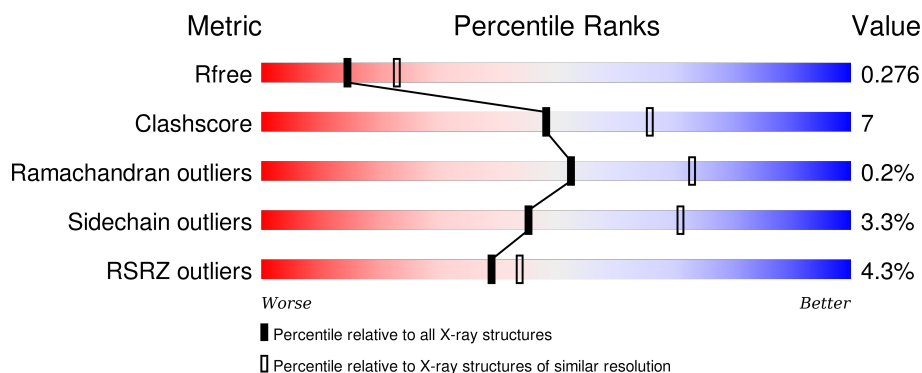
1 Overall quality at a glance ⓘ

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	292	<div> <div>2%</div> <div>69% 11% • 18%</div> </div>
1	B	292	<div> <div>5%</div> <div>67% 17% • 15%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	904	A	801	-	-	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3988 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 Serine/threonine-protein kinase B-raf.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	239	Total	C	N	O	S	0	0	0
			1911	1215	340	344	12			
1	B	249	Total	C	N	O	S	0	0	0
			2001	1271	356	362	12			

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	432	MET	-	expression tag	UNP P15056
A	433	LYS	-	expression tag	UNP P15056
A	434	LYS	-	expression tag	UNP P15056
A	435	GLY	-	expression tag	UNP P15056
A	436	HIS	-	expression tag	UNP P15056
A	437	HIS	-	expression tag	UNP P15056
A	438	HIS	-	expression tag	UNP P15056
A	439	HIS	-	expression tag	UNP P15056
A	440	HIS	-	expression tag	UNP P15056
A	441	HIS	-	expression tag	UNP P15056
A	442	GLY	-	expression tag	UNP P15056
A	443	SER	-	expression tag	UNP P15056
A	446	ALA	SER	engineered mutation	UNP P15056
A	447	ALA	SER	engineered mutation	UNP P15056
A	543	ALA	ILE	engineered mutation	UNP P15056
A	544	SER	ILE	engineered mutation	UNP P15056
A	551	LYS	ILE	engineered mutation	UNP P15056
A	562	ARG	GLN	engineered mutation	UNP P15056
A	588	ASN	LEU	engineered mutation	UNP P15056
A	600	GLU	VAL	engineered mutation	UNP P15056
A	630	SER	LYS	engineered mutation	UNP P15056
A	667	GLU	PHE	engineered mutation	UNP P15056
A	673	SER	TYR	engineered mutation	UNP P15056
A	688	ARG	ALA	engineered mutation	UNP P15056
A	706	SER	-	expression tag	UNP P15056

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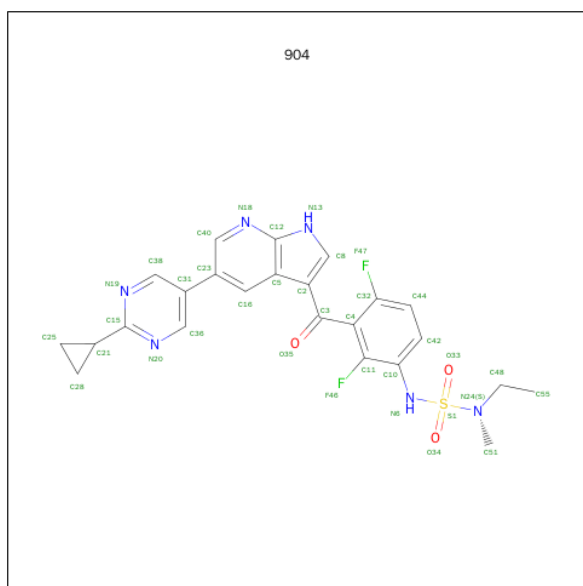
Chain	Residue	Modelled	Actual	Comment	Reference
A	707	PHE	-	expression tag	UNP P15056
A	708	PRO	-	expression tag	UNP P15056
A	709	ARG	-	expression tag	UNP P15056
A	710	ILE	-	expression tag	UNP P15056
A	711	LEU	-	expression tag	UNP P15056
A	712	ALA	-	expression tag	UNP P15056
A	713	GLU	-	expression tag	UNP P15056
A	714	ILE	-	expression tag	UNP P15056
A	715	GLU	-	expression tag	UNP P15056
A	716	GLU	-	expression tag	UNP P15056
A	717	LEU	-	expression tag	UNP P15056
A	718	ALA	-	expression tag	UNP P15056
A	719	ARG	-	expression tag	UNP P15056
A	720	GLU	-	expression tag	UNP P15056
A	721	LEU	-	expression tag	UNP P15056
A	722	SER	-	expression tag	UNP P15056
A	723	GLY	-	expression tag	UNP P15056
B	432	MET	-	expression tag	UNP P15056
B	433	LYS	-	expression tag	UNP P15056
B	434	LYS	-	expression tag	UNP P15056
B	435	GLY	-	expression tag	UNP P15056
B	436	HIS	-	expression tag	UNP P15056
B	437	HIS	-	expression tag	UNP P15056
B	438	HIS	-	expression tag	UNP P15056
B	439	HIS	-	expression tag	UNP P15056
B	440	HIS	-	expression tag	UNP P15056
B	441	HIS	-	expression tag	UNP P15056
B	442	GLY	-	expression tag	UNP P15056
B	443	SER	-	expression tag	UNP P15056
B	446	ALA	SER	engineered mutation	UNP P15056
B	447	ALA	SER	engineered mutation	UNP P15056
B	543	ALA	ILE	engineered mutation	UNP P15056
B	544	SER	ILE	engineered mutation	UNP P15056
B	551	LYS	ILE	engineered mutation	UNP P15056
B	562	ARG	GLN	engineered mutation	UNP P15056
B	588	ASN	LEU	engineered mutation	UNP P15056
B	600	GLU	VAL	engineered mutation	UNP P15056
B	630	SER	LYS	engineered mutation	UNP P15056
B	667	GLU	PHE	engineered mutation	UNP P15056
B	673	SER	TYR	engineered mutation	UNP P15056
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Chain	Residue	Modelled	Actual	Comment	Reference
B	707	PHE	-	expression tag	UNP P15056
B	708	PRO	-	expression tag	UNP P15056
B	709	ARG	-	expression tag	UNP P15056
B	710	ILE	-	expression tag	UNP P15056
B	711	LEU	-	expression tag	UNP P15056
B	712	ALA	-	expression tag	UNP P15056
B	713	GLU	-	expression tag	UNP P15056
B	714	ILE	-	expression tag	UNP P15056
B	715	GLU	-	expression tag	UNP P15056
B	716	GLU	-	expression tag	UNP P15056
B	717	LEU	-	expression tag	UNP P15056
B	718	ALA	-	expression tag	UNP P15056
B	719	ARG	-	expression tag	UNP P15056
B	720	GLU	-	expression tag	UNP P15056
B	721	LEU	-	expression tag	UNP P15056
B	722	SER	-	expression tag	UNP P15056
B	723	GLY	-	expression tag	UNP P15056

- Molecule 2 is N'-(3-{[5-(2-cyclopropylpyrimidin-5-yl)-1H-pyrrolo[2,3-b]pyridin-3-yl]carbonyl}-2,4-difluorophenyl)-N-ethyl-N-methylsulfuric diamide (three-letter code: 904) (formula: C₂₄H₂₂F₂N₆O₃S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	S	
			36	24	2	6	3	1	

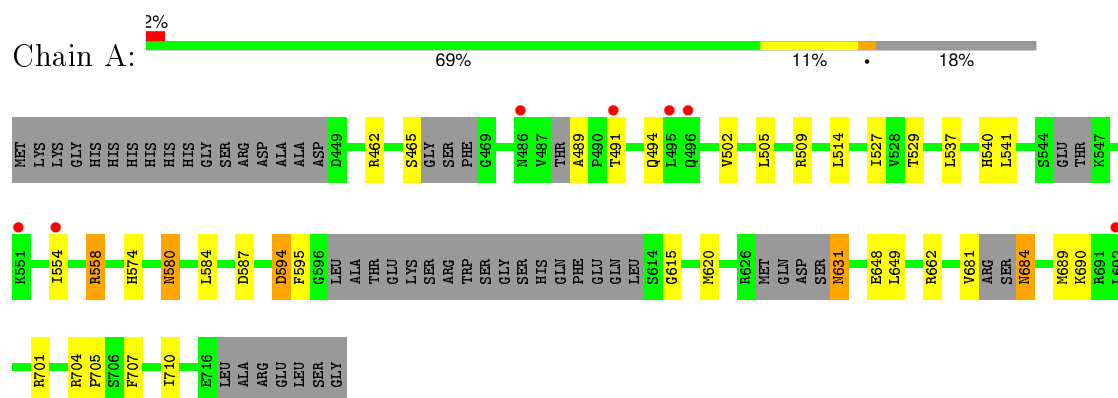
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	25	Total 25	O 25	0	0
3	B	15	Total 15	O 15	0	0

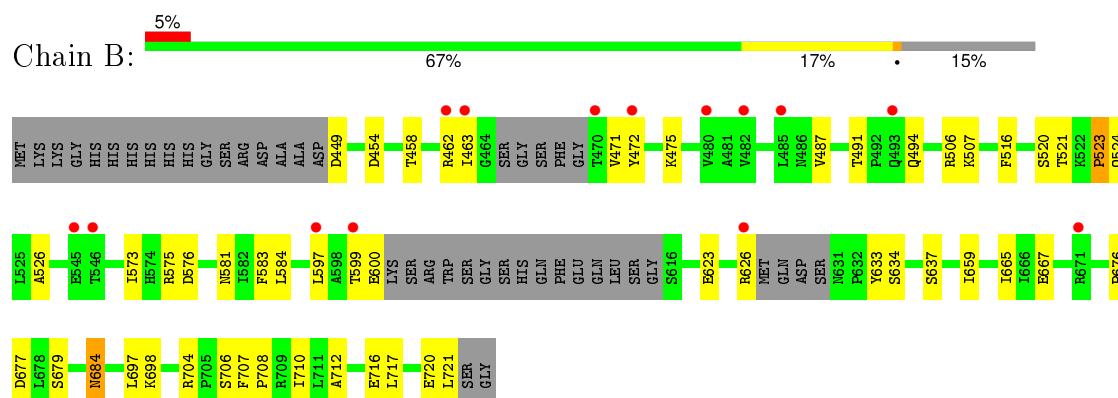
3 Residue-property plots [i](#)

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: Serine/threonine-protein kinase B-raf



- Molecule 1: Serine/threonine-protein kinase B-raf



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	51.33Å 104.82Å 110.23Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	75.96 – 2.47 75.96 – 2.47	Depositor EDS
% Data completeness (in resolution range)	99.9 (75.96-2.47) 99.9 (75.96-2.47)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.10 (at 2.48Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.7.3_928)	Depositor
R, R_{free}	0.234 , 0.273 0.233 , 0.276	Depositor DCC
R_{free} test set	1128 reflections (5.40%)	DCC
Wilson B-factor (Å ²)	54.4	Xtriage
Anisotropy	0.609	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 51.6	EDS
Estimated twinning fraction	0.055 for -h,l,k	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Outliers	0 of 22008 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	3988	wwPDB-VP
Average B, all atoms (Å ²)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.94% 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: 904

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	0.24	0/1947	0.41	0/2617
1	B	0.23	0/2040	0.41	0/2749
All	All	0.23	0/3987	0.41	0/5366

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	1911	0	1920	28	0
1	B	2001	0	2020	31	0
2	A	36	0	21	8	0
3	A	25	0	0	2	0
3	B	15	0	0	1	0
All	All	3988	0	3961	58	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.

The worst 5 of 58 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:681:VAL:HG21	1:A:690:LYS:HD2	1.57	0.84
1:A:505:LEU:HD22	2:A:801:904:H18	1.59	0.83
1:A:594:ASP:H	2:A:801:904:H1	1.31	0.78
1:B:623:GLU:OE2	1:B:704:ARG:NH2	2.28	0.67
1:A:527:ILE:HG21	2:A:801:904:H19	1.77	0.66

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	225/292 (77%)	218 (97%)	7 (3%)	0	100	100
1	B	241/292 (82%)	233 (97%)	7 (3%)	1 (0%)	39	59
All	All	466/584 (80%)	451 (97%)	14 (3%)	1 (0%)	52	73

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	523	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	209/254 (82%)	202 (97%)	7 (3%)	45	71

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	219/254 (86%)	212 (97%)	7 (3%)	46	72
All	All	428/508 (84%)	414 (97%)	14 (3%)	45	71

5 of 14 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	689	MET
1	B	449	ASP
1	B	667	GLU
1	A	684	ASN
1	B	637	SER

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](#)

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	904	A	801	-	36,40,40	1.09	3 (8%)	44,60,60	1.18	2 (4%)

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	904	A	801	-	-	1/24/31/31	0/4/5/5

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	904	C2-C3	-3.68	1.45	1.50
2	A	801	904	O33-S1	2.05	1.45	1.42
2	A	801	904	C40-N18	2.18	1.35	1.31

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	801	904	N19-C15-N20	-2.01	123.26	126.11
2	A	801	904	C32-C4-C11	5.04	119.37	115.27

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	801	904	N6-S1-N24-C51

There are no ring outliers.

1 monomer is involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	801	904	8	0

5.7 Other polymers [i](#)

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	239/292 (81%)	0.43	7 (2%) 55 59	33, 66, 114, 138	0
1	B	249/292 (85%)	0.49	14 (5%) 28 31	32, 73, 119, 142	0
All	All	488/584 (83%)	0.46	21 (4%) 39 44	32, 70, 116, 142	0

The worst 5 of 21 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	495	LEU	5.1
1	B	545	GLU	4.6
1	B	599	THR	4.2
1	A	692	LEU	3.9
1	B	462	ARG	3.5

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	904	A	801	36/36	0.95	0.27	2.82	74,80,120,122	0

6.5 Other polymers ⓘ

There are no such residues in this entry.