Full wwPDB X-ray Structure Validation Report (i)

Dec 20, 2016 – 05:27 PM EST

PDB ID	:	5T8I
Title	:	PI3Kdelta in complex with the inhibitor GS-9901
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Deposited on	:	2016-09-07
Resolution	:	2.60 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

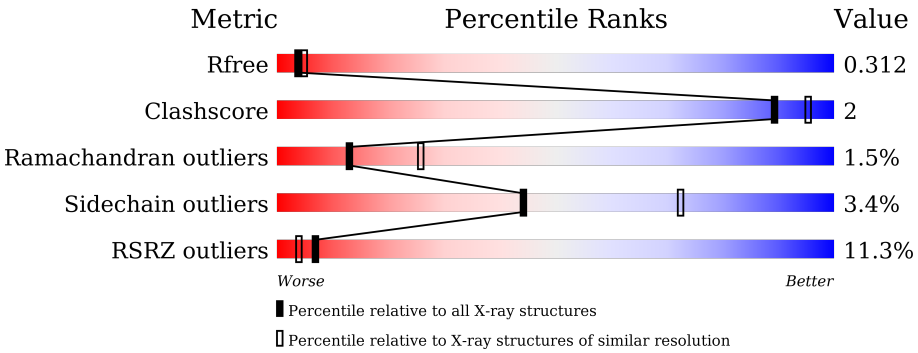
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20028442
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20028442

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 2.60 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	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)

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 <=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	939	10% 78% 7% • 14%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 13091 atoms, of which 6529 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.

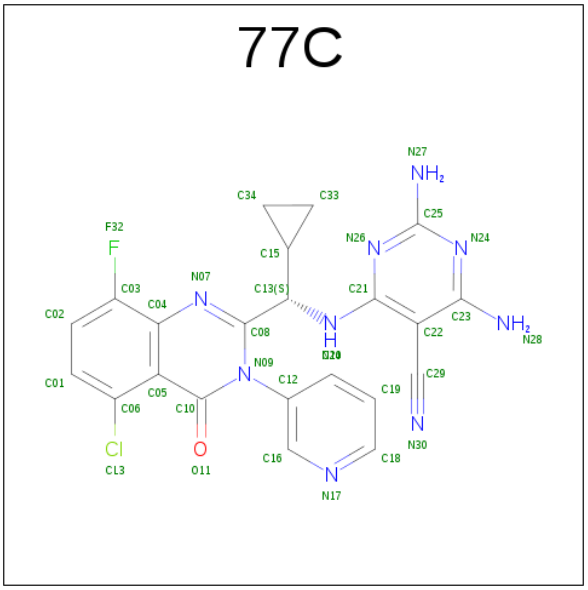
- Molecule 1 is a protein called Phosphatidylinositol 4,5-bisphosphate 3-kinase catalytic subunit delta isoform.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	808	13040	4183	6512	1108	1182	55	0	6	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	508	GLN	-	insertion	UNP O35904

- Molecule 2 is 2,4-diamino-6-{[(S)-[5-chloro-8-fluoro-4-oxo-3-(pyridin-3-yl)-3,4-dihydroquinazolin-2-yl](cyclopropyl)methyl]amino}pyrimidine-5-carbonitrile (three-letter code: 77C) (formula: $C_{22}H_{17}ClFN_9O$).



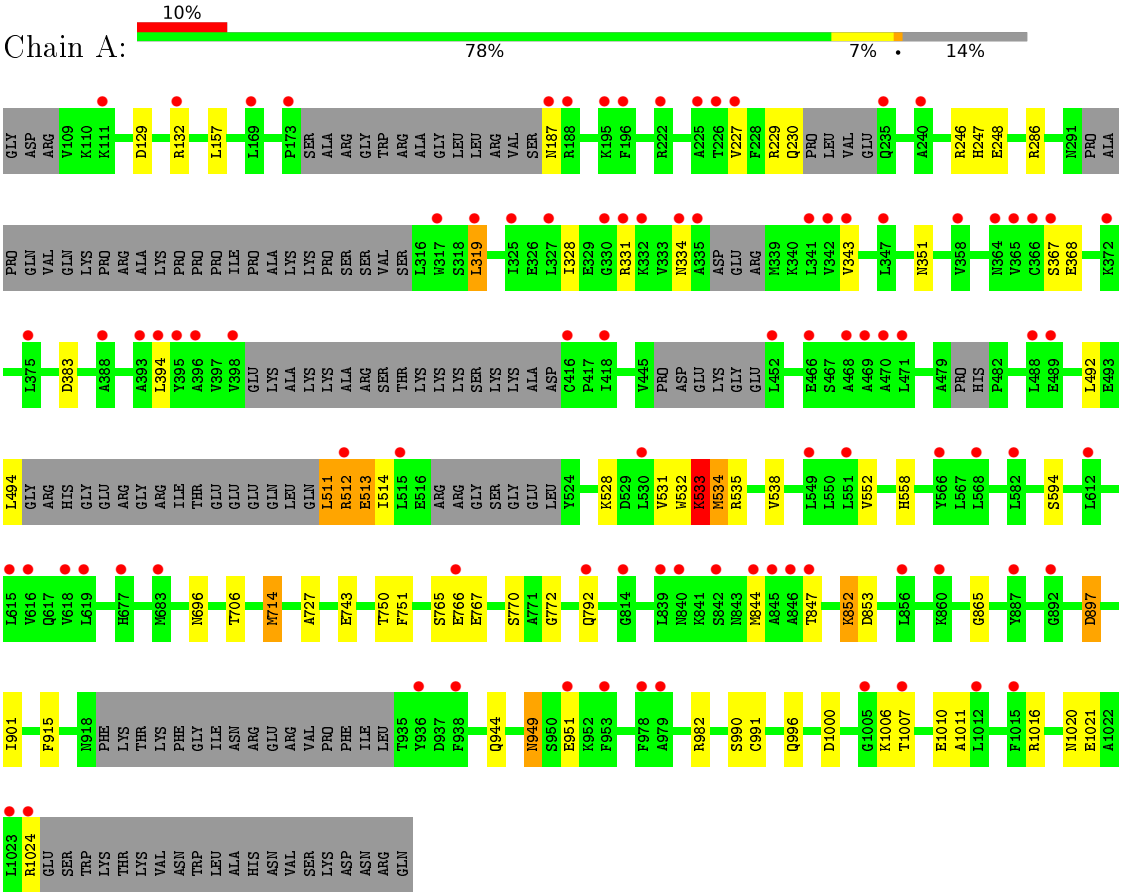
Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
			Total	C	Cl	F	H	N	O		
2	A	1	51	22	1	1	17	9	1	0	0

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: Phosphatidylinositol 4,5-bisphosphate 3-kinase catalytic subunit delta isoform

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	64.05Å 142.20Å 222.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.88 – 2.60 45.89 – 2.61	Depositor EDS
% Data completeness (in resolution range)	91.2 (45.88-2.60) 91.3 (45.89-2.61)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.25 (at 2.61Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.252 , 0.312 0.255 , 0.312	Depositor DCC
R_{free} test set	1999 reflections (6.94%)	DCC
Wilson B-factor (Å^2)	70.0	Xtriage
Anisotropy	0.268	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 64.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	13091	wwPDB-VP
Average B, all atoms (Å^2)	97.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.44% 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: 77C

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	0.23	0/6693	0.42	1/9029 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	714	MET	CG-SD-CE	12.07	119.51	100.20

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	6528	6512	6492	31	1
2	A	34	17	0	0	0
All	All	6562	6529	6492	31	1

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 2.

All (31) 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:129:ASP:O	1:A:132:ARG:NH1	2.25	0.70
1:A:367:SER:HA	1:A:368:GLU:HB2	1.83	0.60
1:A:1006:LYS:NZ	1:A:1007:THR:O	2.37	0.58
1:A:897:ASP:OD1	1:A:897:ASP:N	2.37	0.57
1:A:1016:ARG:O	1:A:1020:ASN:ND2	2.38	0.57
1:A:982:ARG:NH1	1:A:991:CYS:O	2.36	0.57
1:A:246:ARG:NH1	1:A:248:GLU:OE1	2.40	0.55
1:A:533:LYS:HZ2	1:A:538:VAL:CG2	2.19	0.54
1:A:512:ARG:O	1:A:514:ILE:N	2.41	0.54
1:A:383:ASP:OD1	1:A:558:HIS:ND1	2.42	0.53
1:A:750:THR:OG1	1:A:751:PHE:N	2.45	0.50
1:A:533:LYS:O	1:A:535:ARG:N	2.46	0.49
1:A:982:ARG:NH2	1:A:990:SER:O	2.46	0.49
1:A:852:LYS:NZ	1:A:853:ASP:OD2	2.45	0.49
1:A:532:TRP:C	1:A:533:LYS:HE2	2.34	0.48
1:A:533:LYS:HZ2	1:A:538:VAL:HG23	1.78	0.47
1:A:511:LEU:O	1:A:513:GLU:N	2.47	0.47
1:A:844:MET:O	1:A:847:THR:N	2.48	0.47
1:A:528:LYS:HA	1:A:531:VAL:HG12	1.96	0.46
1:A:533:LYS:HD2	1:A:534:MET:N	2.31	0.46
1:A:944:GLN:NE2	1:A:949:ASN:OD1	2.48	0.46
1:A:367:SER:CA	1:A:368:GLU:HB2	2.47	0.45
1:A:1021:GLU:O	1:A:1024:ARG:NH1	2.49	0.44
1:A:531:VAL:HG13	1:A:552:VAL:HG11	1.98	0.44
1:A:511:LEU:HG	1:A:512:ARG:N	2.33	0.43
1:A:1006:LYS:HZ1	1:A:1011:ALA:N	2.18	0.42
1:A:343:VAL:HG22	1:A:394:LEU:HD12	2.01	0.42
1:A:765:SER:HB3	1:A:772:GLY:HA3	2.02	0.42
1:A:528:LYS:HA	1:A:531:VAL:CG1	2.49	0.41
1:A:996:GLN:NE2	1:A:1000:ASP:OD1	2.49	0.41
1:A:157:LEU:O	1:A:286:ARG:NH1	2.55	0.41

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:714:MET:SD	1:A:714:MET:CE[4_566]	1.79	0.41

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	792/939 (84%)	734 (93%)	46 (6%)	12 (2%)	13 26

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	512	ARG
1	A	513	GLU
1	A	533	LYS
1	A	534	MET
1	A	319	LEU
1	A	767	GLU
1	A	865	GLY
1	A	229	ARG
1	A	727	ALA
1	A	227	VAL
1	A	328	ILE
1	A	766	GLU

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	721/827 (87%)	697 (97%)	24 (3%)	45 73

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	187	ASN
1	A	230	GLN
1	A	247	HIS
1	A	319	LEU
1	A	331	ARG
1	A	334	ASN
1	A	351	ASN
1	A	492	LEU
1	A	494	LEU
1	A	511	LEU
1	A	533	LYS
1	A	594	SER
1	A	696	ASN
1	A	706	THR
1	A	743	GLU
1	A	770	SER
1	A	792	GLN
1	A	852	LYS
1	A	897	ASP
1	A	901	ILE
1	A	915	PHE
1	A	949	ASN
1	A	951	GLU
1	A	1010	GLU

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	77C	A	1101	-	36,38,38	1.58	9 (25%)	37,56,56	1.07	2 (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
2	77C	A	1101	-	-	0/12/20/20	0/4/5/5

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1101	77C	C12-N09	-2.66	1.42	1.46
2	A	1101	77C	C22-C23	-2.23	1.39	1.42
2	A	1101	77C	C23-N28	2.05	1.39	1.34
2	A	1101	77C	C25-N27	2.10	1.38	1.34
2	A	1101	77C	C02-C03	2.17	1.39	1.36
2	A	1101	77C	C10-N09	2.23	1.41	1.37
2	A	1101	77C	C08-C13	2.61	1.54	1.50
2	A	1101	77C	C21-N14	3.17	1.40	1.35
2	A	1101	77C	C10-C05	4.88	1.49	1.41

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1101	77C	C03-C04-N07	-2.91	117.48	119.55
2	A	1101	77C	C25-N26-C21	2.02	119.17	114.63

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, 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	808/939 (86%)	0.86	91 (11%) 7 4	68, 89, 104, 112	0

All (91) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	332	LYS	7.4
1	A	366	CYS	6.7
1	A	394	LEU	5.8
1	A	334	ASN	5.8
1	A	847	THR	5.2
1	A	530	LEU	5.2
1	A	235	GLN	5.1
1	A	330	GLY	4.9
1	A	196	PHE	4.9
1	A	468	ALA	4.9
1	A	846	ALA	4.7
1	A	845	ALA	4.7
1	A	936	TYR	4.6
1	A	842	SER	4.5
1	A	470	ALA	4.5
1	A	396	ALA	4.1
1	A	367	SER	4.1
1	A	792	GLN	3.9
1	A	365	VAL	3.8
1	A	471	LEU	3.8
1	A	1005	GLY	3.8
1	A	341	LEU	3.7
1	A	343	VAL	3.6
1	A	469	ALA	3.6
1	A	953	PHE	3.4
1	A	416	CYS	3.4
1	A	331	ARG	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	364	ASN	3.3
1	A	488	LEU	3.3
1	A	1023	LEU	3.2
1	A	187	ASN	3.2
1	A	616	VAL	3.1
1	A	1012	LEU	3.1
1	A	342	VAL	3.0
1	A	839	LEU	3.0
1	A	466	GLU	3.0
1	A	840	ASN	2.9
1	A	892	GLY	2.8
1	A	515	LEU	2.8
1	A	512	ARG	2.8
1	A	418	ILE	2.8
1	A	978	PHE	2.7
1	A	1024	ARG	2.7
1	A	358	VAL	2.7
1	A	327	LEU	2.7
1	A	388	ALA	2.6
1	A	225	ALA	2.6
1	A	372	LYS	2.6
1	A	452	LEU	2.5
1	A	766	GLU	2.5
1	A	325	ILE	2.5
1	A	395	TYR	2.5
1	A	619	LEU	2.5
1	A	240	ALA	2.5
1	A	335	ALA	2.4
1	A	227	VAL	2.4
1	A	1007	THR	2.4
1	A	683	MET	2.4
1	A	375	LEU	2.4
1	A	393	ALA	2.3
1	A	398	VAL	2.3
1	A	132	ARG	2.3
1	A	222	ARG	2.3
1	A	860	LYS	2.3
1	A	195	LYS	2.3
1	A	568	LEU	2.3
1	A	566	TYR	2.2
1	A	319	LEU	2.2
1	A	347	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	612	LEU	2.2
1	A	489	GLU	2.2
1	A	549	LEU	2.2
1	A	856	LEU	2.2
1	A	173	PRO	2.2
1	A	188	ARG	2.2
1	A	1015	PHE	2.2
1	A	111	LYS	2.1
1	A	317	TRP	2.1
1	A	844	MET	2.1
1	A	951	GLU	2.1
1	A	169	LEU	2.1
1	A	551	LEU	2.1
1	A	226	THR	2.1
1	A	814	GLY	2.1
1	A	938	PHE	2.1
1	A	582	LEU	2.1
1	A	615	LEU	2.1
1	A	677	HIS	2.1
1	A	887	TYR	2.1
1	A	979	ALA	2.0
1	A	618	VAL	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, 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	LLDF	B-factors(Å^2)	Q<0.9
2	77C	A	1101	34/34	0.95	0.22	-0.06	73,79,96,99	0

6.5 Other polymers (i)

There are no such residues in this entry.