wwPDB X-ray Structure Validation Summary Report (i)

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PDB ID	:	5T7F
Title	:	PI3Kdelta in complex with the inhibitor GS-643624
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Deposited on	:	2016-09-04
Resolution	:	2.60 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 (i) symbol.

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

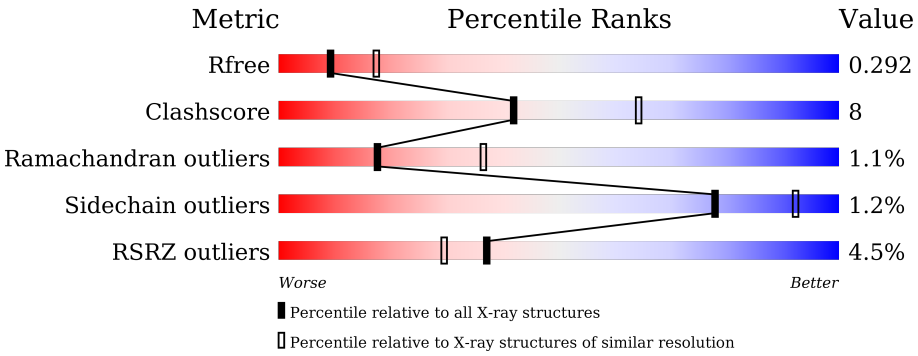
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20028442
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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	4% 71% 15% • 13%
1	B	939	4% 70% 16% •• 13%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 13339 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.

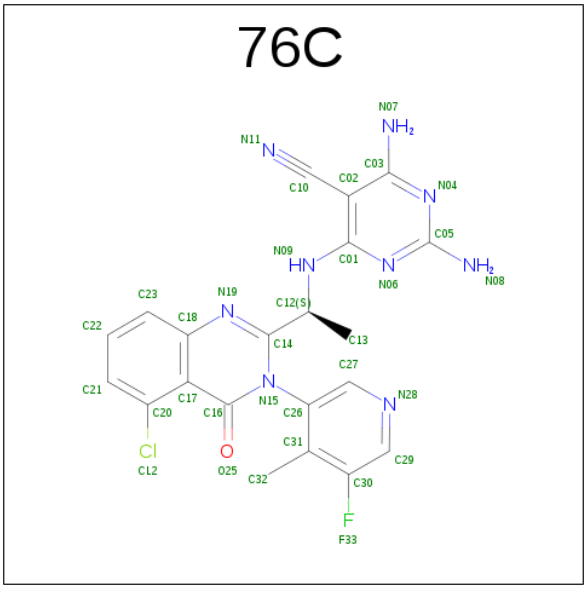
- Molecule 1 is a protein called Phosphatidylinositol 4,5-bisphosphate 3-kinase catalytic subunit delta isoform.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	819	Total	C	N	O	S	0	0	0
			6603	4233	1121	1195	54			
1	B	816	Total	C	N	O	S	0	0	0
			6575	4216	1114	1191	54			

There are 2 discrepancies between the modelled and reference sequences:

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

- Molecule 2 is 2,4-bis(azanyl)-6-[[(1 {S})-1-[5-chloranyl-3-(5-fluoranyl-4-methyl-pyridin-3-yl)-4-oxidanylidene-quinazolin-2-yl]ethyl]amino]pyrimidine-5-carbonitrile (three-letter code: 76C) (formula: $C_{21}H_{17}ClFN_9O$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	Cl	F	N	O	0	0
			33	21	1	1	9	1		
2	B	1	Total	C	Cl	F	N	O	0	0
			33	21	1	1	9	1		

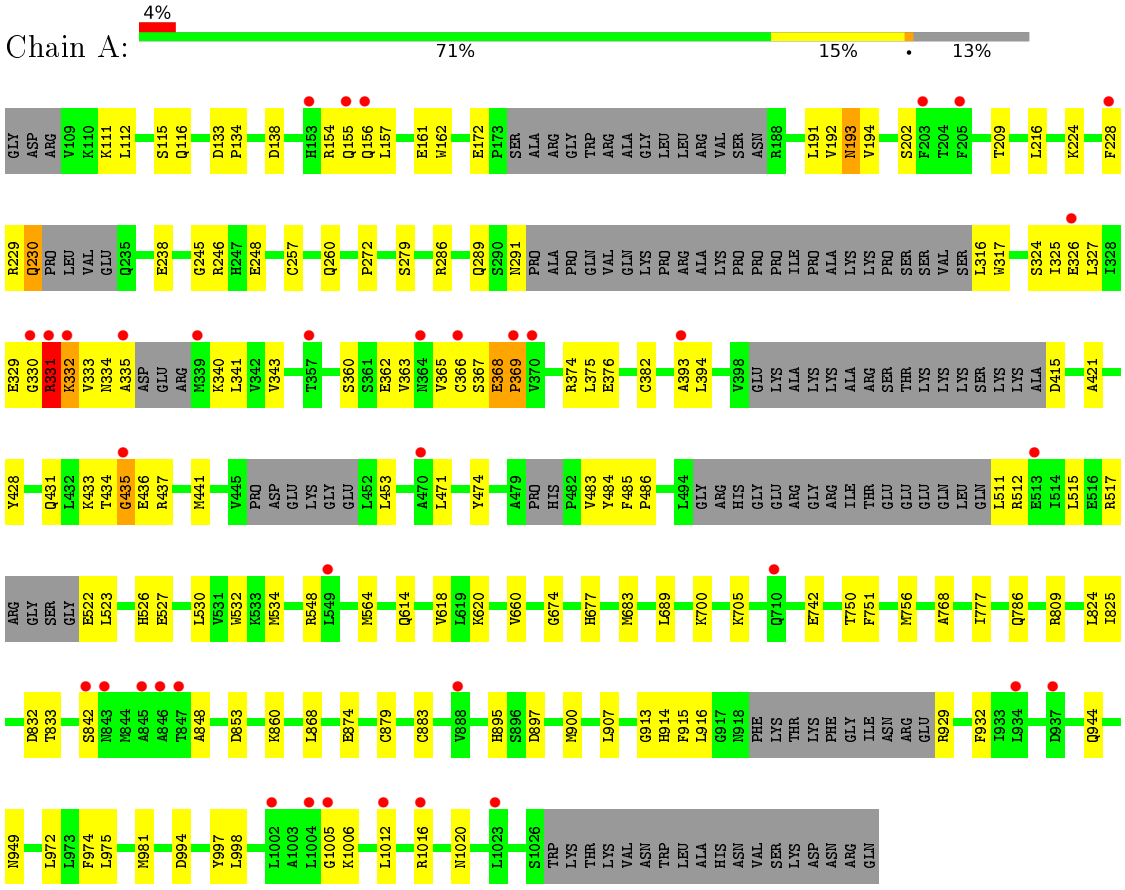
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	48	Total	O	0	0
			48	48		
3	B	47	Total	O	0	0
			47	47		

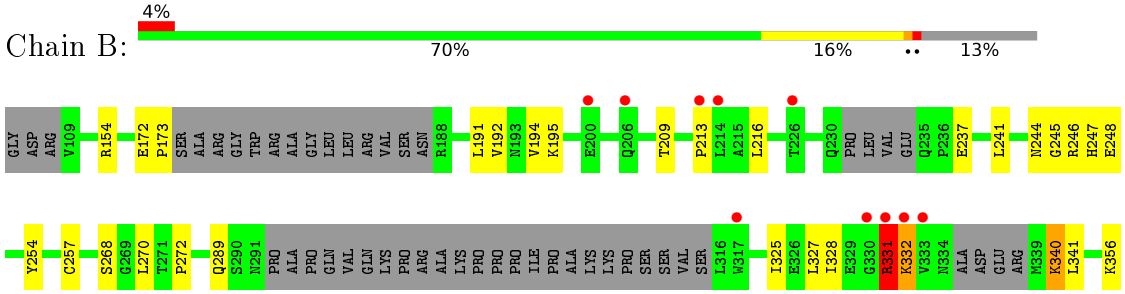
3 Residue-property plots (i)

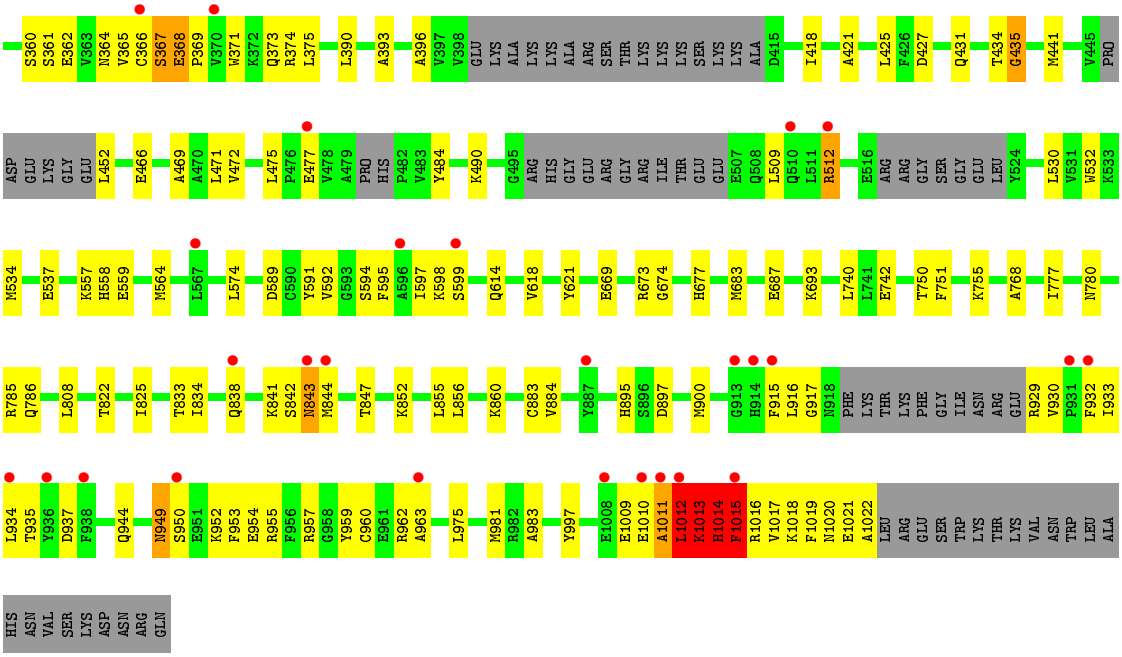
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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



• Molecule 1: Phosphatidylinositol 4,5-bisphosphate 3-kinase catalytic subunit delta isoform




S360 S361 E362 V363 N364 V365 C366 S367 E368 P369 V370 W371 K372 Q373 R374 L375 L390 A393 A396 V397 V398 GLU LYS ALA LYS LYS ALA ARG SER THR LYS LYS LYS SER LYS LYS ALA D415 I418 A421 L425 F426 D427 Q431 T434 G435 M441 V445 PRO
ASP GLU LYS GLY GLU L452 E466 A469 A470 L471 V472 L475 P476 E477 V478 A479 PRO HIS P482 V483 Y484 K490 G495 ARG HIS GLY GLU ARG GLY ARG ILE THR GLU GLU E507 Q508 L509 Q510 L511 R512 E516 ARG ARG GLY SER GLY GLU LEU Y524 L530 V531 W532 K533
M534 E537 K557 H558 E559 M564 L567 L574 D589 C590 Y591 V592 G593 S594 F595 A596 I597 K598 S599 Q614 V618 Y621 E669 R673 G674 H677 M683 E687 K693 L740 L741 E742 T750 F751 K755 A768 I777 N780
R785 Q786 L808 T822 I825 T833 I834 Q838 K841 S842 N843 M844 T847 K852 L855 L856 K860 C883 V884 Y887 H895 S896 D897 M900 G913 H914 F915 L916 G917 N918 PHE LYS THR LYS PHE GLY ILE ASN ARG GLU R929 V930 P931 F932 I933
L934 T935 Y936 D937 F938 Q944 N949 S950 E951 K952 F953 E954 R955 F956 R957 G958 Y959 C960 E961 R962 A963 L975 M981 R982 A983 Y997 E1008 E1009 E1010 A1011 L1012 K1013 H1014 F1015 R1016 V1017 K1018 F1019 N1020 E1021 A1022 LEU ARG GLU SER TRP LYS THR LYS VAL ASN TRP LEU ALA
HIS ASN VAL SER LYS ASP ASN ARG GLN

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	64.23Å 142.79Å 221.07Å 90.00° 90.06° 90.00°	Depositor
Resolution (Å)	45.90 – 2.60 45.87 – 2.60	Depositor EDS
% Data completeness (in resolution range)	91.4 (45.90-2.60) 85.9 (45.87-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.70 (at 2.61Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.230 , 0.294 0.233 , 0.292	Depositor DCC
R_{free} test set	1878 reflections (3.56%)	DCC
Wilson B-factor (Å^2)	47.4	Xtriage
Anisotropy	0.154	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 31.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.467 for h,-k,-l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	13339	wwPDB-VP
Average B, all atoms (Å^2)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.96% 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: 76C

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	0/6741	0.42	1/9090 (0.0%)
1	B	0.27	1/6715 (0.0%)	0.47	3/9059 (0.0%)
All	All	0.26	1/13456 (0.0%)	0.44	4/18149 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	5

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	332	LYS	CB-CG	-5.12	1.38	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	331	ARG	NE-CZ-NH1	-7.28	116.66	120.30
1	B	332	LYS	CB-CG-CD	-6.59	94.46	111.60
1	A	331	ARG	CG-CD-NE	5.85	124.08	111.80
1	B	331	ARG	N-CA-C	5.15	124.91	111.00

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	1012	LEU	Peptide
1	B	1013	LYS	Peptide
1	B	1014	HIS	Peptide
1	B	331	ARG	Peptide
1	B	366	CYS	Peptide

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	6603	0	6597	97	0
1	B	6575	0	6565	124	1
2	A	33	0	0	0	0
2	B	33	0	0	0	0
3	A	48	0	0	3	0
3	B	47	0	0	2	0
All	All	13339	0	13162	221	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 8.

The worst 5 of 221 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:331:ARG:HD3	1:A:368:GLU:HB3	1.56	0.85
1:A:193:ASN:ND2	1:A:202:SER:OG	2.10	0.84
1:A:883:CYS:HB3	1:A:932:PHE:HZ	1.44	0.81
1:B:557:LYS:HE3	1:B:559:GLU:HG2	1.65	0.77
1:A:324:SER:OG	1:A:374:ARG:NH1	2.18	0.76

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:B:356:LYS:NZ	1:B:843:ASN:O[3_555]	2.02	0.18

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	794/939 (85%)	752 (95%)	36 (4%)	6 (1%)	24 46
1	B	794/939 (85%)	740 (93%)	43 (5%)	11 (1%)	14 28
All	All	1588/1878 (85%)	1492 (94%)	79 (5%)	17 (1%)	17 36

5 of 17 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	367	SER
1	B	1012	LEU
1	A	333	VAL
1	A	366	CYS
1	B	755	LYS

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	726/827 (88%)	719 (99%)	7 (1%)	82 94
1	B	723/827 (87%)	712 (98%)	11 (2%)	72 90
All	All	1449/1654 (88%)	1431 (99%)	18 (1%)	78 92

5 of 18 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	332	LYS

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Mol	Chain	Res	Type
1	B	340	LYS
1	B	1012	LEU
1	A	522	GLU
1	B	237	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	247	HIS
1	B	1020	ASN
1	B	526	HIS
1	A	291	ASN
1	B	373	GLN

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)

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	76C	A	1101	-	36,36,36	1.51	8 (22%)	32,53,53	1.37	4 (12%)
2	76C	B	1101	-	36,36,36	1.51	8 (22%)	32,53,53	1.37	4 (12%)

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	76C	A	1101	-	-	0/10/14/14	0/4/4/4
2	76C	B	1101	-	-	0/10/14/14	0/4/4/4

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1101	76C	C26-N15	-2.18	1.43	1.45
2	B	1101	76C	C26-N15	-2.16	1.43	1.45
2	B	1101	76C	C02-C03	-2.09	1.39	1.42
2	A	1101	76C	C02-C03	-2.08	1.39	1.42
2	A	1101	76C	C16-N15	2.07	1.41	1.37

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1101	76C	C26-C27-N28	2.15	124.58	122.20
2	B	1101	76C	C26-C27-N28	2.16	124.59	122.20
2	B	1101	76C	C31-C26-N15	2.65	122.65	119.45
2	A	1101	76C	C31-C26-N15	2.65	122.66	119.45
2	B	1101	76C	C13-C12-N09	3.02	113.70	109.08

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

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	155:GLN	C	156:GLN	N	6.51
1	A	156:GLN	C	157:LEU	N	6.22

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	819/939 (87%)	0.29	37 (4%)	37	29	38, 61, 89, 110	0
1	B	816/939 (86%)	0.24	37 (4%)	37	29	37, 61, 92, 118	0
All	All	1635/1878 (87%)	0.26	74 (4%)	37	29	37, 61, 90, 118	0

The worst 5 of 74 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	366	CYS	8.8
1	A	330	GLY	8.3
1	B	1015	PHE	7.7
1	B	932	PHE	5.1
1	B	366	CYS	4.9

6.2 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

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	76C	B	1101	33/33	0.94	0.20	0.50	36,46,56,73	0
2	76C	A	1101	33/33	0.95	0.18	0.11	36,45,56,70	0

6.5 Other polymers (i)

There are no such residues in this entry.