Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:37 PM GMT

PDB ID	:	4TV3
Title	:	Isolated p110a subunit of PI3Ka provides a platform for structure-based drug design
Authors	:	Chen, P.; Deng, Y.-L.; Bergqvist, S.; Falk, M.; Liu, W.; Timofeevski, S.
Deposited on	:	2014-06-25
Resolution	:	2.85 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 ①) were used in the production of this report:

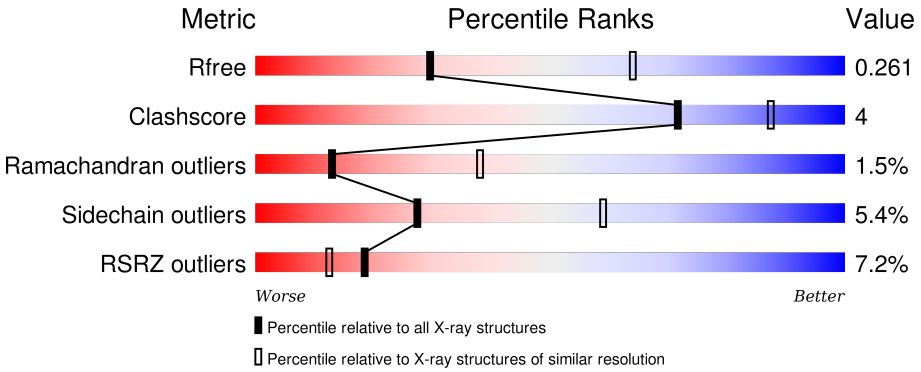
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.85 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	2228 (2.90-2.82)
Clashscore	102246	2499 (2.90-2.82)
Ramachandran outliers	100387	2439 (2.90-2.82)
Sidechain outliers	100360	2442 (2.90-2.82)
RSRZ outliers	91569	2236 (2.90-2.82)

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	946	7% 80% 12% • 7%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6636 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.

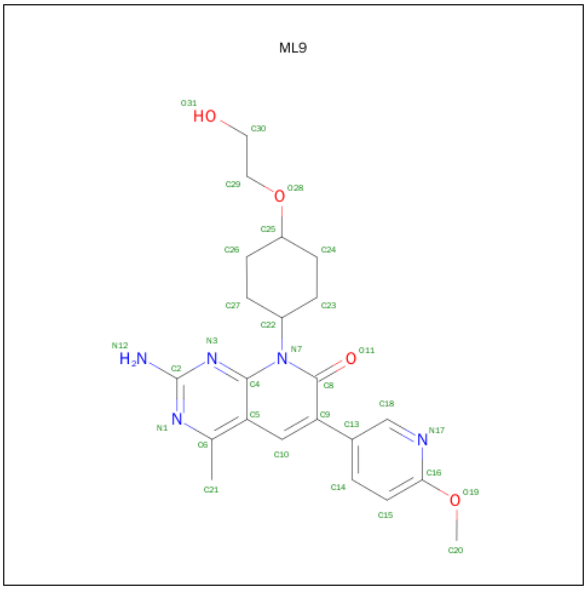
- Molecule 1 is a protein called Phosphatidylinositol 4,5-bisphosphate 3-kinase catalytic subunit alpha isoform.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	879	6601	4231	1106	1206	58	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	103	GLY	-	expression tag	UNP P42336
A	104	SER	-	expression tag	UNP P42336

- Molecule 2 is 2-amino-8-[trans-4-(2-hydroxyethoxy)cyclohexyl]-6-(6-methoxypyridin-3-yl)-4-methylpyrido[2,3-d]pyrimidin-7(8H)-one (three-letter code: ML9) (formula: $C_{22}H_{27}N_5O_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	31	22	5	4	0	0

- Molecule 3 is water.

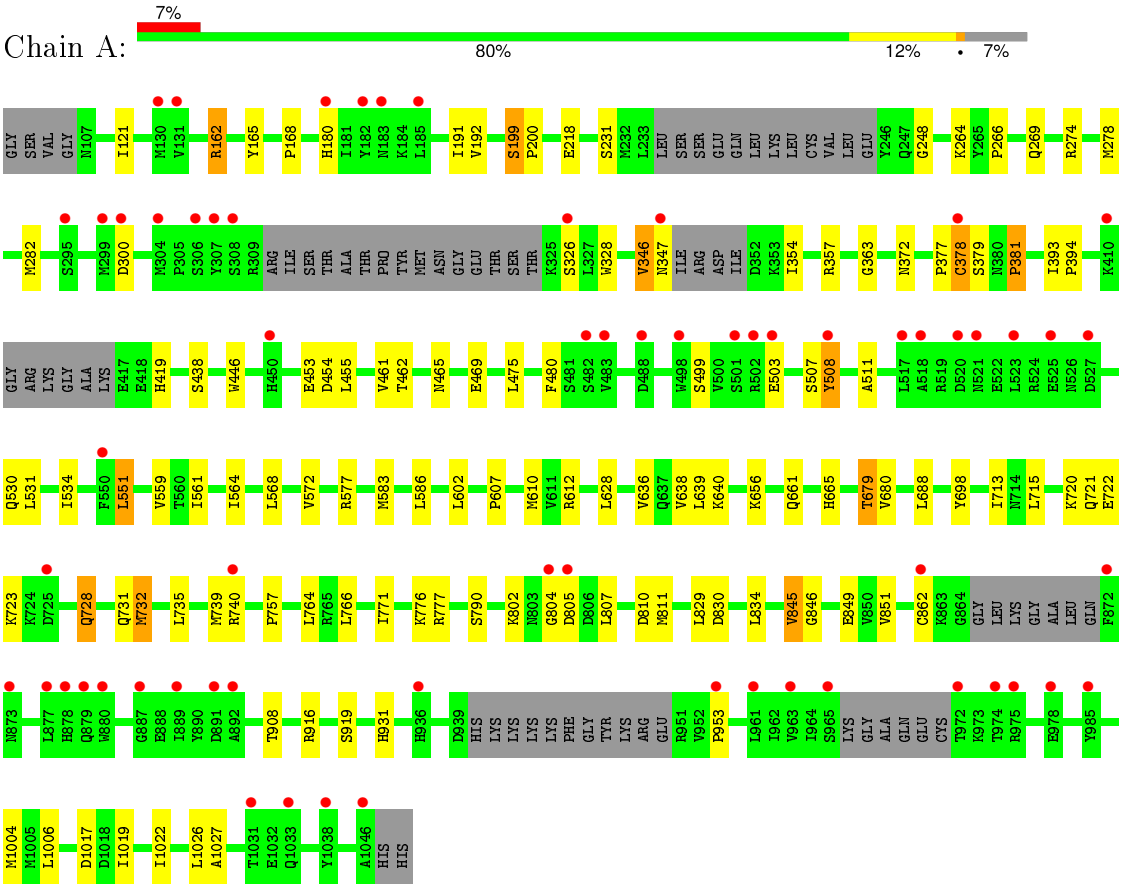
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	4	Total O 4 4	0	0

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 alpha isoform

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	58.04Å 136.77Å 142.64Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.41 – 2.85 34.19 – 2.85	Depositor EDS
% Data completeness (in resolution range)	99.4 (34.41-2.85) 99.9 (34.19-2.85)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$< I/\sigma(I) >$ [1]	2.86 (at 2.85Å)	Xtriage
Refinement program	BUSTER 2.11.4	Depositor
R, R_{free}	0.208 , 0.250 0.221 , 0.261	Depositor DCC
R_{free} test set	1361 reflections (5.28%)	DCC
Wilson B-factor (Å^2)	70.4	Xtriage
Anisotropy	0.101	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 81.8	EDS
Estimated twinning fraction	0.019 for -h,l,k	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Outliers	0 of 27115 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	6636	wwPDB-VP
Average B, all atoms (Å^2)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.57% 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, 0.375 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: ML9

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	0.52	0/6751	0.70	2/9207 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	507	SER	C-N-CA	7.62	140.74	121.70
1	A	377	PRO	C-N-CA	5.71	135.98	121.70

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	6601	0	5945	54	0
2	A	31	0	27	2	0
3	A	4	0	0	0	0
All	All	6636	0	5972	54	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 4.

All (54) 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:807:LEU:HD12	1:A:846:GLY:HA3	1.60	0.83
1:A:180:HIS:CD2	1:A:830:ASP:HB2	2.26	0.70
1:A:739:MET:HG2	1:A:766:LEU:HD11	1.76	0.65
1:A:534:ILE:HG21	1:A:551:LEU:HD11	1.81	0.63
1:A:628:LEU:HD23	1:A:656:LYS:HG2	1.81	0.62
1:A:199:SER:HB2	1:A:200:PRO:CD	2.30	0.61
1:A:346:VAL:HG22	1:A:347:ASN:H	1.64	0.61
1:A:180:HIS:HD2	1:A:830:ASP:HB2	1.67	0.58
1:A:199:SER:HB2	1:A:200:PRO:HD2	1.86	0.56
1:A:807:LEU:CD1	1:A:846:GLY:HA3	2.35	0.55
1:A:454:ASP:CG	1:A:455:LEU:H	2.09	0.55
1:A:266:PRO:HG2	1:A:269:GLN:HB2	1.90	0.53
1:A:461:VAL:HG21	1:A:679:THR:HG23	1.91	0.53
1:A:628:LEU:CD2	1:A:656:LYS:HG2	2.39	0.52
1:A:908:THR:HB	1:A:953:PRO:HG2	1.93	0.51
1:A:728:GLN:O	1:A:732:MET:HB2	2.10	0.51
1:A:269:GLN:HA	1:A:274:ARG:HH21	1.76	0.51
1:A:1022:ILE:O	1:A:1026:LEU:HB2	2.10	0.51
1:A:162:ARG:HH22	1:A:300:ASP:H	1.59	0.50
1:A:640:LYS:HE2	1:A:680:VAL:HG11	1.92	0.50
1:A:568:LEU:HG	1:A:583:MET:HE1	1.94	0.49
1:A:802:LYS:HE3	1:A:805:ASP:HB2	1.95	0.49
1:A:713:ILE:HG12	1:A:845:VAL:HG11	1.96	0.48
1:A:849:GLU:O	2:A:1101:ML9:H21B	2.14	0.48
1:A:776:LYS:HE2	1:A:804:GLY:HA3	1.96	0.47
1:A:191:ILE:HG22	1:A:282:MET:SD	2.54	0.47
1:A:568:LEU:HG	1:A:583:MET:CE	2.44	0.47
1:A:379:SER:O	1:A:381:PRO:HD3	2.14	0.47
1:A:328:TRP:CD1	1:A:394:PRO:HB3	2.49	0.47
1:A:121:ILE:HG12	1:A:688:LEU:HB3	1.97	0.46
1:A:851:VAL:HG23	2:A:1101:ML9:H21	1.98	0.45
1:A:916:ARG:HD3	1:A:931:HIS:ND1	2.31	0.45
1:A:531:LEU:HA	1:A:534:ILE:HD12	1.98	0.45
1:A:199:SER:CB	1:A:200:PRO:CD	2.94	0.45
1:A:636:VAL:O	1:A:639:LEU:HB2	2.17	0.45
1:A:661:GLN:NE2	1:A:698:TYR:HB2	2.32	0.45
1:A:1006:LEU:HD21	1:A:1019:ILE:HD11	1.99	0.44
1:A:508:TYR:HD2	1:A:508:TYR:H	1.65	0.44
1:A:561:ILE:O	1:A:564:ILE:HG22	2.18	0.43
1:A:354:ILE:HD11	1:A:381:PRO:HB3	1.99	0.43
1:A:602:LEU:O	1:A:612:ARG:NH2	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:731:GLN:HB3	1:A:771:ILE:HD13	2.00	0.43
1:A:372:ASN:N	1:A:372:ASN:HD22	2.17	0.43
1:A:363:GLY:N	1:A:607:PRO:HG3	2.34	0.43
1:A:583:MET:HA	1:A:586:LEU:HD12	2.02	0.42
1:A:638:VAL:HG11	1:A:1004:MET:HG2	2.01	0.42
1:A:499:SER:O	1:A:503:GLU:HB2	2.21	0.41
1:A:572:VAL:CG2	1:A:583:MET:HE3	2.51	0.41
1:A:572:VAL:HG21	1:A:583:MET:HG2	2.02	0.41
1:A:218:GLU:OE2	1:A:248:GLY:HA3	2.21	0.41
1:A:165:TYR:O	1:A:168:PRO:HD3	2.21	0.40
1:A:665:HIS:CG	1:A:757:PRO:HG3	2.56	0.40
1:A:393:ILE:HD13	1:A:480:PHE:CZ	2.57	0.40
1:A:446:TRP:CZ2	1:A:465:ASN:HA	2.57	0.40

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	863/946 (91%)	791 (92%)	59 (7%)	13 (2%)	13 38

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	378	CYS
1	A	508	TYR
1	A	199	SER
1	A	381	PRO
1	A	453	GLU
1	A	511	ALA
1	A	722	GLU
1	A	862	CYS

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Mol	Chain	Res	Type
1	A	264	LYS
1	A	723	LYS
1	A	231	SER
1	A	1027	ALA
1	A	346	VAL

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	624/860 (73%)	590 (95%)	34 (5%)	27 59

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	162	ARG
1	A	192	VAL
1	A	278	MET
1	A	326	SER
1	A	357	ARG
1	A	378	CYS
1	A	419	HIS
1	A	438	SER
1	A	462	THR
1	A	469	GLU
1	A	475	LEU
1	A	530	GLN
1	A	551	LEU
1	A	559	VAL
1	A	577	ARG
1	A	610	MET
1	A	679	THR
1	A	715	LEU
1	A	720	LYS
1	A	721	GLN
1	A	728	GLN

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Mol	Chain	Res	Type
1	A	732	MET
1	A	735	LEU
1	A	740	ARG
1	A	764	LEU
1	A	777	ARG
1	A	790	SER
1	A	810	ASP
1	A	811	MET
1	A	829	LEU
1	A	834	LEU
1	A	845	VAL
1	A	919	SER
1	A	1017	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	345	ASN
1	A	372	ASN
1	A	419	HIS
1	A	530	GLN
1	A	661	GLN
1	A	760	GLN
1	A	825	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)

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	ML9	A	1101	-	33,34,34	1.04	2 (6%)	34,48,48	0.90	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	ML9	A	1101	-	-	0/14/24/24	0/4/4/4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1101	ML9	C10-C9	-2.11	1.34	1.37
2	A	1101	ML9	C8-N7	4.39	1.44	1.38

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1101	ML9	C10-C9-C8	2.25	119.86	116.60
2	A	1101	ML9	C2-N1-C6	2.79	119.37	117.01

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1101	ML9	2	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	879/946 (92%)	0.35	63 (7%) 18 12	37, 70, 118, 162	0

All (63) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	307	TYR	6.8
1	A	521	ASN	6.5
1	A	300	ASP	6.4
1	A	502	ARG	5.4
1	A	972	THR	4.9
1	A	873	ASN	4.5
1	A	889	ILE	4.2
1	A	1033	GLN	4.1
1	A	877	LEU	4.1
1	A	299	MET	4.0
1	A	295	SER	3.7
1	A	974	THR	3.7
1	A	862	CYS	3.7
1	A	482	SER	3.7
1	A	306	SER	3.6
1	A	891	ASP	3.5
1	A	975	ARG	3.5
1	A	520	ASP	3.5
1	A	518	ALA	3.4
1	A	878	HIS	3.4
1	A	326	SER	3.4
1	A	892	ALA	3.3
1	A	130	MET	3.2
1	A	978	GLU	3.1
1	A	503	GLU	3.1
1	A	183	ASN	3.1
1	A	517	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	347	ASN	3.1
1	A	498	TRP	3.0
1	A	182	TYR	2.9
1	A	308	SER	2.9
1	A	1046	ALA	2.9
1	A	953	PRO	2.8
1	A	880	TRP	2.7
1	A	961	LEU	2.6
1	A	872	PHE	2.6
1	A	550	PHE	2.6
1	A	488	ASP	2.6
1	A	501	SER	2.6
1	A	508	TYR	2.6
1	A	185	LEU	2.5
1	A	985	TYR	2.3
1	A	725	ASP	2.3
1	A	805	ASP	2.3
1	A	936	HIS	2.3
1	A	410	LYS	2.3
1	A	450	HIS	2.2
1	A	523	LEU	2.2
1	A	887	GLY	2.2
1	A	304	MET	2.2
1	A	131	VAL	2.2
1	A	965	SER	2.2
1	A	740	ARG	2.2
1	A	525	GLU	2.2
1	A	483	VAL	2.2
1	A	1038	TYR	2.2
1	A	180	HIS	2.2
1	A	527	ASP	2.1
1	A	378	CYS	2.1
1	A	804	GLY	2.1
1	A	963	VAL	2.1
1	A	879	GLN	2.0
1	A	1031	THR	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	ML9	A	1101	31/31	0.94	0.20	-0.04	62,69,91,97	0

6.5 Other polymers (i)

There are no such residues in this entry.