



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:11 AM UTC

PDB ID : 4TUU / pdb_00004tuu
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 : 2014-06-24
Resolution : 2.64 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

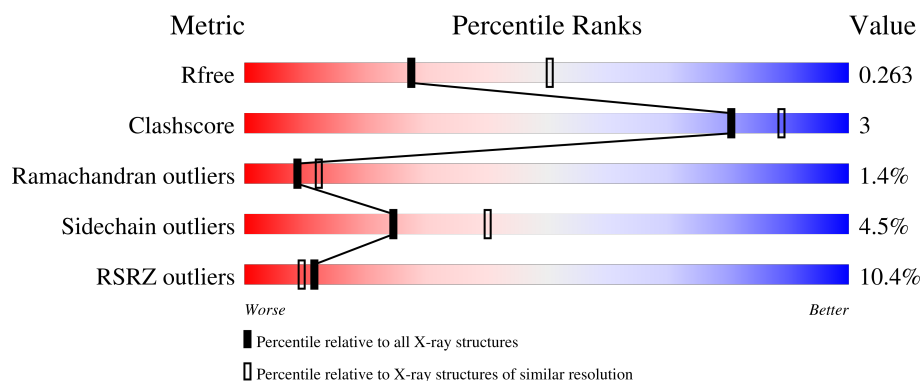
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.64 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}	180053	2053 (2.66-2.62)
Clashscore	190562	2097 (2.66-2.62)
Ramachandran outliers	187476	2066 (2.66-2.62)
Sidechain outliers	187428	2066 (2.66-2.62)
RSRZ outliers	180081	2052 (2.66-2.62)

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 of 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 $\leq 5\%$. 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	946	10% 81% 10% 7%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6631 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 sub-unit alpha isoform.

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

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

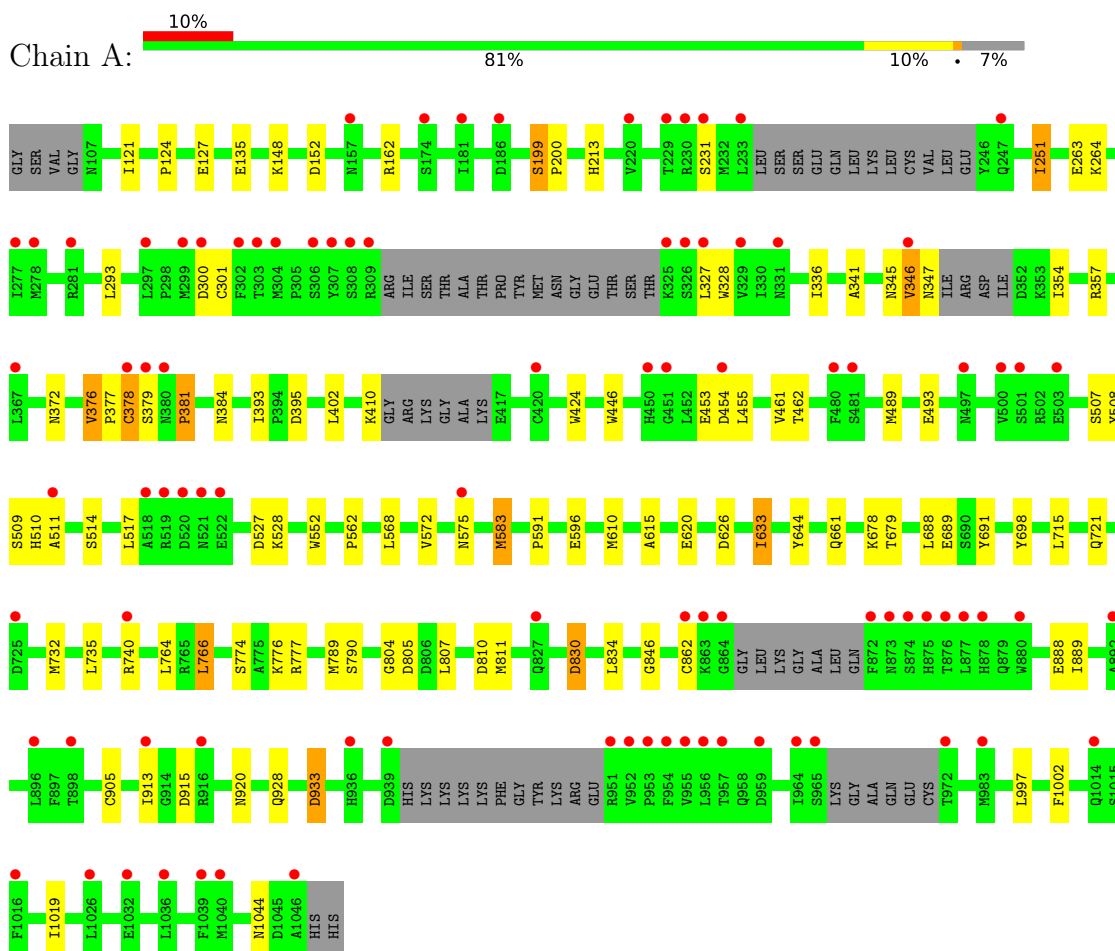
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	30	Total	O	0	0
			30	30		

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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: Phosphatidylinositol 4,5-bisphosphate 3-kinase catalytic subunit alpha isoform



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	57.69Å 136.45Å 143.08Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.64 – 2.64 35.64 – 2.64	Depositor EDS
% Data completeness (in resolution range)	100.0 (35.64-2.64) 99.9 (35.64-2.64)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.49 (at 2.65Å)	Xtriage
Refinement program	BUSTER 2.11.4	Depositor
R, R_{free}	0.209 , 0.245 0.225 , 0.263	Depositor DCC
R_{free} test set	1720 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	62.3	Xtriage
Anisotropy	0.009	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 71.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	0.000 for -h,l,k	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6631	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.51% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	0.91	4/6751 (0.1%)	1.41	39/9207 (0.4%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	633	ILE	CG1-CD1	6.78	1.78	1.51
1	A	777	ARG	CA-CB	5.34	1.56	1.52
1	A	583	MET	SD-CE	-5.11	1.66	1.79
1	A	721	GLN	CA-C	5.08	1.55	1.52

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	507	SER	CA-C-N	10.78	141.10	121.70
1	A	507	SER	C-N-CA	10.78	141.10	121.70
1	A	346	VAL	CA-C-N	6.70	133.76	121.70
1	A	346	VAL	C-N-CA	6.70	133.76	121.70
1	A	152	ASP	CA-CB-CG	6.26	118.86	112.60
1	A	527	ASP	CA-CB-CG	6.25	118.85	112.60
1	A	377	PRO	CA-C-N	5.97	129.10	120.38
1	A	377	PRO	C-N-CA	5.97	129.10	120.38
1	A	810	ASP	CA-C-N	5.95	128.58	120.54
1	A	810	ASP	C-N-CA	5.95	128.58	120.54
1	A	327	LEU	CA-C-N	5.90	131.81	122.60
1	A	327	LEU	C-N-CA	5.90	131.81	122.60
1	A	509	SER	N-CA-C	5.80	119.98	113.02
1	A	528	LYS	N-CA-C	-5.75	105.76	112.89
1	A	678	LYS	CA-C-N	5.74	128.54	120.28
1	A	678	LYS	C-N-CA	5.74	128.54	120.28
1	A	263	GLU	CA-C-N	5.64	132.31	121.54
1	A	263	GLU	C-N-CA	5.64	132.31	121.54
1	A	888	GLU	CA-C-N	5.60	129.31	120.47
1	A	888	GLU	C-N-CA	5.60	129.31	120.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	933	ASP	CA-CB-CG	5.53	118.13	112.60
1	A	920	ASN	N-CA-C	-5.48	107.60	114.56
1	A	774	SER	CA-C-N	5.39	127.50	120.28
1	A	774	SER	C-N-CA	5.39	127.50	120.28
1	A	913	ILE	CA-C-N	5.32	125.15	120.10
1	A	913	ILE	C-N-CA	5.32	125.15	120.10
1	A	376	VAL	N-CA-CB	-5.28	106.07	111.87
1	A	889	ILE	CA-C-N	5.27	127.65	120.54
1	A	889	ILE	C-N-CA	5.27	127.65	120.54
1	A	830	ASP	CA-CB-CG	5.25	117.85	112.60
1	A	905	CYS	CA-C-N	5.24	127.16	120.56
1	A	905	CYS	C-N-CA	5.24	127.16	120.56
1	A	790	SER	CA-C-N	5.17	127.93	120.38
1	A	790	SER	C-N-CA	5.17	127.93	120.38
1	A	328	TRP	N-CA-C	-5.15	106.23	112.88
1	A	691	TYR	CA-C-N	5.09	127.61	120.28
1	A	691	TYR	C-N-CA	5.09	127.61	120.28
1	A	615	ALA	CA-C-N	5.07	127.41	120.46
1	A	615	ALA	C-N-CA	5.07	127.41	120.46

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	33	0
2	A	30	0	0	0	0
All	All	6631	0	5945	33	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 3.

All (33) 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:633:ILE:CD1	1:A:633:ILE:CG1	1.78	1.60
1:A:568:LEU:HG	1:A:583:MET:HE1	1.48	0.93
1:A:124:PRO:HG2	1:A:127:GLU:HG3	1.73	0.70
1:A:357:ARG:HE	1:A:372:ASN:HD21	1.45	0.65
1:A:395:ASP:HB3	1:A:575:ASN:O	1.98	0.63
1:A:776:LYS:HE2	1:A:804:GLY:HA3	1.82	0.61
1:A:807:LEU:HD12	1:A:846:GLY:HA3	1.83	0.60
1:A:596:GLU:HG2	1:A:997:LEU:HD13	1.87	0.57
1:A:199:SER:HB2	1:A:200:PRO:HD2	1.88	0.55
1:A:357:ARG:NE	1:A:372:ASN:HD21	2.05	0.54
1:A:135:GLU:OE2	1:A:644:TYR:HB3	2.08	0.53
1:A:661:GLN:NE2	1:A:698:TYR:HB2	2.24	0.52
1:A:562:PRO:HG3	1:A:591:PRO:HG2	1.91	0.52
1:A:568:LEU:HG	1:A:583:MET:CE	2.32	0.52
1:A:379:SER:O	1:A:381:PRO:HD3	2.10	0.51
1:A:489:MET:HE3	1:A:493:GLU:HG2	1.94	0.50
1:A:766:LEU:H	1:A:766:LEU:HD12	1.76	0.49
1:A:341:ALA:HB3	1:A:381:PRO:HB2	1.96	0.47
1:A:454:ASP:CG	1:A:455:LEU:H	2.23	0.47
1:A:346:VAL:HG22	1:A:347:ASN:H	1.80	0.47
1:A:514:SER:HB3	1:A:517:LEU:HD12	1.96	0.47
1:A:121:ILE:HD11	1:A:689:GLU:HA	1.98	0.46
1:A:251:ILE:HD13	1:A:293:LEU:HD22	1.99	0.45
1:A:336:ILE:HD13	1:A:402:LEU:HD22	1.98	0.44
1:A:354:ILE:HG12	1:A:378:CYS:HA	1.99	0.44
1:A:162:ARG:HH22	1:A:300:ASP:HB2	1.82	0.44
1:A:552:TRP:HZ3	1:A:583:MET:HE2	1.82	0.44
1:A:121:ILE:HG12	1:A:688:LEU:HB3	2.00	0.43
1:A:572:VAL:HG21	1:A:583:MET:HG2	2.00	0.43
1:A:776:LYS:HE2	1:A:804:GLY:CA	2.48	0.42
1:A:424:TRP:CE2	1:A:446:TRP:HB2	2.55	0.41
1:A:199:SER:CB	1:A:200:PRO:HD2	2.51	0.41
1:A:1002:PHE:HB3	1:A:1019:ILE:HG12	2.03	0.41

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	863/946 (91%)	801 (93%)	50 (6%)	12 (1%)	9	12

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	264	LYS
1	A	508	TYR
1	A	199	SER
1	A	231	SER
1	A	511	ALA
1	A	830	ASP
1	A	862	CYS
1	A	915	ASP
1	A	933	ASP
1	A	453	GLU
1	A	381	PRO
1	A	510	HIS

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	624/860 (73%)	596 (96%)	28 (4%)	24	40

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	148	LYS
1	A	213	HIS
1	A	251	ILE
1	A	301	CYS
1	A	345	ASN

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Mol	Chain	Res	Type
1	A	376	VAL
1	A	378	CYS
1	A	384	ASN
1	A	393	ILE
1	A	410	LYS
1	A	461	VAL
1	A	462	THR
1	A	610	MET
1	A	620	GLU
1	A	626	ASP
1	A	679	THR
1	A	715	LEU
1	A	732	MET
1	A	735	LEU
1	A	740	ARG
1	A	764	LEU
1	A	766	LEU
1	A	789	MET
1	A	805	ASP
1	A	811	MET
1	A	834	LEU
1	A	928	GLN
1	A	1044	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	183	ASN
1	A	269	GLN
1	A	362	HIS
1	A	370	ASN
1	A	372	ASN
1	A	419	HIS
1	A	643	GLN
1	A	738	GLN
1	A	936	HIS

5.3.3 RNA ⓘ

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

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, 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	879/946 (92%)	0.69	91 (10%) 11 9	35, 62, 106, 142	0

All (91) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	939	ASP	6.7
1	A	1046	ALA	5.7
1	A	233	LEU	5.0
1	A	872	PHE	4.9
1	A	959	ASP	4.8
1	A	451	GLY	4.7
1	A	956	LEU	4.4
1	A	380	ASN	4.3
1	A	521	ASN	4.2
1	A	954	PHE	4.0
1	A	955	VAL	3.9
1	A	953	PRO	3.7
1	A	309	ARG	3.7
1	A	247	GLN	3.6
1	A	951	ARG	3.6
1	A	864	GLY	3.5
1	A	873	ASN	3.5
1	A	518	ALA	3.5
1	A	297	LEU	3.4
1	A	186	ASP	3.4
1	A	379	SER	3.4
1	A	896	LEU	3.3
1	A	307	TYR	3.3
1	A	522	GLU	3.3
1	A	874	SER	3.3
1	A	302	PHE	3.2
1	A	520	ASP	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	278	MET	3.1
1	A	300	ASP	3.1
1	A	725	ASP	3.1
1	A	1040	MET	3.1
1	A	308	SER	3.1
1	A	325	LYS	3.0
1	A	327	LEU	3.0
1	A	877	LEU	3.0
1	A	875	HIS	3.0
1	A	936	HIS	2.9
1	A	863	LYS	2.9
1	A	952	VAL	2.9
1	A	346	VAL	2.9
1	A	1026	LEU	2.8
1	A	862	CYS	2.8
1	A	827	GLN	2.8
1	A	306	SER	2.8
1	A	892	ALA	2.7
1	A	1032	GLU	2.7
1	A	500	VAL	2.7
1	A	174	SER	2.7
1	A	229	THR	2.7
1	A	1039	PHE	2.7
1	A	231	SER	2.6
1	A	876	THR	2.6
1	A	378	CYS	2.6
1	A	1014	GLN	2.6
1	A	281	ARG	2.5
1	A	277	ILE	2.5
1	A	367	LEU	2.5
1	A	481	SER	2.5
1	A	1036	LEU	2.5
1	A	299	MET	2.4
1	A	1016	PHE	2.4
1	A	303	THR	2.4
1	A	964	ILE	2.4
1	A	157	ASN	2.4
1	A	497	ASN	2.4
1	A	454	ASP	2.4
1	A	220	VAL	2.4
1	A	575	ASN	2.4
1	A	420	CYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	450	HIS	2.3
1	A	304	MET	2.3
1	A	916	ARG	2.3
1	A	519	ARG	2.3
1	A	501	SER	2.3
1	A	329	VAL	2.3
1	A	181	ILE	2.2
1	A	913	ILE	2.2
1	A	511	ALA	2.2
1	A	503	GLU	2.2
1	A	898	THR	2.2
1	A	230	ARG	2.2
1	A	326	SER	2.2
1	A	480	PHE	2.1
1	A	880	TRP	2.1
1	A	957	THR	2.1
1	A	331	ASN	2.1
1	A	965	SER	2.1
1	A	878	HIS	2.1
1	A	972	THR	2.0
1	A	983	MET	2.0
1	A	740	ARG	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.