



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 01:11 PM UTC

PDB ID : 4XI2 / pdb_00004xi2
Title : Crystal Structure of an auto-inhibited form of Bruton's Tryrosine Kinase
Authors : Vogan, E.M.; Harrison, S.C.
Deposited on : 2015-01-06
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

<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

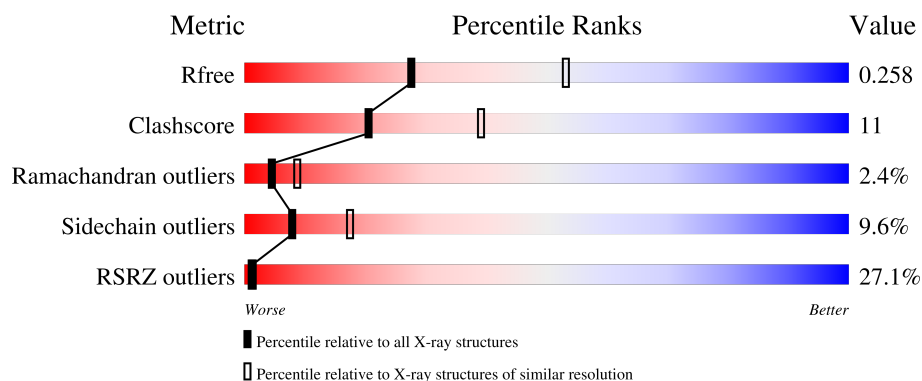
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (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 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	446	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6835 atoms, of which 3375 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 Tyrosine-protein kinase BTK.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	421	Total	C	H	N	O	S	54	0	0
			6833	2215	3375	577	642	24			

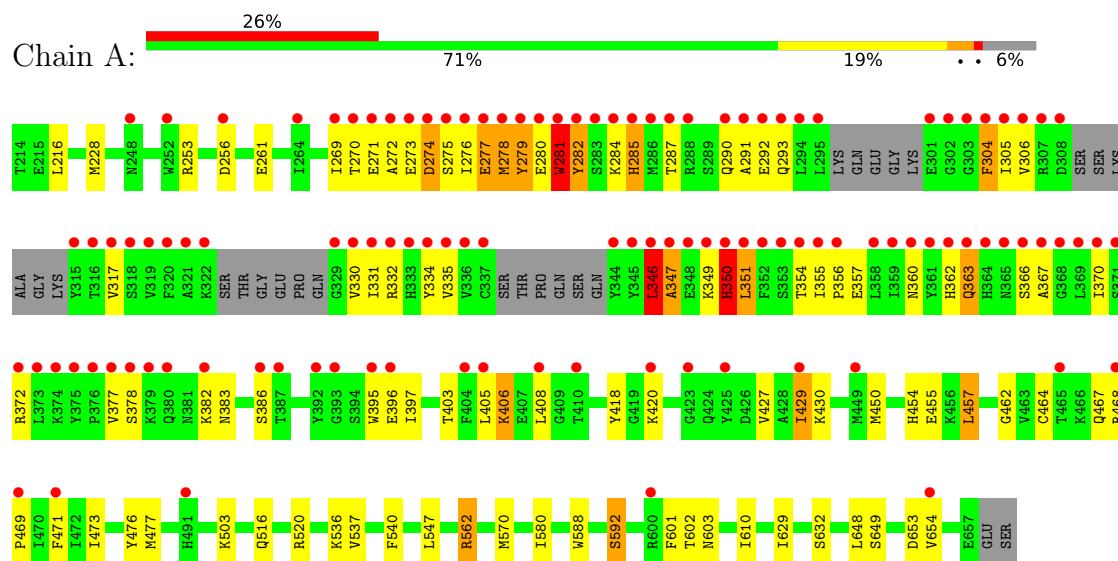
- Molecule 2 is GOLD ION (CCD ID: AU) (formula: Au).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Au	0	0
			2	2		

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: Tyrosine-protein kinase BTK



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	132.20Å 132.20Å 107.63Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	43.27 – 2.60 43.27 – 2.60	Depositor EDS
% Data completeness (in resolution range)	89.2 (43.27-2.60) 91.7 (43.27-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.46 (at 2.61Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1839)	Depositor
R, R_{free}	0.230 , 0.248 0.235 , 0.258	Depositor DCC
R_{free} test set	1525 reflections (4.77%)	wwPDB-VP
Wilson B-factor (Å ²)	73.2	Xtriage
Anisotropy	0.066	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 81.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.024 for -h,-k,l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6835	wwPDB-VP
Average B, all atoms (Å ²)	122.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.02% 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

Bond lengths and bond angles in the following residue types are not validated in this section: AU

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	0.47	3/3540 (0.1%)	0.84	16/4774 (0.3%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	285	HIS	ND1-CE1	5.52	1.38	1.32
1	A	362	HIS	ND1-CE1	5.26	1.37	1.32
1	A	350	HIS	ND1-CE1	5.23	1.37	1.32

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	293	GLN	OE1-CD-NE2	-9.83	112.77	122.60
1	A	290	GLN	OE1-CD-NE2	-9.77	112.83	122.60
1	A	363	GLN	OE1-CD-NE2	-9.73	112.87	122.60
1	A	278	MET	N-CA-C	8.03	119.66	111.07
1	A	350	HIS	CB-CG-CD2	-6.69	122.50	131.20
1	A	293	GLN	CG-CD-NE2	6.68	126.42	116.40
1	A	290	GLN	CG-CD-NE2	6.67	126.40	116.40
1	A	363	GLN	CG-CD-NE2	6.62	126.33	116.40
1	A	362	HIS	CB-CG-CD2	-6.53	122.72	131.20
1	A	285	HIS	CB-CG-CD2	-6.35	122.95	131.20
1	A	363	GLN	N-CA-C	-6.07	105.88	113.28
1	A	304	PHE	N-CA-C	5.88	117.16	108.86
1	A	285	HIS	CB-CG-ND1	5.67	131.20	122.70
1	A	350	HIS	CB-CG-ND1	5.66	131.19	122.70
1	A	362	HIS	CB-CG-ND1	5.57	131.05	122.70
1	A	378	SER	N-CA-C	5.11	118.28	110.36

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	3458	3375	3375	76	6
2	A	2	0	0	0	0
All	All	3460	3375	3375	76	6

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 11.

All (76) 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:292:GLU:HG2	1:A:331:ILE:HD12	1.21	1.18
1:A:292:GLU:CG	1:A:331:ILE:HD12	1.99	0.91
1:A:292:GLU:HA	1:A:331:ILE:CD1	2.01	0.90
1:A:349:LYS:NZ	1:A:350:HIS:HB2	1.86	0.90
1:A:292:GLU:HA	1:A:331:ILE:HD13	1.61	0.82
1:A:292:GLU:HG2	1:A:331:ILE:CD1	2.06	0.81
1:A:354:THR:C	1:A:356:PRO:HD2	2.13	0.73
1:A:429:ILE:C	1:A:429:ILE:HD12	2.14	0.73
1:A:349:LYS:HZ2	1:A:350:HIS:HB2	1.52	0.73
1:A:429:ILE:HD12	1:A:430:LYS:N	2.06	0.71
1:A:349:LYS:HZ3	1:A:350:HIS:HB2	1.54	0.70
1:A:304:PHE:O	1:A:305:ILE:CG2	2.43	0.67
1:A:355:ILE:N	1:A:356:PRO:HD2	2.10	0.67
1:A:429:ILE:HD11	1:A:471:PHE:CD2	2.30	0.67
1:A:349:LYS:HG3	1:A:350:HIS:N	2.10	0.66
1:A:306:VAL:HG22	1:A:317:VAL:HG22	1.79	0.64
1:A:292:GLU:CG	1:A:331:ILE:CD1	2.73	0.62
1:A:304:PHE:O	1:A:305:ILE:HG23	2.00	0.62
1:A:354:THR:CB	1:A:356:PRO:HD2	2.30	0.62
1:A:562:ARG:NH1	1:A:603:ASN:OD1	2.33	0.62
1:A:304:PHE:C	1:A:305:ILE:HG23	2.26	0.61
1:A:276:ILE:CG2	1:A:282:TYR:CD1	2.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:355:ILE:N	1:A:356:PRO:CD	2.65	0.59
1:A:334:TYR:CD2	1:A:346:LEU:HD21	2.38	0.58
1:A:629:ILE:O	1:A:632:SER:OG	2.19	0.58
1:A:253:ARG:NH2	1:A:261:GLU:OE1	2.37	0.58
1:A:349:LYS:HG3	1:A:350:HIS:H	1.69	0.58
1:A:292:GLU:CA	1:A:331:ILE:CD1	2.79	0.57
1:A:349:LYS:CG	1:A:350:HIS:H	2.17	0.57
1:A:335:VAL:O	1:A:346:LEU:O	2.24	0.56
1:A:349:LYS:CG	1:A:350:HIS:N	2.68	0.56
1:A:281:TRP:H	1:A:281:TRP:CD1	2.21	0.55
1:A:276:ILE:HG21	1:A:282:TYR:CD1	2.42	0.54
1:A:354:THR:HB	1:A:356:PRO:HD2	1.90	0.54
1:A:562:ARG:NH2	1:A:601:PHE:O	2.41	0.54
1:A:291:ALA:HB1	1:A:305:ILE:HD11	1.91	0.53
1:A:588:TRP:O	1:A:592:SER:OG	2.26	0.53
1:A:356:PRO:O	1:A:360:ASN:OD1	2.26	0.53
1:A:408:LEU:HD11	1:A:476:TYR:HE1	1.73	0.53
1:A:334:TYR:HD2	1:A:346:LEU:HD21	1.73	0.52
1:A:363:GLN:O	1:A:372:ARG:HD2	2.12	0.50
1:A:464:CYS:SG	1:A:471:PHE:HB2	2.52	0.50
1:A:330:VAL:HG22	1:A:331:ILE:N	2.27	0.49
1:A:304:PHE:C	1:A:305:ILE:CG2	2.85	0.49
1:A:279:TYR:CD1	1:A:279:TYR:N	2.82	0.47
1:A:457:LEU:HD22	1:A:540:PHE:CE1	2.50	0.46
1:A:468:ARG:HA	1:A:469:PRO:C	2.40	0.46
1:A:349:LYS:CD	1:A:350:HIS:H	2.29	0.46
1:A:370:ILE:O	1:A:370:ILE:HG22	2.16	0.45
1:A:405:LEU:HG	1:A:406:LYS:HD2	1.99	0.45
1:A:334:TYR:HB3	1:A:346:LEU:HG	1.99	0.45
1:A:277:GLU:H	1:A:277:GLU:HG2	1.39	0.45
1:A:397:ILE:HG13	1:A:473:ILE:HD13	2.00	0.44
1:A:477:MET:HE1	1:A:536:LYS:HG3	2.00	0.44
1:A:276:ILE:HG22	1:A:282:TYR:CG	2.52	0.44
1:A:454:HIS:HB3	1:A:457:LEU:HB2	2.00	0.44
1:A:279:TYR:H	1:A:279:TYR:HD1	1.63	0.44
1:A:351:LEU:HD12	1:A:351:LEU:HA	1.71	0.44
1:A:366:SER:O	1:A:367:ALA:C	2.60	0.43
1:A:304:PHE:O	1:A:305:ILE:HG22	2.16	0.43
1:A:455:GLU:O	1:A:536:LYS:HD3	2.19	0.43
1:A:274:ASP:HB3	1:A:279:TYR:OH	2.20	0.41
1:A:405:LEU:HD22	1:A:420:LYS:HE3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:346:LEU:HB3	1:A:347:ALA:H	1.63	0.41
1:A:408:LEU:HD11	1:A:418:TYR:HB2	2.02	0.41
1:A:429:ILE:HD11	1:A:471:PHE:CG	2.55	0.41
1:A:284:LYS:HG2	1:A:285:HIS:H	1.85	0.41
1:A:349:LYS:HD2	1:A:350:HIS:H	1.84	0.41
1:A:270:THR:OG1	1:A:271:GLU:N	2.53	0.41
1:A:292:GLU:CB	1:A:331:ILE:HD12	2.47	0.41
1:A:273:GLU:O	1:A:274:ASP:C	2.64	0.41
1:A:282:TYR:CE2	1:A:284:LYS:N	2.84	0.41
1:A:356:PRO:O	1:A:360:ASN:CG	2.64	0.41
1:A:395:TRP:CG	1:A:396:GLU:N	2.88	0.40
1:A:450:MET:HE1	1:A:462:GLY:HA2	2.03	0.40
1:A:284:LYS:HG2	1:A:285:HIS:N	2.37	0.40

All (6) 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:332:ARG:HG3	1:A:370:ILE:CD1[4_556]	0.79	0.81
1:A:332:ARG:HG3	1:A:370:ILE:HD11[4_556]	0.93	0.67
1:A:332:ARG:HG3	1:A:370:ILE:HD13[4_556]	0.94	0.66
1:A:332:ARG:CG	1:A:370:ILE:CD1[4_556]	1.71	0.49
1:A:332:ARG:HG3	1:A:370:ILE:HD12[4_556]	1.24	0.36
1:A:332:ARG:CG	1:A:370:ILE:HD11[4_556]	1.51	0.09

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	411/446 (92%)	374 (91%)	27 (7%)	10 (2%)	4 9

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	272	ALA
1	A	274	ASP
1	A	287	THR
1	A	275	SER
1	A	346	LEU
1	A	347	ALA
1	A	280	GLU
1	A	282	TYR
1	A	383	ASN
1	A	281	TRP

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	376/397 (95%)	340 (90%)	36 (10%)	8 17

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	216	LEU
1	A	228	MET
1	A	256	ASP
1	A	269	ILE
1	A	277	GLU
1	A	278	MET
1	A	279	TYR
1	A	281	TRP
1	A	346	LEU
1	A	350	HIS
1	A	351	LEU
1	A	357	GLU
1	A	377	VAL
1	A	382	LYS
1	A	386	SER
1	A	403	THR
1	A	406	LYS

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Mol	Chain	Res	Type
1	A	427	VAL
1	A	429	ILE
1	A	457	LEU
1	A	467	GLN
1	A	503	LYS
1	A	516	GLN
1	A	520	ARG
1	A	537	VAL
1	A	547	LEU
1	A	562	ARG
1	A	570	MET
1	A	580	ILE
1	A	592	SER
1	A	602	THR
1	A	610	ILE
1	A	648	LEU
1	A	649	SER
1	A	653	ASP
1	A	654	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	532	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

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, 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	421/446 (94%)	1.43	114 (27%) 1 1	56, 103, 235, 245	6 (1%)

All (114) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	320	PHE	8.1
1	A	294	LEU	7.4
1	A	344	TYR	7.3
1	A	272	ALA	7.3
1	A	286	MET	7.2
1	A	303	GLY	7.1
1	A	278	MET	6.8
1	A	301	GLU	6.7
1	A	322	LYS	6.7
1	A	285	HIS	6.7
1	A	276	ILE	6.6
1	A	337	CYS	6.5
1	A	318	SER	6.2
1	A	367	ALA	6.2
1	A	335	VAL	5.9
1	A	316	THR	5.9
1	A	315	TYR	5.8
1	A	330	VAL	5.8
1	A	291	ALA	5.7
1	A	321	ALA	5.7
1	A	295	LEU	5.6
1	A	375	TYR	5.6
1	A	361	TYR	5.4
1	A	347	ALA	5.4
1	A	362	HIS	5.3
1	A	305	ILE	5.3
1	A	351	LEU	5.3

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Mol	Chain	Res	Type	RSRZ
1	A	356	PRO	5.2
1	A	345	TYR	5.2
1	A	358	LEU	5.2
1	A	377	VAL	5.1
1	A	308	ASP	5.1
1	A	279	TYR	5.0
1	A	293	GLN	5.0
1	A	395	TRP	5.0
1	A	370	ILE	5.0
1	A	349	LYS	4.9
1	A	304	PHE	4.9
1	A	378	SER	4.9
1	A	352	PHE	4.7
1	A	359	ILE	4.6
1	A	373	LEU	4.6
1	A	307	ARG	4.5
1	A	371	SER	4.5
1	A	350	HIS	4.3
1	A	363	GLN	4.3
1	A	281	TRP	4.2
1	A	379	LYS	4.2
1	A	275	SER	4.2
1	A	355	ILE	4.2
1	A	277	GLU	4.2
1	A	283	SER	4.0
1	A	365	ASN	4.0
1	A	332	ARG	3.8
1	A	306	VAL	3.8
1	A	248	ASN	3.7
1	A	302	GLY	3.7
1	A	348	GLU	3.6
1	A	396	GLU	3.6
1	A	284	LYS	3.5
1	A	408	LEU	3.5
1	A	329	GLY	3.5
1	A	368	GLY	3.4
1	A	360	ASN	3.4
1	A	425	TYR	3.3
1	A	376	PRO	3.3
1	A	366	SER	3.3
1	A	269	ILE	3.3
1	A	334	TYR	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	271	GLU	3.2
1	A	654	VAL	3.2
1	A	282	TYR	3.2
1	A	280	GLU	3.1
1	A	372	ARG	3.1
1	A	469	PRO	3.0
1	A	354	THR	3.0
1	A	333	HIS	3.0
1	A	274	ASP	3.0
1	A	465	THR	2.9
1	A	319	VAL	2.9
1	A	331	ILE	2.9
1	A	364	HIS	2.9
1	A	382	LYS	2.9
1	A	288	ARG	2.9
1	A	600	ARG	2.8
1	A	405	LEU	2.8
1	A	290	GLN	2.8
1	A	336	VAL	2.8
1	A	404	PHE	2.8
1	A	392	TYR	2.7
1	A	264	ILE	2.7
1	A	292	GLU	2.7
1	A	256	ASP	2.6
1	A	252	TRP	2.6
1	A	423	GLY	2.5
1	A	429	ILE	2.5
1	A	374	LYS	2.4
1	A	386	SER	2.4
1	A	369	LEU	2.4
1	A	346	LEU	2.3
1	A	468	ARG	2.3
1	A	491	HIS	2.2
1	A	273	GLU	2.2
1	A	387	THR	2.2
1	A	317	VAL	2.2
1	A	287	THR	2.2
1	A	353	SER	2.2
1	A	449	MET	2.2
1	A	471	PHE	2.1
1	A	393	GLY	2.1
1	A	380	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	420	LYS	2.0
1	A	410	THR	2.0
1	A	270	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 oligosaccharides 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. 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	B-factors(Å ²)	Q<0.9
2	AU	A	702	1/1	0.88	0.23	218,218,218,218	0
2	AU	A	701	1/1	0.98	0.11	191,191,191,191	1

6.5 Other polymers [i](#)

There are no such residues in this entry.