



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:03 AM UTC

PDB ID : 3UQG / pdb_00003uqg
Title : c-SRC kinase domain in complex with bumpless BKI analog UW1243
Authors : Merritt, E.A.; Larson, E.T.
Deposited on : 2011-11-20
Resolution : 2.20 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
Mogul : 2022.3.0, CSD as543be (2022)
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

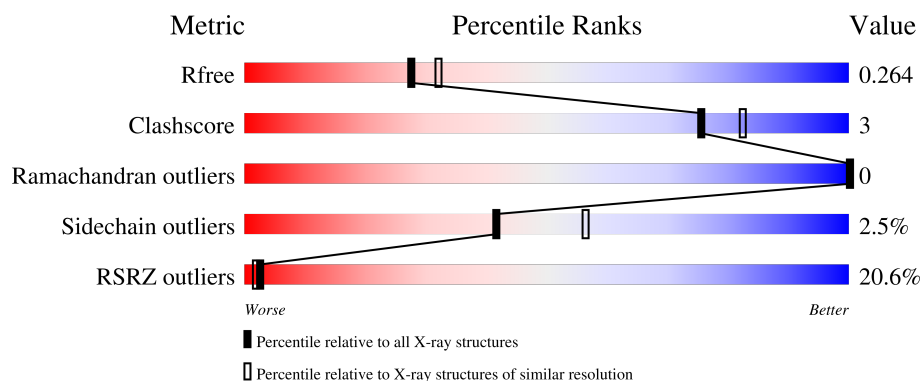
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	286	19% 82% 10% 8%
1	B	286	19% 83% 7% 10%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 4194 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.

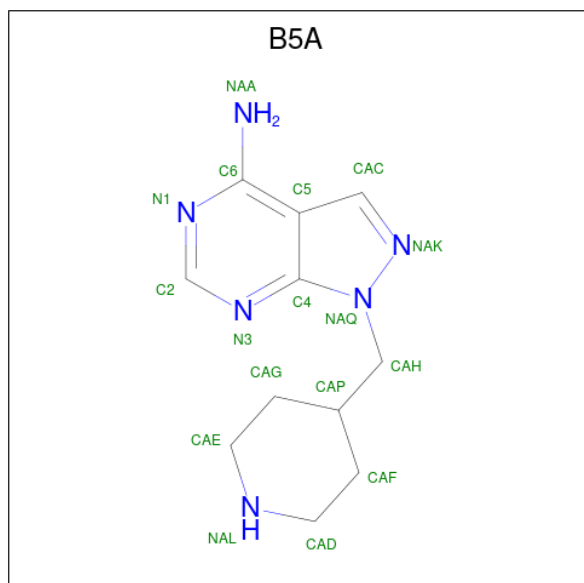
- Molecule 1 is a protein called Proto-oncogene tyrosine-protein kinase Src.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	263	Total	C	N	O	S	0	1	0
			2104	1351	351	385	17			
1	B	257	Total	C	N	O	S	0	0	0
			2028	1303	338	372	15			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	248	GLY	-	expression tag	UNP P00523
A	249	HIS	-	expression tag	UNP P00523
A	250	MET	-	expression tag	UNP P00523
B	248	GLY	-	expression tag	UNP P00523
B	249	HIS	-	expression tag	UNP P00523
B	250	MET	-	expression tag	UNP P00523

- Molecule 2 is 1-(piperidin-4-ylmethyl)-1H-pyrazolo[3,4-d]pyrimidin-4-amine (CCD ID: B5A) (formula: C₁₁H₁₆N₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	N	0	0
			17	11	6		
2	B	1	Total	C	N	0	0
			17	11	6		

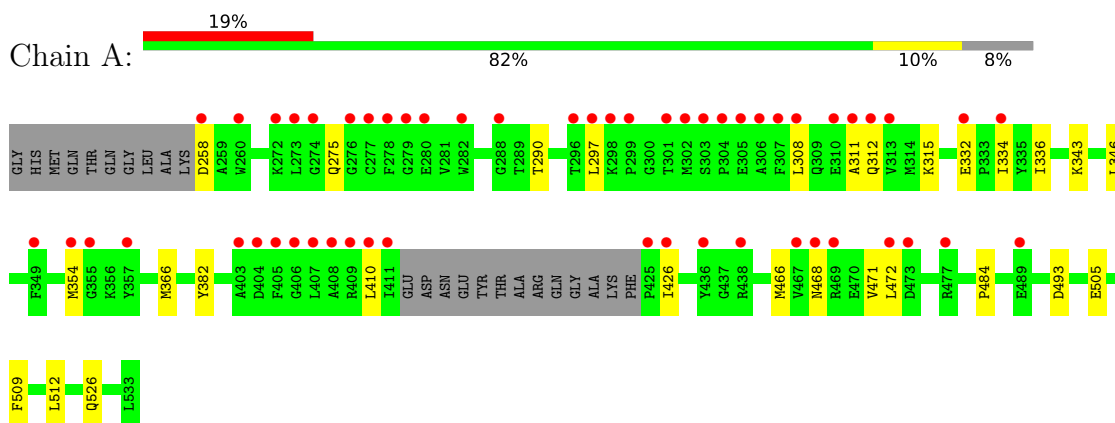
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	17	Total	O	0	0
			17	17		
3	B	11	Total	O	0	0
			11	11		

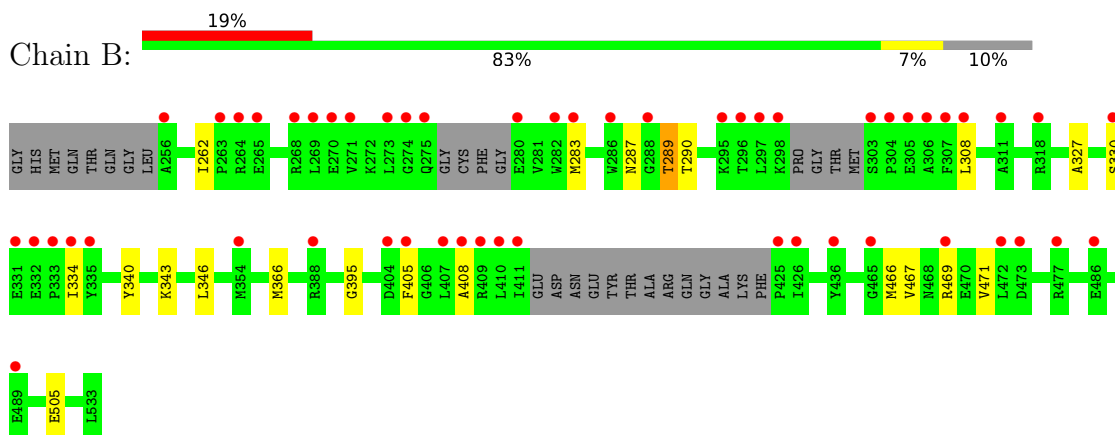
3 Residue-property plots [i](#)

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: Proto-oncogene tyrosine-protein kinase Src



- Molecule 1: Proto-oncogene tyrosine-protein kinase Src



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	42.54Å 63.72Å 74.98Å 78.17° 89.34° 90.08°	Depositor
Resolution (Å)	53.21 – 2.20 53.21 – 2.20	Depositor EDS
% Data completeness (in resolution range)	97.5 (53.21-2.20) 97.5 (53.21-2.20)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.67 (at 2.20Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.229 , 0.259 0.237 , 0.264	Depositor DCC
R_{free} test set	1905 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	34.1	Xtriage
Anisotropy	0.227	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 40.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.025 for h,-k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	4194	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 16.65% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: B5A

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	0.75	1/2158 (0.0%)	0.82	0/2923
1	B	0.75	0/2075	0.80	0/2814
All	All	0.75	1/4233 (0.0%)	0.81	0/5737

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	484	PRO	CA-C	5.90	1.55	1.51

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	2104	0	2086	14	0
1	B	2028	0	1981	11	0
2	A	17	0	16	0	0
2	B	17	0	16	0	0
3	A	17	0	0	1	0
3	B	11	0	0	0	0
All	All	4194	0	4099	25	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 (25) 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:297:LEU:HD23	1:A:334:ILE:HD13	1.47	0.97
1:A:258:ASP:OD1	1:A:315:LYS:NZ	2.27	0.67
1:B:466:MET:HE2	1:B:471:VAL:HG22	1.79	0.65
1:A:382:TYR:CE1	1:A:410:LEU:HD13	2.34	0.62
1:A:466:MET:HE2	1:A:471:VAL:HG22	1.81	0.61
1:A:308:LEU:HD23	1:A:312:GLN:HG2	1.82	0.61
1:B:343:LYS:HD3	1:B:395:GLY:O	2.06	0.56
1:B:283:MET:HE2	1:B:340:TYR:OH	2.07	0.55
1:A:526:GLN:HG2	3:A:17:HOH:O	2.07	0.54
1:A:426:ILE:HG21	1:A:468:ASN:HB3	1.91	0.52
1:B:346:LEU:CD1	1:B:366:MET:HE2	2.41	0.50
1:B:405:PHE:HB3	1:B:408:ALA:HB3	1.94	0.48
1:B:346:LEU:CD1	1:B:366:MET:CE	2.94	0.45
1:A:410:LEU:O	1:A:410:LEU:HG	2.16	0.45
1:A:334:ILE:H	1:A:334:ILE:HD12	1.83	0.44
1:B:287:ASN:O	1:B:289:THR:HG22	2.17	0.44
1:B:330:SER:O	1:B:334:ILE:HD12	2.18	0.43
1:B:346:LEU:HD13	1:B:366:MET:HE2	2.00	0.43
1:A:426:ILE:HD11	1:A:472:LEU:CD2	2.49	0.43
1:A:311:ALA:HB2	1:A:336:ILE:HD13	2.01	0.43
1:A:346:LEU:CD1	1:A:366:MET:HE2	2.49	0.42
1:B:467:VAL:O	1:B:471:VAL:HG23	2.20	0.42
1:A:354:MET:O	1:A:354:MET:HE3	2.20	0.41
1:A:509:PHE:HA	1:A:512:LEU:HD12	2.03	0.41
1:B:262:ILE:HG12	1:B:327:ALA:HB1	2.01	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	260/286 (91%)	253 (97%)	7 (3%)	0	100	100
1	B	249/286 (87%)	243 (98%)	6 (2%)	0	100	100
All	All	509/572 (89%)	496 (97%)	13 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	225/245 (92%)	219 (97%)	6 (3%)	39	53
1	B	212/245 (86%)	207 (98%)	5 (2%)	43	58
All	All	437/490 (89%)	426 (98%)	11 (2%)	42	56

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	275	GLN
1	A	290	THR
1	A	332	GLU
1	A	343	LYS
1	A	493	ASP
1	A	505	GLU
1	B	289	THR
1	B	290	THR
1	B	308	LEU
1	B	469	ARG
1	B	505	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	324	GLN
1	A	397	ASN
1	B	309	GLN
1	B	324	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 ⓘ

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	B5A	A	1	-	19,19,19	5.03	4 (21%)	25,26,26	3.03	10 (40%)
2	B5A	B	1	-	19,19,19	4.85	4 (21%)	25,26,26	2.98	11 (44%)

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	B5A	A	1	-	-	2/4/12/12	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	B5A	B	1	-	-	2/4/12/12	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1	B5A	NAQ-NAK	-20.00	1.23	1.37
2	B	1	B5A	NAQ-NAK	-19.15	1.24	1.37
2	A	1	B5A	C5-CAC	-7.44	1.33	1.42
2	B	1	B5A	C5-CAC	-7.23	1.33	1.42
2	A	1	B5A	CAH-NAQ	3.46	1.48	1.45
2	B	1	B5A	C4-NAQ	-3.16	1.33	1.35
2	B	1	B5A	CAH-NAQ	3.12	1.48	1.45
2	A	1	B5A	C4-NAQ	-2.41	1.33	1.35

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1	B5A	CAC-NAK-NAQ	8.32	110.21	106.06
2	B	1	B5A	CAC-NAK-NAQ	7.67	109.88	106.06
2	A	1	B5A	N3-C4-NAQ	6.26	135.11	125.34
2	B	1	B5A	N3-C4-NAQ	5.92	134.59	125.34
2	B	1	B5A	C5-CAC-NAK	-5.23	107.41	111.38
2	A	1	B5A	C5-CAC-NAK	-4.98	107.60	111.38
2	B	1	B5A	N1-C2-N3	-4.49	121.78	128.58
2	A	1	B5A	C6-C5-C4	4.29	119.09	115.55
2	A	1	B5A	N1-C2-N3	-4.18	122.25	128.58
2	A	1	B5A	C5-C4-N3	-4.18	119.53	126.89
2	B	1	B5A	C5-C4-N3	-3.89	120.03	126.89
2	B	1	B5A	C6-C5-C4	3.70	118.61	115.55
2	B	1	B5A	C2-N3-C4	3.33	119.97	111.83
2	A	1	B5A	C2-N3-C4	3.33	119.96	111.83
2	A	1	B5A	C5-C4-NAQ	-3.20	105.36	107.26
2	B	1	B5A	C5-C4-NAQ	-3.15	105.39	107.26
2	B	1	B5A	CAH-NAQ-C4	-2.96	124.05	127.89
2	B	1	B5A	CAH-NAQ-NAK	2.72	124.66	119.10
2	A	1	B5A	CAH-NAQ-NAK	2.22	123.63	119.10
2	A	1	B5A	C6-C5-CAC	-2.15	135.08	139.39
2	B	1	B5A	C6-C5-CAC	-2.01	135.36	139.39

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1	B5A	NAQ-CAH-CAP-CAG
2	B	1	B5A	NAQ-CAH-CAP-CAG
2	A	1	B5A	NAQ-CAH-CAP-CAF
2	B	1	B5A	NAQ-CAH-CAP-CAF

There are no ring outliers.

No monomer is involved in short contacts.

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	263/286 (91%)	1.27	54 (20%) 2 2	39, 60, 115, 136	1 (0%)
1	B	257/286 (89%)	1.22	53 (20%) 2 2	39, 58, 115, 127	0
All	All	520/572 (90%)	1.24	107 (20%) 2 2	39, 59, 115, 136	1 (0%)

All (107) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	278	PHE	6.0
1	B	275	GLN	5.5
1	A	411	ILE	5.0
1	B	298	LYS	5.0
1	A	297	LEU	4.9
1	A	405	PHE	4.6
1	A	296	THR	4.4
1	B	472	LEU	4.4
1	B	307	PHE	4.4
1	A	308	LEU	4.3
1	A	299	PRO	4.1
1	A	305	GLU	4.1
1	A	425	PRO	4.1
1	A	276	GLY	4.0
1	B	411	ILE	4.0
1	A	438[A]	ARG	4.0
1	B	306	ALA	4.0
1	B	304	PRO	3.9
1	B	297	LEU	3.9
1	B	354	MET	3.9
1	A	307	PHE	3.9
1	A	302	MET	3.8
1	B	288	GLY	3.8
1	B	311	ALA	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	277	CYS	3.7
1	B	274	GLY	3.6
1	B	425	PRO	3.6
1	A	304	PRO	3.6
1	B	308	LEU	3.5
1	A	408	ALA	3.4
1	B	303	SER	3.4
1	A	313	VAL	3.3
1	A	407	LEU	3.3
1	A	303	SER	3.3
1	B	264	ARG	3.3
1	B	334	ILE	3.3
1	A	436	TYR	3.3
1	A	409	ARG	3.2
1	B	407	LEU	3.2
1	B	333	PRO	3.2
1	A	355	GLY	3.2
1	B	436	TYR	3.2
1	A	406	GLY	3.1
1	A	473	ASP	3.1
1	A	410	LEU	3.1
1	B	268	ARG	3.1
1	A	334	ILE	3.1
1	A	403	ALA	3.1
1	A	332	GLU	3.0
1	B	305	GLU	3.0
1	A	469	ARG	3.0
1	A	472	LEU	3.0
1	A	306	ALA	2.9
1	A	311	ALA	2.9
1	A	354	MET	2.9
1	B	408	ALA	2.9
1	B	256	ALA	2.9
1	B	269	LEU	2.9
1	A	272	LYS	2.8
1	A	279	GLY	2.8
1	B	271	VAL	2.8
1	A	301	THR	2.8
1	A	298	LYS	2.8
1	B	332	GLU	2.7
1	B	331	GLU	2.7
1	B	283	MET	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	477	ARG	2.6
1	A	467	VAL	2.6
1	A	477	ARG	2.6
1	A	260	TRP	2.6
1	B	405	PHE	2.6
1	A	468	ASN	2.5
1	B	296	THR	2.5
1	A	312	GLN	2.5
1	B	426	ILE	2.5
1	A	258	ASP	2.5
1	B	335	TYR	2.4
1	A	426	ILE	2.4
1	A	282	TRP	2.4
1	B	280	GLU	2.4
1	A	404	ASP	2.4
1	B	263	PRO	2.4
1	B	473	ASP	2.3
1	A	288	GLY	2.3
1	B	465	GLY	2.3
1	B	286	TRP	2.3
1	A	274	GLY	2.3
1	B	282	TRP	2.3
1	B	388	ARG	2.3
1	B	486	GLU	2.3
1	A	273	LEU	2.3
1	B	469	ARG	2.3
1	A	489	GLU	2.2
1	B	273	LEU	2.2
1	A	280	GLU	2.2
1	B	265	GLU	2.2
1	B	330	SER	2.2
1	A	357	TYR	2.2
1	B	409	ARG	2.2
1	B	410	LEU	2.2
1	A	310	GLU	2.2
1	B	404	ASP	2.1
1	A	349	PHE	2.1
1	B	270	GLU	2.1
1	B	295	LYS	2.1
1	B	318	ARG	2.1
1	B	489	GLU	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($\text{\AA}^2$)	Q<0.9
2	B5A	A	1	17/17	0.86	0.18	58,62,92,94	0
2	B5A	B	1	17/17	0.87	0.20	76,83,101,102	0

6.5 Other polymers [i](#)

There are no such residues in this entry.