



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:10 PM GMT

PDB ID : 3T4N
Title : Structure of the regulatory fragment of *Saccharomyces cerevisiae* AMPK in complex with ADP
Authors : Mayer, F.V.; Heath, R.; Underwood, E.; Sanders, M.J.; Carmena, D.; McCartney, R.; Leiper, F.C.; Xiao, B.; Jing, C.; Walker, P.A.; Haire, L.F.; Ogrodowicz, R.; Martin, S.R.; Schmdit, M.C.; Gamblin, S.J.; Carling, D.
Deposited on : 2011-07-26
Resolution : 2.30 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 ⓘ](#)) 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

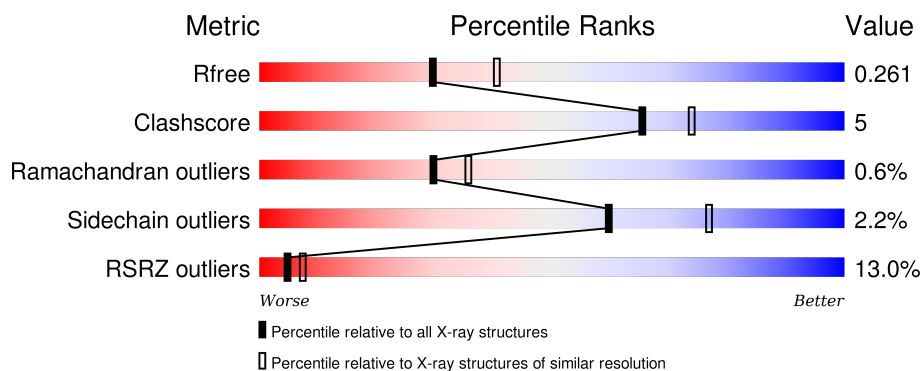
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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 $\leq 5\%$. 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	179	<div> <div>16%</div> <div>66%</div> <div>12%</div> <div>22%</div> </div>
2	B	113	<div> <div>26%</div> <div>84%</div> <div>8%</div> <div>8%</div> </div>
3	C	323	<div> <div>5%</div> <div>80%</div> <div>15%</div> <div>• •</div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 4699 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 Carbon catabolite-derepressing protein kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	139	Total	C	N	O	S	0	0	0
			1121	733	185	198	5			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	455	GLY	-	EXPRESSION TAG	UNP P06782
A	456	PRO	-	EXPRESSION TAG	UNP P06782

- Molecule 2 is a protein called SNF1 protein kinase subunit beta-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	104	Total	C	N	O	S	0	0	0
			826	535	134	154	3			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	303	MET	-	INITIATING METHIONINE	UNP P34164

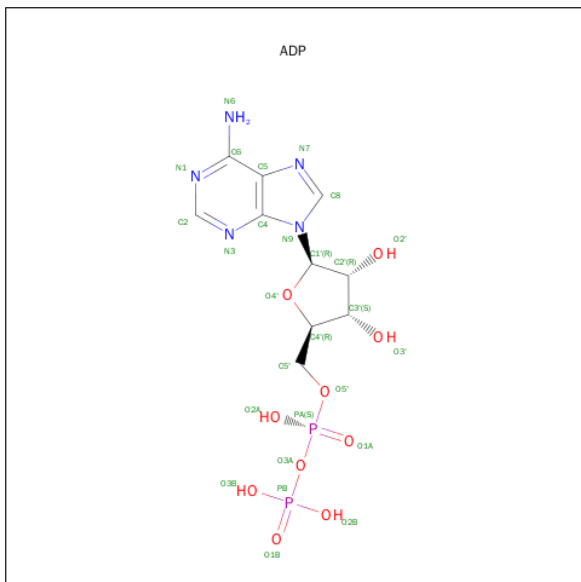
- Molecule 3 is a protein called Nuclear protein SNF4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	311	Total	C	N	O	S	0	0	0
			2392	1531	391	460	10			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	1	MET	-	EXPRESSION TAG	UNP P12904
C	2	ALA	-	EXPRESSION TAG	UNP P12904

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $\text{C}_{10}\text{H}_{15}\text{N}_5\text{O}_{10}\text{P}_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

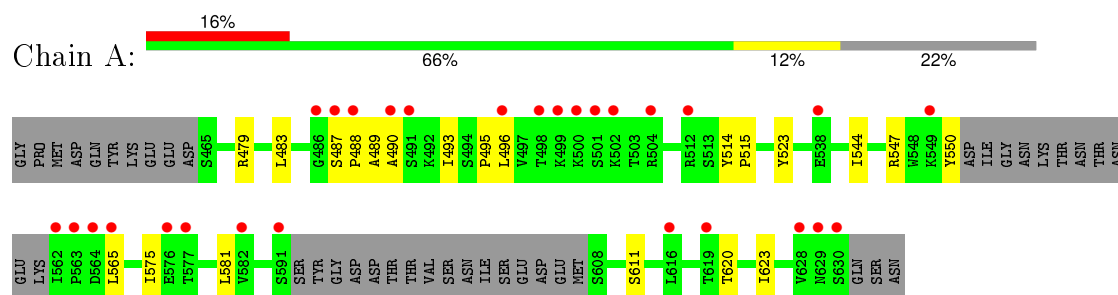
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	81	Total O 81 81	0	0
5	B	54	Total O 54 54	0	0
5	C	198	Total O 198 198	0	0

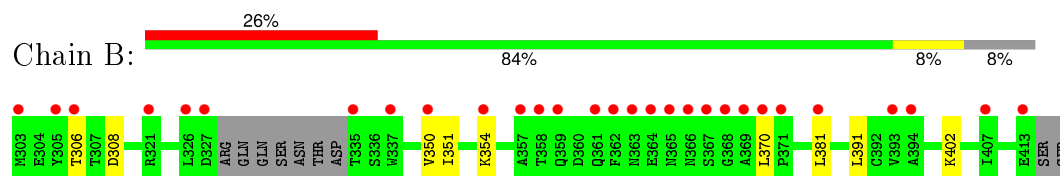
3 Residue-property plots [i](#)

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.

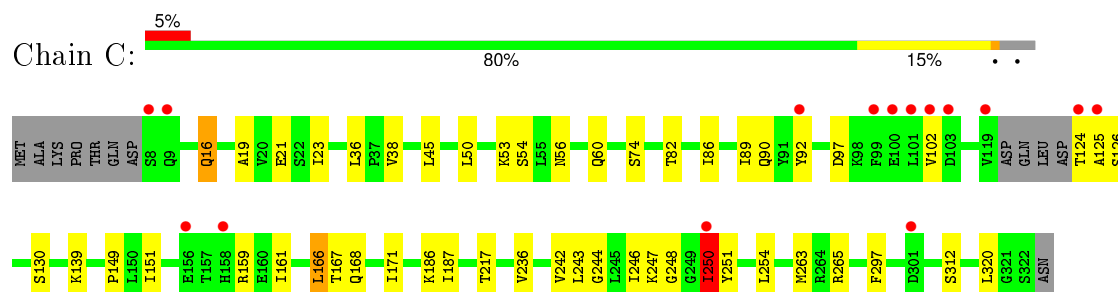
- Molecule 1: Carbon catabolite-derepressing protein kinase



- Molecule 2: SNF1 protein kinase subunit beta-2



- Molecule 3: Nuclear protein SNF4



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	88.60 Å 251.21 Å 79.59 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.30 29.60 – 2.30	Depositor EDS
% Data completeness (in resolution range)	94.7 (30.00-2.30) 94.7 (29.60-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.53 (at 2.31 Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.221 , 0.268 0.216 , 0.261	Depositor DCC
R_{free} test set	1944 reflections (5.42%)	DCC
Wilson B-factor (Å ²)	41.1	Xtriage
Anisotropy	0.055	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 45.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 37813 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4699	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.10% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: ADP

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	0.35	0/1150	0.48	0/1558
2	B	0.36	0/848	0.51	0/1166
3	C	0.39	0/2426	0.54	1/3297 (0.0%)
All	All	0.37	0/4424	0.52	1/6021 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	166	LEU	CA-CB-CG	5.36	127.62	115.30

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	1121	0	1140	16	0
2	B	826	0	809	7	0
3	C	2392	0	2412	30	0
4	C	27	0	12	0	0
5	A	81	0	0	0	0
5	B	54	0	0	0	0
5	C	198	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	4699	0	4373	44	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 5.

All (44) 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)
3:C:166:LEU:HD13	3:C:171:ILE:HD11	1.63	0.81
1:A:611:SER:HB2	3:C:161:ILE:HG21	1.64	0.80
1:A:620:THR:HG23	2:B:391:LEU:HD23	1.71	0.71
3:C:50:LEU:HD12	3:C:53:LYS:HE2	1.79	0.64
3:C:89:ILE:HD11	3:C:246:ILE:HG12	1.79	0.64
3:C:56:ASN:O	3:C:60:GLN:HG2	1.98	0.63
1:A:489:ALA:HB1	1:A:493:ILE:HD12	1.81	0.61
3:C:166:LEU:CD1	3:C:171:ILE:HD11	2.33	0.59
3:C:168:GLN:HE22	3:C:312:SER:HB3	1.68	0.58
1:A:611:SER:HB2	3:C:161:ILE:CG2	2.33	0.56
3:C:126:SER:HB2	3:C:151:ILE:HD13	1.87	0.55
3:C:250:ILE:O	3:C:254:LEU:HG	2.08	0.53
2:B:306:THR:HG23	2:B:308:ASP:H	1.72	0.53
3:C:236:VAL:HG21	3:C:297:PHE:CE2	2.44	0.53
2:B:351:ILE:HA	2:B:354:LYS:HE3	1.90	0.52
3:C:126:SER:O	3:C:139:LYS:HE2	2.11	0.51
2:B:350:VAL:HG13	2:B:351:ILE:HD12	1.94	0.49
3:C:92:TYR:CE1	3:C:102:VAL:HG22	2.50	0.47
3:C:19:ALA:O	3:C:23:ILE:HG12	2.15	0.47
3:C:90:GLN:OE1	3:C:217:THR:HG21	2.15	0.47
3:C:45:LEU:HD13	3:C:54:SER:HB2	1.96	0.46
2:B:402:LYS:NZ	3:C:36:LEU:O	2.37	0.46
3:C:82:THR:O	3:C:86:ILE:HG12	2.16	0.46
1:A:623:ILE:HD11	2:B:381:LEU:HD21	1.98	0.46
3:C:56:ASN:OD1	3:C:247:LYS:HE2	2.17	0.45
3:C:86:ILE:HD13	3:C:242:VAL:HG21	1.97	0.45
1:A:483:LEU:HG	1:A:490:ALA:HB1	1.99	0.45
3:C:149:PRO:HB2	3:C:151:ILE:CD1	2.47	0.45
3:C:89:ILE:HA	3:C:89:ILE:HD13	1.82	0.44
1:A:514:TYR:HB3	1:A:515:PRO:CD	2.49	0.43
3:C:16:GLN:NE2	3:C:187:ILE:H	2.17	0.43
3:C:167:THR:HB	5:C:360:HOH:O	2.19	0.42
2:B:402:LYS:HD3	3:C:38:VAL:HA	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:514:TYR:HB3	1:A:515:PRO:HD2	2.00	0.42
1:A:550:TYR:CE1	3:C:74:SER:OG	2.72	0.42
1:A:523:TYR:CZ	1:A:544:ILE:HG12	2.55	0.42
1:A:479:ARG:NH2	1:A:495:PRO:HD3	2.34	0.41
3:C:125:ALA:O	3:C:149:PRO:HD2	2.21	0.41
1:A:575:ILE:HD11	1:A:581:LEU:HB2	2.01	0.41
1:A:490:ALA:HA	3:C:263:MET:CE	2.50	0.41
1:A:496:LEU:HD22	3:C:244:GLY:HA2	2.01	0.41
3:C:236:VAL:O	3:C:265:ARG:NH2	2.51	0.41
1:A:487:SER:HA	1:A:488:PRO:HD3	1.89	0.40
1:A:547:ARG:HG2	1:A:565:LEU:HB3	2.03	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	133/179 (74%)	130 (98%)	3 (2%)	0	100	100
2	B	100/113 (88%)	95 (95%)	5 (5%)	0	100	100
3	C	307/323 (95%)	302 (98%)	2 (1%)	3 (1%)	19	21
All	All	540/615 (88%)	527 (98%)	10 (2%)	3 (1%)	30	36

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	251	TYR
3	C	248	GLY
3	C	250	ILE

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	124/162 (76%)	124 (100%)	0	100	100
2	B	94/108 (87%)	93 (99%)	1 (1%)	80	90
3	C	271/297 (91%)	261 (96%)	10 (4%)	41	55
All	All	489/567 (86%)	478 (98%)	11 (2%)	60	77

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

Mol	Chain	Res	Type
2	B	370	LEU
3	C	16	GLN
3	C	21	GLU
3	C	97	ASP
3	C	124	THR
3	C	130	SER
3	C	159	ARG
3	C	186	LYS
3	C	243	LEU
3	C	250	ILE
3	C	320	LEU

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	485	GLN
3	C	9	GLN
3	C	16	GLN
3	C	28	ASN
3	C	168	GLN
3	C	214	GLN
3	C	218	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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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$
4	ADP	C	324	-	22,29,29	1.03	1 (4%)	27,45,45	1.94	6 (22%)

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
4	ADP	C	324	-	-	0/12/32/32	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	324	ADP	C5-C4	3.15	1.47	1.40

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
4	C	324	ADP	N3-C2-N1	-7.78	122.94	128.89
4	C	324	ADP	C1'-N9-C4	-2.60	123.02	126.94
4	C	324	ADP	PA-O3A-PB	-2.40	124.60	132.67
4	C	324	ADP	C4-C5-N7	-2.34	107.32	109.48
4	C	324	ADP	C2-N1-C6	2.00	122.35	118.77
4	C	324	ADP	O3B-PB-O2B	2.16	115.60	107.38

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 [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	139/179 (77%)	0.96	28 (20%) 1 2	24, 54, 68, 73	0
2	B	104/113 (92%)	1.38	29 (27%) 1 1	30, 56, 70, 74	0
3	C	311/323 (96%)	0.25	15 (4%) 34 43	23, 35, 55, 65	0
All	All	554/615 (90%)	0.64	72 (12%) 5 7	23, 42, 67, 74	0

All (72) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	335	THR	7.9
2	B	326	LEU	7.4
2	B	368	GLY	6.4
2	B	365	ASN	5.5
1	A	562	ILE	5.5
1	A	563	PRO	5.1
1	A	491	SER	4.8
2	B	303	MET	4.7
1	A	499	LYS	4.6
2	B	367	SER	4.5
1	A	591	SER	4.2
2	B	366	ASN	4.2
1	A	498	THR	4.1
1	A	501	SER	4.1
1	A	502	LYS	4.1
2	B	337	TRP	3.9
1	A	628	VAL	3.8
2	B	354	LYS	3.8
2	B	358	THR	3.6
3	C	99	PHE	3.6
1	A	565	LEU	3.6
2	B	363	ASN	3.5
1	A	577	THR	3.4

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Mol	Chain	Res	Type	RSRZ
2	B	321	ARG	3.4
2	B	369	ALA	3.3
3	C	250	ILE	3.3
2	B	362	PHE	3.3
3	C	92	TYR	3.3
2	B	357	ALA	3.3
1	A	629	ASN	3.2
2	B	327	ASP	3.2
3	C	100	GLU	3.2
1	A	487	SER	3.1
3	C	125	ALA	3.0
3	C	124	THR	3.0
3	C	158	HIS	3.0
1	A	490	ALA	3.0
1	A	486	GLY	2.9
3	C	103	ASP	2.9
2	B	350	VAL	2.9
2	B	370	LEU	2.8
3	C	301	ASP	2.8
1	A	496	LEU	2.7
2	B	407	ILE	2.7
1	A	619	THR	2.7
1	A	500	LYS	2.7
3	C	119	VAL	2.7
2	B	413	GLU	2.7
2	B	393	VAL	2.7
2	B	361	GLN	2.6
1	A	616	LEU	2.6
2	B	364	GLU	2.6
3	C	9	GLN	2.5
3	C	102	VAL	2.5
2	B	306	THR	2.4
1	A	538	GLU	2.4
2	B	359	GLN	2.4
1	A	504	ARG	2.3
1	A	564	ASP	2.2
3	C	101	LEU	2.2
2	B	371	PRO	2.2
1	A	630	SER	2.2
1	A	549	LYS	2.2
2	B	394	ALA	2.1
1	A	582	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	488	PRO	2.1
1	A	576	GLU	2.1
3	C	156	GLU	2.1
1	A	512	ARG	2.1
2	B	381	LEU	2.1
3	C	8	SER	2.0
2	B	305	TYR	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, 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	LLDF	B-factors(\AA^2)	Q<0.9
4	ADP	C	324	27/27	0.95	0.13	-0.66	39,41,52,53	0

6.5 Other polymers [i](#)

There are no such residues in this entry.