



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 06:10 AM GMT

PDB ID : 3H4J
Title : crystal structure of pombe AMPK KDAID fragment
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Deposited on : 2009-04-20
Resolution : 2.80 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

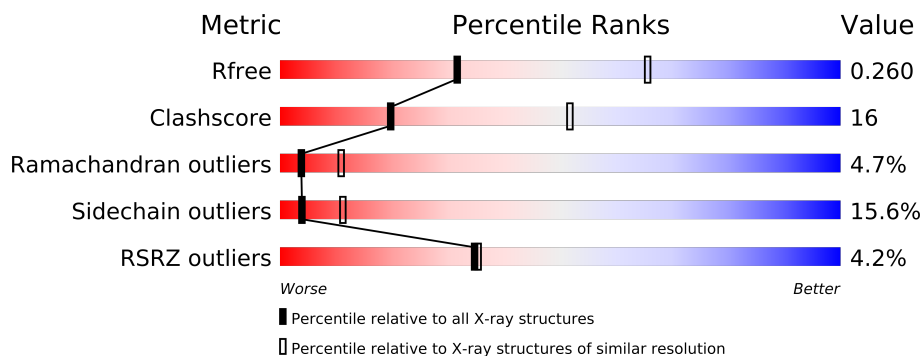
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.80 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}	66092	1799 (2.80-2.80)
Clashscore	79885	2295 (2.80-2.80)
Ramachandran outliers	78287	2252 (2.80-2.80)
Sidechain outliers	78261	2254 (2.80-2.80)
RSRZ outliers	66119	1802 (2.80-2.80)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	336	
1	B	336	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5364 atoms, of which 0 are hydrogen and 0 are deuterium.

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 SNF1-like protein kinase ssp2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	330	Total	C	N	O	S	0	0	0
			2686	1716	464	490	16			
1	A	316	Total	C	N	O	S	0	0	0
			2574	1645	442	472	15			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	24	MET	-	EXPRESSION TAG	UNP O74536
B	352	LEU	-	EXPRESSION TAG	UNP O74536
B	353	GLU	-	EXPRESSION TAG	UNP O74536
B	354	HIS	-	EXPRESSION TAG	UNP O74536
B	355	HIS	-	EXPRESSION TAG	UNP O74536
B	356	HIS	-	EXPRESSION TAG	UNP O74536
B	357	HIS	-	EXPRESSION TAG	UNP O74536
B	358	HIS	-	EXPRESSION TAG	UNP O74536
B	359	HIS	-	EXPRESSION TAG	UNP O74536
A	24	MET	-	EXPRESSION TAG	UNP O74536
A	352	LEU	-	EXPRESSION TAG	UNP O74536
A	353	GLU	-	EXPRESSION TAG	UNP O74536
A	354	HIS	-	EXPRESSION TAG	UNP O74536
A	355	HIS	-	EXPRESSION TAG	UNP O74536
A	356	HIS	-	EXPRESSION TAG	UNP O74536
A	357	HIS	-	EXPRESSION TAG	UNP O74536
A	358	HIS	-	EXPRESSION TAG	UNP O74536
A	359	HIS	-	EXPRESSION TAG	UNP O74536

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	23	Total	O	0	0
			23	23		

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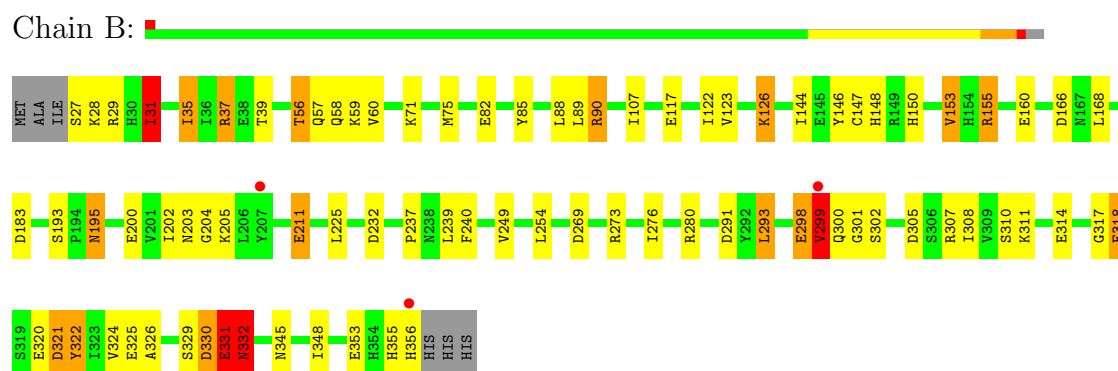
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	81	Total	O	0	0
			81	81		

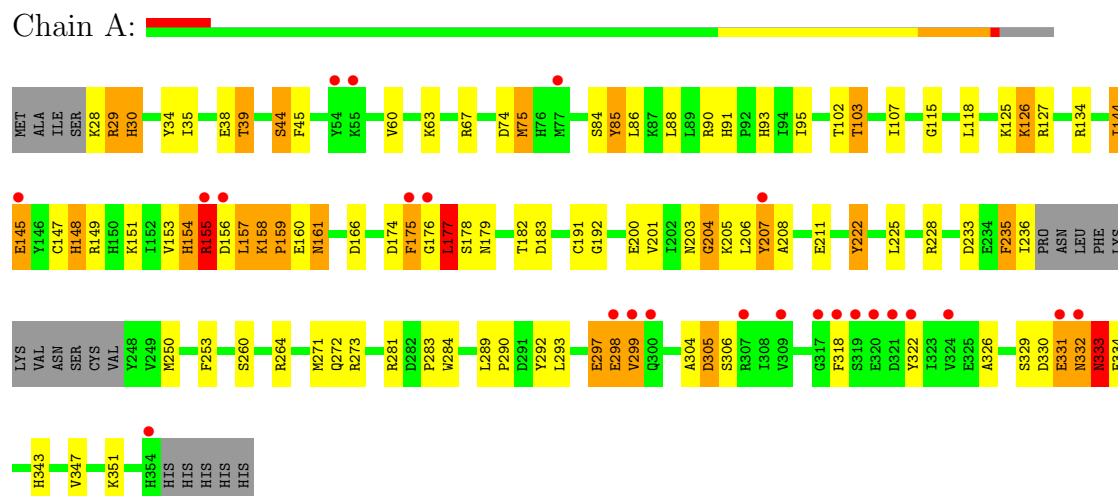
3 Residue-property plots

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: SNF1-like protein kinase ssp2



- Molecule 1: SNF1-like protein kinase ssp2



4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α , β , γ	128.96Å 128.96Å 106.87Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	39.26 – 2.80 39.26 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.9 (39.26-2.80) 99.8 (39.26-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.47 (at 2.69Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.218 , 0.257 0.221 , 0.260	Depositor DCC
R_{free} test set	1399 reflections (5.04%)	DCC
Wilson B-factor (Å ²)	71.1	Xtriage
Anisotropy	0.413	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 68.9	EDS
Estimated twinning fraction	0.038 for h,-h-k,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 27815 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5364	wwPDB-VP
Average B, all atoms (Å ²)	102.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.72% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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	0.45	0/2627	0.83	8/3545 (0.2%)
1	B	0.51	0/2744	0.85	7/3705 (0.2%)
All	All	0.48	0/5371	0.84	15/7250 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	299	VAL	CB-CA-C	-8.47	95.30	111.40
1	A	75	MET	N-CA-C	-7.86	89.77	111.00
1	B	299	VAL	CB-CA-C	-7.36	97.43	111.40
1	A	154	HIS	N-CA-C	-6.99	92.12	111.00
1	B	331	GLU	N-CA-C	6.82	129.41	111.00
1	B	205	LYS	N-CA-C	-6.34	93.89	111.00
1	A	183	ASP	CB-CG-OD2	6.33	124.00	118.30
1	B	299	VAL	N-CA-C	-6.27	94.08	111.00
1	A	177	LEU	CA-CB-CG	6.10	129.34	115.30
1	B	126	LYS	N-CA-C	-6.04	94.68	111.00
1	B	298	GLU	N-CA-C	5.67	126.32	111.00
1	B	332	ASN	N-CA-C	5.57	126.03	111.00
1	A	155	ARG	N-CA-C	5.45	125.71	111.00
1	A	182	THR	CB-CA-C	-5.26	97.39	111.60
1	A	192	GLY	N-CA-C	-5.19	100.13	113.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	235	PHE	Peptide

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2574	0	0	47	0
1	B	2686	0	7	41	0
2	A	23	0	0	5	0
2	B	81	0	0	7	0
All	All	5364	0	7	85	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 16.

All (85) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:71:LYS:CG	2:B:408:HOH:O	2.05	1.01
1:B:311:LYS:NZ	2:B:372:HOH:O	2.04	0.90
1:A:235:PHE:C	1:A:236:ILE:CG2	2.45	0.84
1:B:57:GLN:NE2	2:B:373:HOH:O	2.10	0.83
1:A:235:PHE:O	1:A:236:ILE:CG2	2.30	0.79
1:A:126:LYS:CG	1:A:127:ARG:N	2.51	0.73
1:A:29:ARG:NE	2:A:17:HOH:O	2.24	0.69
1:B:195:ASN:N	1:B:195:ASN:OD1	2.28	0.67
1:B:155:ARG:NH1	2:B:405:HOH:O	2.29	0.66
1:A:144:ILE:CG2	1:A:145:GLU:N	2.60	0.65
1:A:235:PHE:O	1:A:236:ILE:CG1	2.47	0.63
1:A:222:TYR:CD2	1:A:222:TYR:C	2.72	0.63
1:A:125:LYS:NZ	2:A:380:HOH:O	2.31	0.63
1:A:155:ARG:O	1:A:157:LEU:N	2.31	0.63
1:A:331:GLU:O	1:A:333:ASN:N	2.32	0.63
1:B:298:GLU:C	1:B:299:VAL:O	2.36	0.62
1:A:91:HIS:CD2	1:A:93:HIS:N	2.70	0.60
1:A:326:ALA:O	1:A:333:ASN:OD1	2.20	0.60

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:159:PRO:O	1:A:161:ASN:N	2.36	0.59
1:B:193:SER:OG	1:A:233:ASP:OD1	2.20	0.59
1:B:146:TYR:OH	1:B:345:ASN:ND2	2.36	0.58
1:B:330:ASP:O	1:B:331:GLU:CB	2.51	0.58
1:B:202:ILE:O	1:B:204:GLY:N	2.36	0.58
1:A:177:LEU:O	1:A:178:SER:CB	2.51	0.57
1:B:305:ASP:OD2	1:B:307:ARG:N	2.38	0.57
1:A:177:LEU:CD2	1:A:177:LEU:N	2.68	0.56
1:A:144:ILE:CG1	1:A:148:HIS:NE2	2.69	0.55
1:B:211:GLU:O	1:B:273:ARG:NH1	2.40	0.54
1:A:264:ARG:NH2	2:A:373:HOH:O	2.41	0.54
1:B:147:CYS:O	1:B:150:HIS:N	2.41	0.54
1:A:28:LYS:NZ	2:A:368:HOH:O	2.40	0.54
1:B:203:ASN:ND2	1:A:203:ASN:O	2.44	0.51
1:B:320:GLU:O	1:B:324:VAL:N	2.43	0.51
2:B:406:HOH:O	1:A:228:ARG:CD	2.58	0.51
1:B:280:ARG:NH2	1:B:293:LEU:O	2.44	0.50
1:A:44:SER:OG	1:A:63:LYS:NZ	2.46	0.49
1:B:305:ASP:OD2	1:B:305:ASP:C	2.51	0.49
1:A:34:TYR:CD1	1:A:34:TYR:N	2.81	0.49
1:B:27:SER:N	2:B:418:HOH:O	2.46	0.48
1:A:260:SER:OG	1:A:264:ARG:NH1	2.46	0.48
1:A:235:PHE:O	1:A:236:ILE:CB	2.60	0.48
1:A:30:HIS:CE1	2:A:368:HOH:O	2.66	0.48
1:A:85:TYR:OH	1:A:151:LYS:O	2.32	0.47
1:B:317:GLY:O	1:B:318:PHE:O	2.32	0.47
1:B:321:ASP:O	1:B:325:GLU:N	2.48	0.47
1:B:28:LYS:O	1:B:29:ARG:CB	2.62	0.47
1:A:204:GLY:O	1:A:207:TYR:CZ	2.67	0.47
1:A:44:SER:OG	1:A:45:PHE:N	2.48	0.46
1:B:89:LEU:O	1:B:90:ARG:CD	2.64	0.46
1:A:305:ASP:O	1:A:306:SER:OG	2.34	0.46
1:B:240:PHE:N	2:B:402:HOH:O	2.49	0.46
1:B:298:GLU:O	1:B:299:VAL:O	2.34	0.45
1:A:304:ALA:O	1:A:305:ASP:C	2.55	0.45
1:B:35:ILE:CD1	1:B:37:ARG:CZ	2.95	0.45
1:B:332:ASN:N	1:B:332:ASN:OD1	2.50	0.44
1:A:144:ILE:O	1:A:147:CYS:N	2.51	0.44
1:B:31:ILE:CG1	1:B:31:ILE:O	2.66	0.44
1:A:331:GLU:O	1:A:332:ASN:C	2.55	0.44
1:A:67:ARG:NH1	1:A:103:THR:O	2.51	0.43
1:A:153:VAL:O	1:A:153:VAL:CG1	2.65	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:84:SER:C	1:A:86:LEU:N	2.72	0.43
1:B:27:SER:OG	1:B:28:LYS:N	2.51	0.43
1:B:85:TYR:C	1:B:85:TYR:CD2	2.91	0.43
1:A:45:PHE:CD1	1:A:176:GLY:O	2.72	0.43
1:A:297:GLU:CG	1:A:298:GLU:N	2.82	0.43
1:A:39:THR:CG2	1:A:39:THR:O	2.66	0.43
1:A:208:ALA:CB	1:A:211:GLU:OE1	2.67	0.42
1:B:318:PHE:CD1	1:B:318:PHE:N	2.85	0.42
1:B:147:CYS:O	1:B:148:HIS:C	2.57	0.42
1:B:56:THR:O	1:B:57:GLN:CB	2.67	0.42
1:B:269:ASP:OD2	1:B:269:ASP:C	2.58	0.42
1:A:318:PHE:CD2	1:A:322:TYR:CE2	3.08	0.42
1:B:90:ARG:NH1	1:B:90:ARG:CG	2.83	0.42
1:A:211:GLU:O	1:A:273:ARG:NH1	2.52	0.41
1:B:122:ILE:O	1:B:126:LYS:O	2.37	0.41
1:A:67:ARG:NH1	1:A:102:THR:CG2	2.84	0.41
1:B:202:ILE:O	1:B:202:ILE:CD1	2.69	0.41
1:B:153:VAL:O	1:B:155:ARG:N	2.52	0.41
1:B:322:TYR:CD1	1:B:322:TYR:C	2.94	0.41
1:B:353:GLU:C	1:B:355:HIS:N	2.75	0.41
1:B:237:PRO:O	1:A:44:SER:O	2.39	0.40
1:A:158:LYS:NZ	1:A:175:PHE:CE2	2.90	0.40
1:B:202:ILE:C	1:B:204:GLY:N	2.75	0.40
1:A:85:TYR:CD2	1:A:85:TYR:O	2.74	0.40
1:A:134:ARG:NH1	1:A:284:TRP:O	2.55	0.40

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	312/336 (93%)	243 (78%)	50 (16%)	19 (6%)	2	6
1	B	328/336 (98%)	277 (84%)	40 (12%)	11 (3%)	6	19
All	All	640/672 (95%)	520 (81%)	90 (14%)	30 (5%)	4	11

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	299	VAL
1	B	318	PHE
1	B	331	GLU
1	A	159	PRO
1	A	160	GLU
1	A	332	ASN
1	A	333	ASN
1	B	300	GLN
1	B	301	GLY
1	B	314	GLU
1	B	329	SER
1	B	332	ASN
1	A	38	GLU
1	A	44	SER
1	A	74	ASP
1	A	253	PHE
1	B	302	SER
1	B	326	ALA
1	A	297	GLU
1	A	305	ASP
1	A	292	TYR
1	A	126	LYS
1	A	156	ASP
1	A	204	GLY
1	A	351	LYS
1	A	290	PRO
1	A	298	GLU
1	B	31	ILE
1	A	115	GLY
1	A	283	PRO

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	284/303 (94%)	235 (83%)	49 (17%)	3	8
1	B	298/303 (98%)	256 (86%)	42 (14%)	5	14

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	582/606 (96%)	491 (84%)	91 (16%)	4 11

All (91) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	31	ILE
1	B	35	ILE
1	B	37	ARG
1	B	39	THR
1	B	56	THR
1	B	58	GLN
1	B	59	LYS
1	B	60	VAL
1	B	75	MET
1	B	82	GLU
1	B	88	LEU
1	B	90	ARG
1	B	107	ILE
1	B	117	GLU
1	B	123	VAL
1	B	144	ILE
1	B	153	VAL
1	B	155	ARG
1	B	160	GLU
1	B	166	ASP
1	B	168	LEU
1	B	183	ASP
1	B	195	ASN
1	B	200	GLU
1	B	211	GLU
1	B	225	LEU
1	B	232	ASP
1	B	239	LEU
1	B	249	VAL
1	B	254	LEU
1	B	276	ILE
1	B	291	ASP
1	B	293	LEU
1	B	299	VAL
1	B	308	ILE
1	B	310	SER
1	B	321	ASP

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Mol	Chain	Res	Type
1	B	322	TYR
1	B	330	ASP
1	B	332	ASN
1	B	348	ILE
1	B	356	HIS
1	A	29	ARG
1	A	30	HIS
1	A	35	ILE
1	A	39	THR
1	A	60	VAL
1	A	75	MET
1	A	85	TYR
1	A	88	LEU
1	A	90	ARG
1	A	95	ILE
1	A	103	THR
1	A	107	ILE
1	A	118	LEU
1	A	144	ILE
1	A	145	GLU
1	A	148	HIS
1	A	149	ARG
1	A	154	HIS
1	A	155	ARG
1	A	157	LEU
1	A	158	LYS
1	A	161	ASN
1	A	166	ASP
1	A	174	ASP
1	A	175	PHE
1	A	177	LEU
1	A	179	ASN
1	A	191	CYS
1	A	200	GLU
1	A	201	VAL
1	A	205	LYS
1	A	206	LEU
1	A	207	TYR
1	A	222	TYR
1	A	225	LEU
1	A	250	MET
1	A	271	MET

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Mol	Chain	Res	Type
1	A	272	GLN
1	A	281	ARG
1	A	289	LEU
1	A	293	LEU
1	A	299	VAL
1	A	329	SER
1	A	330	ASP
1	A	331	GLU
1	A	333	ASN
1	A	334	GLU
1	A	343	HIS
1	A	347	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

There are no ligands in this entry.

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	316/336 (94%)	0.23	24 (7%) 14 12	54, 109, 201, 271	0
1	B	330/336 (98%)	-0.14	3 (0%) 81 81	41, 70, 165, 232	0
All	All	646/672 (96%)	0.04	27 (4%) 35 35	41, 90, 189, 271	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	299	VAL	7.2
1	A	155	ARG	7.0
1	A	77	MET	5.5
1	A	207	TYR	5.0
1	A	354	HIS	3.3
1	A	175	PHE	3.2
1	A	55	LYS	3.1
1	A	321	ASP	3.0
1	A	307	ARG	2.9
1	A	319	SER	2.9
1	A	331	GLU	2.8
1	A	145	GLU	2.8
1	A	176	GLY	2.7
1	A	298	GLU	2.5
1	A	156	ASP	2.5
1	A	309	VAL	2.5
1	A	318	PHE	2.3
1	A	324	VAL	2.3
1	A	320	GLU	2.3
1	A	317	GLY	2.3
1	B	299	VAL	2.2
1	A	322	TYR	2.2
1	B	356	HIS	2.1
1	A	332	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	207	TYR	2.1
1	A	54	TYR	2.0
1	A	300	GLN	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.