



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:13 AM UTC

PDB ID : 2BDW / pdb_00002bdw
Title : Crystal Structure of the Auto-Inhibited Kinase Domain of Calcium/Calmodulin Activated Kinase II
Authors : Rosenberg, O.S.; Kuriyan, J.
Deposited on : 2005-10-20
Resolution : 1.80 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

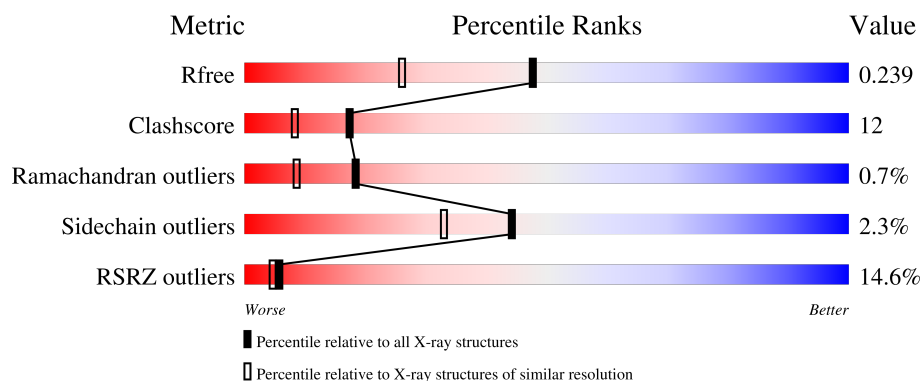
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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}	180053	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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 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	362	8% 69% 15% • 15%
1	B	362	17% 59% 24% • 15%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5354 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 Hypothetical protein K11E8.1d.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	309	Total	C	N	O	S	0	0	0
			2461	1569	431	452	9			
1	B	309	Total	C	N	O	S	0	0	0
			2462	1570	433	450	9			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-18	GLY	-	cloning artifact	UNP Q9NG91
A	-17	PRO	-	cloning artifact	UNP Q9NG91
A	-16	HIS	-	cloning artifact	UNP Q9NG91
A	-15	MET	-	cloning artifact	UNP Q9NG91
A	-14	ALA	-	cloning artifact	UNP Q9NG91
A	-13	SER	-	cloning artifact	UNP Q9NG91
A	-12	MET	-	cloning artifact	UNP Q9NG91
A	-11	THR	-	cloning artifact	UNP Q9NG91
A	-10	GLY	-	cloning artifact	UNP Q9NG91
A	-9	GLY	-	cloning artifact	UNP Q9NG91
A	-8	GLN	-	cloning artifact	UNP Q9NG91
A	-7	GLN	-	cloning artifact	UNP Q9NG91
A	-6	MET	-	cloning artifact	UNP Q9NG91
A	-5	GLY	-	cloning artifact	UNP Q9NG91
A	-4	ARG	-	cloning artifact	UNP Q9NG91
A	-3	GLY	-	cloning artifact	UNP Q9NG91
A	-2	SER	-	cloning artifact	UNP Q9NG91
A	-1	GLU	-	cloning artifact	UNP Q9NG91
A	0	PHE	-	cloning artifact	UNP Q9NG91
A	45	ASN	ASP	engineered mutation	UNP Q9NG91
B	-18	GLY	-	cloning artifact	UNP Q9NG91
B	-17	PRO	-	cloning artifact	UNP Q9NG91
B	-16	HIS	-	cloning artifact	UNP Q9NG91
B	-15	MET	-	cloning artifact	UNP Q9NG91
B	-14	ALA	-	cloning artifact	UNP Q9NG91

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-13	SER	-	cloning artifact	UNP Q9NG91
B	-12	MET	-	cloning artifact	UNP Q9NG91
B	-11	THR	-	cloning artifact	UNP Q9NG91
B	-10	GLY	-	cloning artifact	UNP Q9NG91
B	-9	GLY	-	cloning artifact	UNP Q9NG91
B	-8	GLN	-	cloning artifact	UNP Q9NG91
B	-7	GLN	-	cloning artifact	UNP Q9NG91
B	-6	MET	-	cloning artifact	UNP Q9NG91
B	-5	GLY	-	cloning artifact	UNP Q9NG91
B	-4	ARG	-	cloning artifact	UNP Q9NG91
B	-3	GLY	-	cloning artifact	UNP Q9NG91
B	-2	SER	-	cloning artifact	UNP Q9NG91
B	-1	GLU	-	cloning artifact	UNP Q9NG91
B	0	PHE	-	cloning artifact	UNP Q9NG91
B	45	ASN	ASP	engineered mutation	UNP Q9NG91

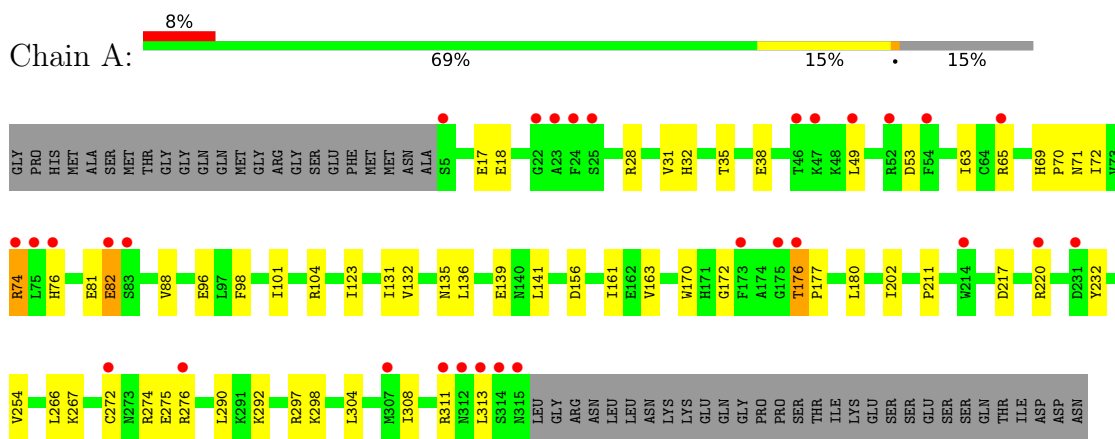
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	277	Total O 277 277	0	0
2	B	154	Total O 154 154	0	0

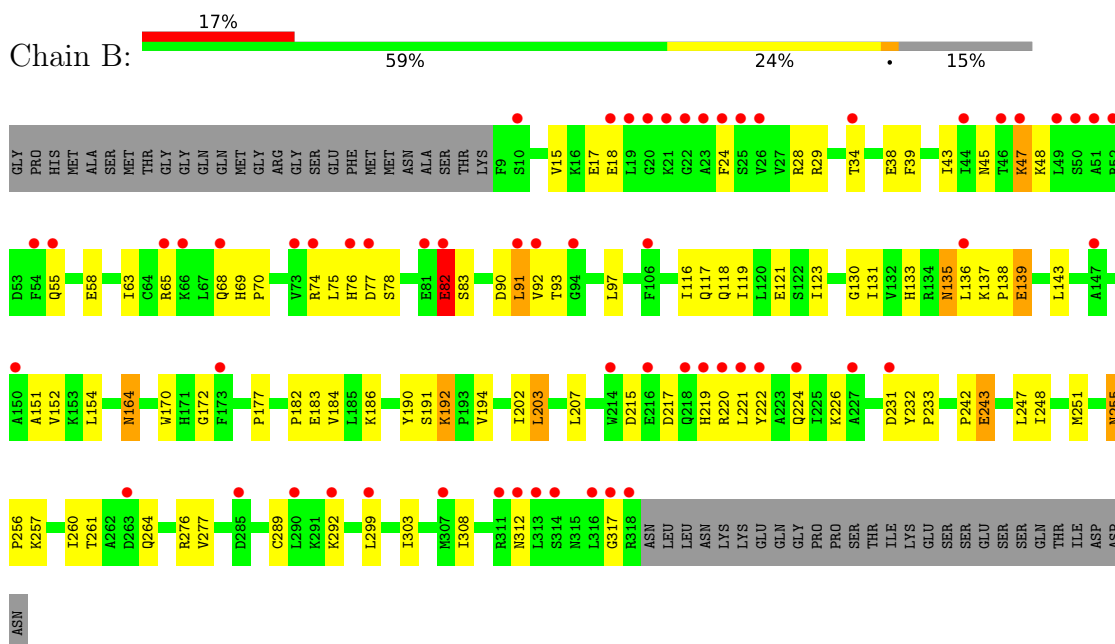
3 Residue-property plots [i](#)

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: Hypothetical protein K11E8.1d



- Molecule 1: Hypothetical protein K11E8.1d



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	46.12Å 77.10Å 119.52Å 90.00° 96.74° 90.00°	Depositor
Resolution (Å)	45.80 – 1.80 45.80 – 1.80	Depositor EDS
% Data completeness (in resolution range)	95.6 (45.80-1.80) 95.7 (45.80-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.23 (at 1.81Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.216 , 0.236 0.218 , 0.239	Depositor DCC
R_{free} test set	7753 reflections (10.17%)	wwPDB-VP
Wilson B-factor (Å ²)	22.1	Xtriage
Anisotropy	0.519	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 46.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5354	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.75% 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	0.44	0/2516	0.87	7/3406 (0.2%)
1	B	0.32	0/2517	0.82	6/3407 (0.2%)
All	All	0.39	0/5033	0.85	13/6813 (0.2%)

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	34	THR	N-CA-C	5.84	117.32	111.07
1	A	74	ARG	N-CA-C	5.76	118.81	110.28
1	A	232	TYR	CA-C-N	5.52	125.45	119.76
1	A	232	TYR	C-N-CA	5.52	125.45	119.76
1	B	232	TYR	CA-C-N	5.49	125.42	119.76
1	B	232	TYR	C-N-CA	5.49	125.42	119.76
1	A	176	THR	CA-C-N	5.22	125.28	119.32
1	A	176	THR	C-N-CA	5.22	125.28	119.32
1	B	255	ASN	CA-C-N	5.21	125.26	119.32
1	B	255	ASN	C-N-CA	5.21	125.26	119.32
1	A	254	VAL	N-CA-C	5.20	115.41	110.42
1	A	211	PRO	N-CA-C	5.08	116.90	110.70
1	B	164	ASN	CB-CA-C	-5.01	110.78	116.54

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	2461	0	2469	46	0
1	B	2462	0	2471	80	0
2	A	277	0	0	10	0
2	B	154	0	0	5	0
All	All	5354	0	4940	123	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 12.

All (123) 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:B:63:ILE:HG23	1:B:131:ILE:HD13	1.49	0.94
1:A:308:ILE:O	1:A:311:ARG:HG2	1.79	0.82
1:A:69:HIS:HD2	1:A:71:ASN:H	1.26	0.81
1:B:45:ASN:OD1	1:B:47:LYS:HD2	1.86	0.76
1:B:74:ARG:HB3	1:B:90:ASP:OD2	1.87	0.75
1:A:69:HIS:CD2	1:A:71:ASN:H	2.05	0.73
1:A:98:PHE:HA	2:A:607:HOH:O	1.87	0.72
1:B:260:ILE:HG21	2:B:473:HOH:O	1.88	0.72
1:B:82:GLU:CD	1:B:83:SER:H	1.98	0.71
1:A:266:LEU:O	1:A:272:CYS:SG	2.51	0.68
1:A:32:HIS:HD2	1:A:35:THR:H	1.39	0.68
1:A:304:LEU:O	1:A:308:ILE:HD13	1.94	0.68
1:B:231:ASP:OD2	1:B:233:PRO:HG3	1.93	0.68
1:B:116:ILE:HG13	1:B:203:LEU:HG	1.77	0.67
1:A:74:ARG:HG2	2:A:585:HOH:O	1.96	0.66
1:A:217:ASP:HB3	1:A:220:ARG:HE	1.59	0.66
1:A:31:VAL:HG22	1:A:38:GLU:HG2	1.79	0.64
1:A:141:LEU:HD11	1:A:202:ILE:HD13	1.79	0.64
1:B:289:CYS:O	1:B:292:LYS:HG2	1.96	0.64
1:B:39:PHE:C	1:B:91:LEU:HD22	2.23	0.63
1:B:183:GLU:CG	1:B:256:PRO:HG3	2.29	0.62
1:B:255:ASN:HD22	1:B:255:ASN:C	2.09	0.61
1:B:68:GLN:O	1:B:68:GLN:HG2	2.00	0.61
1:B:242:PRO:HD2	1:B:243:GLU:OE2	2.01	0.60
1:A:217:ASP:CB	1:A:220:ARG:HE	2.14	0.60
1:A:76:HIS:N	1:A:88:VAL:O	2.35	0.59
1:A:96:GLU:CD	1:A:297:ARG:HH22	2.10	0.59
1:B:251:MET:HG3	2:B:473:HOH:O	2.01	0.59
1:A:72:ILE:HB	2:A:585:HOH:O	2.02	0.58
1:B:257:LYS:HD2	1:B:257:LYS:N	2.18	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:123:ILE:HD11	1:A:136:LEU:HD11	1.85	0.57
1:B:217:ASP:OD2	1:B:219:HIS:HB2	2.03	0.57
1:B:243:GLU:HG3	1:B:277:VAL:HG12	1.86	0.57
1:A:290:LEU:HD21	2:A:607:HOH:O	2.04	0.57
1:A:267:LYS:HA	1:A:272:CYS:SG	2.45	0.56
1:A:292:LYS:NZ	1:B:317:GLY:HA2	2.19	0.56
1:B:247:LEU:HD12	2:B:473:HOH:O	2.06	0.56
1:B:183:GLU:HG2	1:B:256:PRO:CG	2.36	0.55
1:B:299:LEU:O	1:B:303:ILE:HG12	2.06	0.55
1:B:55:GLN:O	1:B:58:GLU:HG2	2.07	0.54
1:B:299:LEU:C	1:B:299:LEU:HD13	2.32	0.54
1:A:313:LEU:C	1:A:313:LEU:HD23	2.32	0.54
1:B:183:GLU:CG	1:B:256:PRO:CG	2.86	0.54
1:B:183:GLU:HG2	1:B:256:PRO:HG2	1.89	0.54
1:B:191:SER:OG	1:B:192:LYS:HD2	2.07	0.54
1:B:92:VAL:O	1:B:92:VAL:HG23	2.07	0.54
1:B:183:GLU:CD	1:B:256:PRO:HG3	2.33	0.53
1:A:304:LEU:C	1:A:304:LEU:HD23	2.34	0.53
1:B:97:LEU:HA	1:B:143:LEU:HD21	1.91	0.53
1:A:63:ILE:HG23	1:A:131:ILE:HD13	1.91	0.52
1:A:217:ASP:HB2	1:A:220:ARG:HH21	1.74	0.52
1:B:130:GLY:HA3	1:B:164:ASN:HD22	1.75	0.52
1:A:176:THR:O	1:A:180:LEU:HG	2.11	0.51
1:B:29:ARG:NH2	1:B:38:GLU:OE2	2.41	0.50
1:B:118:GLN:NE2	1:B:152:VAL:H	2.08	0.50
1:A:170:TRP:CH2	1:A:172:GLY:HA2	2.46	0.50
1:A:72:ILE:O	1:A:74:ARG:HG3	2.12	0.49
1:B:43:ILE:HD12	1:B:43:ILE:N	2.27	0.49
1:A:101:ILE:HB	2:A:607:HOH:O	2.11	0.49
1:B:261:THR:H	1:B:264:GLN:NE2	2.11	0.49
1:B:47:LYS:HZ2	1:B:48:LYS:HG3	1.77	0.49
1:B:221:LEU:C	1:B:221:LEU:HD13	2.38	0.49
1:B:47:LYS:HD3	1:B:48:LYS:N	2.28	0.49
1:B:170:TRP:CH2	1:B:172:GLY:HA2	2.47	0.49
1:A:275:GLU:HG3	2:A:571:HOH:O	2.12	0.49
1:B:255:ASN:HD22	1:B:256:PRO:CD	2.26	0.48
1:B:69:HIS:CG	1:B:70:PRO:HD2	2.48	0.48
1:A:276:ARG:HD3	1:A:276:ARG:N	2.28	0.48
1:B:164:ASN:O	1:B:192:LYS:HE3	2.14	0.48
1:B:207:LEU:HD12	1:B:248:ILE:HD11	1.96	0.48
1:B:119:ILE:O	1:B:123:ILE:HG12	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:308:ILE:HG22	1:B:312:ASN:HD21	1.78	0.48
1:B:255:ASN:HD22	1:B:256:PRO:N	2.11	0.47
1:B:255:ASN:HD22	1:B:256:PRO:HD2	1.79	0.47
1:A:104:ARG:HD3	2:A:602:HOH:O	2.15	0.47
1:B:68:GLN:OE1	1:B:68:GLN:N	2.46	0.47
1:B:15:VAL:CG1	1:B:28:ARG:HE	2.28	0.47
1:B:97:LEU:HA	1:B:143:LEU:CD2	2.45	0.47
1:B:215:ASP:OD2	1:B:220:ARG:HB2	2.15	0.46
1:B:117:GLN:O	1:B:121:GLU:HG3	2.15	0.46
1:A:17:GLU:HB2	1:B:93:THR:HB	1.97	0.46
1:A:49:LEU:HD22	1:A:53:ASP:CB	2.46	0.46
1:B:136:LEU:HG	1:B:202:ILE:CD1	2.45	0.46
1:B:139:GLU:H	1:B:139:GLU:CD	2.22	0.46
1:B:17:GLU:OE2	1:B:29:ARG:HD3	2.16	0.46
1:B:77:ASP:OD1	1:B:78:SER:N	2.48	0.46
1:B:192:LYS:HD2	1:B:192:LYS:H	1.80	0.46
1:B:118:GLN:HE22	1:B:151:ALA:HA	1.81	0.46
1:A:69:HIS:CG	1:A:70:PRO:HD2	2.51	0.45
1:B:182:PRO:O	1:B:186:LYS:HG3	2.16	0.45
1:B:255:ASN:C	1:B:255:ASN:ND2	2.71	0.45
1:B:47:LYS:HD3	1:B:48:LYS:HG3	1.99	0.45
1:B:260:ILE:HG13	1:B:264:GLN:HE21	1.82	0.45
1:B:243:GLU:H	1:B:243:GLU:CD	2.23	0.45
1:B:65:ARG:HG3	1:B:75:LEU:HD23	1.99	0.45
1:A:18:GLU:HA	1:A:28:ARG:HG2	1.99	0.45
1:A:31:VAL:HG22	1:A:38:GLU:CG	2.45	0.45
1:A:65:ARG:HH11	1:A:65:ARG:HG3	1.83	0.44
1:A:274:ARG:HG2	2:A:429:HOH:O	2.18	0.44
1:B:177:PRO:HG2	2:B:412:HOH:O	2.17	0.44
1:B:18:GLU:HB2	1:B:28:ARG:HH12	1.83	0.43
1:B:231:ASP:C	1:B:233:PRO:HD3	2.43	0.43
1:A:292:LYS:HZ3	1:B:317:GLY:HA2	1.83	0.43
1:A:298:LYS:HD2	2:A:580:HOH:O	2.17	0.43
1:B:184:VAL:HG22	1:B:190:TYR:CD2	2.53	0.43
1:B:276:ARG:HH11	1:B:276:ARG:HG2	1.83	0.43
1:A:304:LEU:HD23	1:A:308:ILE:HD13	2.00	0.43
1:B:91:LEU:HD12	1:B:93:THR:HG23	2.00	0.43
1:B:18:GLU:HB2	1:B:28:ARG:NH1	2.34	0.42
1:B:137:LYS:HE3	1:B:139:GLU:HG2	2.00	0.42
1:A:275:GLU:C	1:A:276:ARG:HD3	2.44	0.42
1:A:101:ILE:HD12	2:A:607:HOH:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:137:LYS:HB2	1:B:138:PRO:HD2	2.01	0.42
1:B:91:LEU:HD12	1:B:93:THR:CG2	2.51	0.41
1:A:139:GLU:CD	1:A:297:ARG:HH21	2.29	0.41
1:A:81:GLU:O	1:A:82:GLU:C	2.63	0.41
1:B:133:HIS:CE1	1:B:135:ASN:HB3	2.55	0.41
1:B:191:SER:O	1:B:194:VAL:HG22	2.20	0.41
1:B:222:TYR:O	1:B:226:LYS:HG3	2.21	0.41
1:A:161:ILE:HG13	1:A:163:VAL:HG23	2.03	0.40
1:B:76:HIS:HB2	2:B:471:HOH:O	2.21	0.40
1:A:132:VAL:HG12	1:A:163:VAL:HG23	2.03	0.40
1:B:43:ILE:HD12	1:B:43:ILE:H	1.86	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	307/362 (85%)	298 (97%)	7 (2%)	2 (1%)	18	8
1	B	307/362 (85%)	297 (97%)	8 (3%)	2 (1%)	18	8
All	All	614/724 (85%)	595 (97%)	15 (2%)	4 (1%)	18	8

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	82	GLU
1	B	24	PHE
1	B	82	GLU
1	A	156	ASP

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	265/309 (86%)	263 (99%)	2 (1%)	73	70
1	B	264/309 (85%)	254 (96%)	10 (4%)	29	17
All	All	529/618 (86%)	517 (98%)	12 (2%)	44	33

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	135	ASN
1	A	177	PRO
1	B	47	LYS
1	B	82	GLU
1	B	91	LEU
1	B	135	ASN
1	B	139	GLU
1	B	154	LEU
1	B	192	LYS
1	B	203	LEU
1	B	224	GLN
1	B	243	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	HIS
1	A	69	HIS
1	A	114	HIS
1	A	135	ASN
1	A	164	ASN
1	A	218	GLN
1	A	264	GLN
1	B	55	GLN
1	B	85	HIS
1	B	118	GLN

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Mol	Chain	Res	Type
1	B	135	ASN
1	B	164	ASN
1	B	255	ASN
1	B	264	GLN
1	B	312	ASN

5.3.3 RNA [i](#)

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	309/362 (85%)	0.39	30 (9%) 13 11	12, 22, 43, 71	0
1	B	309/362 (85%)	1.26	60 (19%) 3 2	17, 33, 54, 69	0
All	All	618/724 (85%)	0.83	90 (14%) 6 5	12, 28, 50, 71	0

All (90) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	24	PHE	8.8
1	B	214	TRP	6.9
1	B	219	HIS	5.0
1	B	25	SER	4.3
1	A	272	CYS	4.3
1	B	316	LEU	4.2
1	B	23	ALA	4.0
1	B	22	GLY	3.9
1	A	313	LEU	3.9
1	A	311	ARG	3.8
1	B	47	LYS	3.7
1	B	292	LYS	3.7
1	A	82	GLU	3.6
1	A	173	PHE	3.6
1	A	315	ASN	3.5
1	A	276	ARG	3.5
1	B	216	GLU	3.5
1	A	83	SER	3.4
1	B	65	ARG	3.4
1	A	5	SER	3.4
1	B	312	ASN	3.4
1	B	91	LEU	3.4
1	A	46	THR	3.4
1	B	231	ASP	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	94	GLY	3.3
1	B	317	GLY	3.3
1	B	82	GLU	3.2
1	B	76	HIS	3.2
1	B	18	GLU	3.2
1	B	92	VAL	3.2
1	B	66	LYS	3.2
1	B	318	ARG	3.2
1	B	21	LYS	3.2
1	B	147	ALA	3.1
1	A	22	GLY	3.1
1	A	175	GLY	3.1
1	B	285	ASP	3.0
1	B	222	TYR	2.9
1	B	26	VAL	2.9
1	A	312	ASN	2.9
1	A	75	LEU	2.8
1	B	68	GLN	2.8
1	A	24	PHE	2.8
1	B	218	GLN	2.7
1	B	221	LEU	2.7
1	B	307	MET	2.7
1	B	150	ALA	2.7
1	B	19	LEU	2.7
1	B	34	THR	2.7
1	A	314	SER	2.7
1	B	49	LEU	2.6
1	A	52	ARG	2.6
1	B	77	ASP	2.6
1	B	313	LEU	2.6
1	A	25	SER	2.5
1	B	52	ARG	2.5
1	B	290	LEU	2.5
1	B	51	ALA	2.5
1	A	49	LEU	2.5
1	B	44	ILE	2.5
1	A	307	MET	2.4
1	A	176	THR	2.4
1	A	214	TRP	2.4
1	B	10	SER	2.4
1	B	46	THR	2.3
1	B	74	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	23	ALA	2.3
1	A	47	LYS	2.3
1	B	220	ARG	2.2
1	A	76	HIS	2.2
1	B	227	ALA	2.2
1	B	73	VAL	2.2
1	B	54	PHE	2.2
1	B	173	PHE	2.2
1	B	263	ASP	2.2
1	B	20	GLY	2.2
1	B	106	PHE	2.1
1	A	231	ASP	2.1
1	B	50	SER	2.1
1	A	74	ARG	2.1
1	B	311	ARG	2.1
1	B	81	GLU	2.1
1	B	299	LEU	2.1
1	B	224	GLN	2.1
1	A	65	ARG	2.1
1	A	220	ARG	2.1
1	B	136	LEU	2.0
1	B	314	SER	2.0
1	A	54	PHE	2.0
1	B	55	GLN	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.