



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 01:00 PM UTC

PDB ID : 2QNJ / pdb_00002qnj
Title : Kinase and Ubiquitin-associated domains of MARK3/Par-1
Authors : Murphy, J.M.; Ceccarelli, D.F.J.; Sicheri, F.; Pawson, T.
Deposited on : 2007-07-18
Resolution : 2.70 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

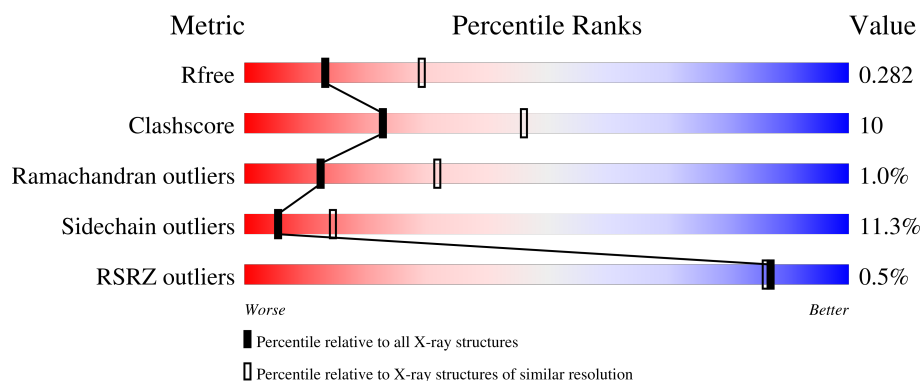
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	328	 73% 20% . . .
1	B	328	 73% 20% 5% .

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5075 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 MAP/microtubule affinity-regulating kinase 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	318	Total	C	N	O	S	0	0	0
			2510	1607	428	462	13			
1	B	322	Total	C	N	O	S	0	0	0
			2518	1611	426	468	13			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	43	GLY	-	expression tag	UNP P27448
A	45	MET	-	expression tag	UNP P27448
A	46	GLY	-	expression tag	UNP P27448
A	47	SER	-	expression tag	UNP P27448
B	43	GLY	-	expression tag	UNP P27448
B	45	MET	-	expression tag	UNP P27448
B	46	GLY	-	expression tag	UNP P27448
B	47	SER	-	expression tag	UNP P27448

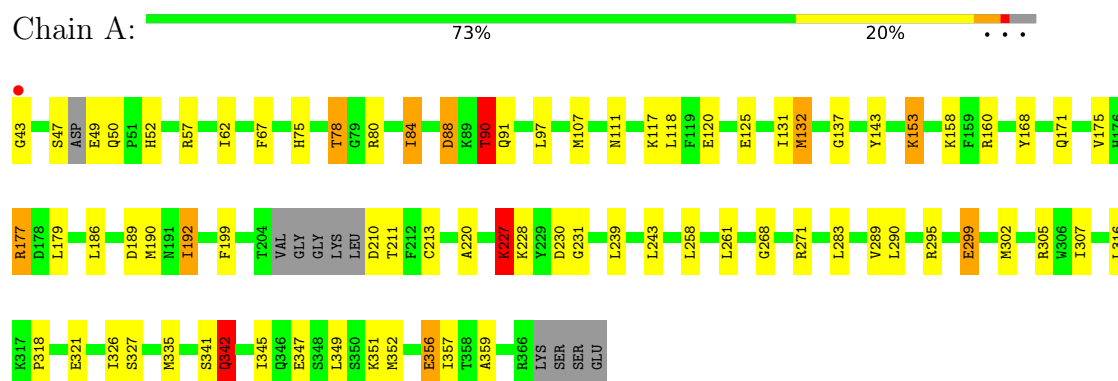
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	20	Total	O	0	0
			20	20		
2	B	27	Total	O	0	0
			27	27		

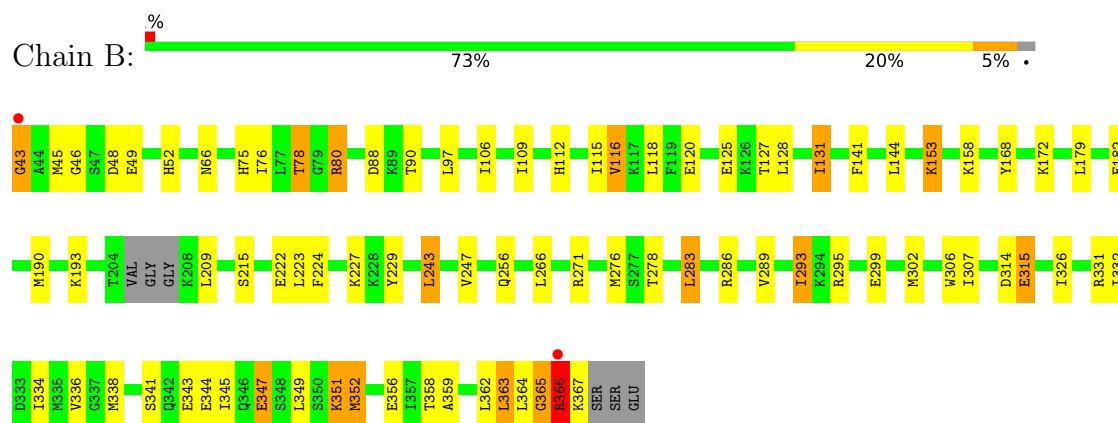
3 Residue-property plots

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: MAP/microtubule affinity-regulating kinase 3



- Molecule 1: MAP/microtubule affinity-regulating kinase 3



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	62.67Å 112.54Å 117.21Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.70 30.00 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.9 (30.00-2.70) 99.8 (30.00-2.70)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.64 (at 2.68Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.215 , 0.279 0.222 , 0.282	Depositor DCC
R_{free} test set	1213 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å ²)	48.0	Xtriage
Anisotropy	0.476	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 36.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.012 for -h,l,k	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	5075	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.47% 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	0.83	0/2557	1.04	7/3452 (0.2%)
1	B	0.84	0/2565	1.09	6/3466 (0.2%)
All	All	0.84	0/5122	1.07	13/6918 (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	43	GLY	N-CA-C	-9.18	86.69	113.30
1	A	321	GLU	CA-C-N	-6.16	114.28	120.31
1	A	321	GLU	C-N-CA	-6.16	114.28	120.31
1	B	343	GLU	N-CA-C	-5.93	104.73	111.07
1	B	365	GLY	N-CA-C	-5.76	96.59	113.30
1	A	231	GLY	CA-C-N	5.74	125.42	119.56
1	A	231	GLY	C-N-CA	5.74	125.42	119.56
1	B	209	LEU	N-CA-C	-5.43	106.53	112.72
1	B	364	LEU	N-CA-C	5.26	119.33	113.02
1	B	46	GLY	N-CA-C	-5.22	105.18	112.18
1	A	220	ALA	CA-C-N	5.05	125.08	119.32
1	A	220	ALA	C-N-CA	5.05	125.08	119.32
1	A	160	ARG	N-CA-C	-5.04	105.70	111.14

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	2510	0	2482	49	2
1	B	2518	0	2476	56	2
2	A	20	0	0	1	0
2	B	27	0	0	0	0
All	All	5075	0	4958	104	2

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 10.

All (104) 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:43:GLY:N	1:B:52:HIS:HE2	1.31	1.26
1:B:75:HIS:HD2	1:B:78:THR:HB	1.28	0.97
1:B:43:GLY:N	1:B:52:HIS:NE2	2.15	0.93
1:B:256:GLN:HA	1:B:256:GLN:HE21	1.33	0.92
1:B:75:HIS:CD2	1:B:78:THR:HB	2.08	0.87
1:A:289:VAL:HB	1:A:295:ARG:HG2	1.56	0.85
1:A:78:THR:HG23	1:A:80:ARG:HD3	1.60	0.84
1:A:75:HIS:HD2	1:A:78:THR:HB	1.46	0.81
1:A:75:HIS:CD2	1:A:78:THR:HB	2.18	0.79
1:A:75:HIS:HD2	1:A:78:THR:CG2	2.00	0.75
1:B:256:GLN:HA	1:B:256:GLN:NE2	2.01	0.74
1:B:299:GLU:HA	1:B:302:MET:CE	2.19	0.72
1:A:302:MET:HE1	1:A:318:PRO:HG3	1.72	0.72
1:A:153:LYS:H	1:A:153:LYS:HD2	1.54	0.71
1:A:111:ASN:HD22	1:A:117:LYS:HD3	1.56	0.70
1:B:78:THR:CG2	1:B:80:ARG:HG2	2.21	0.70
1:B:43:GLY:O	1:B:52:HIS:NE2	2.25	0.69
1:B:78:THR:HG23	1:B:80:ARG:HG2	1.74	0.68
1:A:75:HIS:HD2	1:A:78:THR:CB	2.06	0.67
1:A:177:ARG:HD2	1:A:230:ASP:HA	1.75	0.67
1:A:67:PHE:HA	1:A:91:GLN:NE2	2.08	0.67
1:B:88:ASP:OD1	1:B:90:THR:HB	1.96	0.66
1:B:179:LEU:H	1:B:179:LEU:HD22	1.60	0.66
1:B:334:ILE:HG22	1:B:338:MET:HE3	1.78	0.65
1:A:107:MET:HE1	1:A:132:MET:HE2	1.78	0.65
1:A:120:GLU:HB2	1:A:359:ALA:HB2	1.79	0.64
1:B:158:LYS:HE3	1:B:190:MET:O	1.98	0.64
1:A:177:ARG:HH11	1:A:230:ASP:HB3	1.63	0.62
1:B:341:SER:OG	1:B:344:GLU:HG2	1.99	0.62
1:B:299:GLU:HA	1:B:302:MET:HE3	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:75:HIS:HD2	1:B:78:THR:CB	2.09	0.61
1:B:43:GLY:O	1:B:52:HIS:CD2	2.55	0.60
1:A:67:PHE:HA	1:A:91:GLN:HE22	1.67	0.59
1:A:302:MET:HE1	1:A:318:PRO:CG	2.32	0.59
1:B:224:PHE:HB2	1:B:266:LEU:HD21	1.84	0.59
1:B:289:VAL:HB	1:B:295:ARG:HG2	1.85	0.58
1:A:302:MET:HE1	1:A:318:PRO:CD	2.32	0.58
1:A:299:GLU:HA	1:A:302:MET:HE2	1.85	0.57
1:B:45:MET:HE2	1:B:76:ILE:HD13	1.86	0.57
1:A:177:ARG:HH11	1:A:230:ASP:CB	2.18	0.57
1:B:131:ILE:HD12	1:B:131:ILE:N	2.20	0.56
1:B:120:GLU:HB2	1:B:359:ALA:HB2	1.86	0.55
1:B:365:GLY:HA3	1:B:366:ARG:C	2.31	0.55
1:B:366:ARG:CB	1:B:367:LYS:HA	2.37	0.54
1:B:222:GLU:CD	1:B:295:ARG:HH22	2.15	0.54
1:A:88:ASP:OD1	1:A:90:THR:HB	2.08	0.54
1:B:112:HIS:HB3	1:B:115:ILE:HD12	1.91	0.53
1:A:168:TYR:O	1:A:171:GLN:HG2	2.08	0.53
1:A:345:ILE:HA	1:A:357:ILE:HG21	1.91	0.53
1:B:362:LEU:O	1:B:365:GLY:HA2	2.10	0.52
1:B:283:LEU:HD12	1:B:306:TRP:CE3	2.44	0.52
1:B:299:GLU:HA	1:B:302:MET:HE2	1.90	0.52
1:A:168:TYR:HA	1:A:171:GLN:HG2	1.91	0.52
1:B:106:ILE:HA	1:B:109:ILE:HD12	1.92	0.51
1:A:75:HIS:CD2	1:A:78:THR:CG2	2.89	0.50
1:B:222:GLU:OE2	1:B:295:ARG:NH2	2.45	0.50
1:A:47:SER:O	1:A:49:GLU:N	2.45	0.49
1:A:302:MET:HE1	1:A:318:PRO:HD3	1.94	0.49
1:A:78:THR:CG2	1:A:80:ARG:H	2.25	0.49
1:A:153:LYS:HD2	1:A:153:LYS:N	2.26	0.49
1:A:50:GLN:O	1:A:57:ARG:HD2	2.12	0.49
1:A:177:ARG:NH1	1:A:230:ASP:HB3	2.28	0.48
1:A:351:LYS:O	1:A:352:MET:HB3	2.14	0.48
1:B:352:MET:CE	1:B:358:THR:HG21	2.44	0.48
1:B:131:ILE:N	1:B:131:ILE:CD1	2.77	0.47
1:B:366:ARG:NE	1:B:366:ARG:HA	2.29	0.47
1:B:352:MET:HE1	1:B:358:THR:CG2	2.45	0.46
1:A:271:ARG:NH1	1:B:172:LYS:O	2.48	0.46
1:B:352:MET:HE1	1:B:358:THR:HG21	1.96	0.46
1:A:97:LEU:HD12	1:A:97:LEU:HA	1.79	0.46
1:B:127:THR:HG22	1:B:128:LEU:N	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:158:LYS:HB3	1:A:192:ILE:HD11	1.98	0.46
1:A:335:MET:HE1	1:A:357:ILE:HG23	1.97	0.46
1:B:78:THR:HG22	1:B:80:ARG:H	1.81	0.45
1:B:314:ASP:O	1:B:315:GLU:C	2.58	0.45
1:B:347:GLU:O	1:B:351:LYS:HB2	2.17	0.45
1:B:141:PHE:HA	1:B:144:LEU:HD12	1.99	0.44
1:B:153:LYS:H	1:B:153:LYS:HD2	1.82	0.44
1:A:302:MET:HG2	1:A:316:LEU:HD23	1.99	0.44
1:A:143:TYR:C	1:A:143:TYR:CD1	2.96	0.44
1:A:227:LYS:HB3	1:A:228:LYS:H	1.62	0.44
1:B:243:LEU:HD11	1:B:283:LEU:HD13	1.99	0.44
1:A:78:THR:HG22	1:A:80:ARG:H	1.82	0.43
1:A:199:PHE:CD2	1:A:199:PHE:N	2.85	0.43
1:A:351:LYS:O	1:A:352:MET:CB	2.64	0.43
1:B:356:GLU:H	1:B:356:GLU:HG2	1.61	0.43
1:A:268:GLY:HA3	1:A:290:LEU:HD21	2.00	0.43
1:B:247:VAL:CG2	1:B:276:MET:HE2	2.48	0.43
1:A:189:ASP:O	1:A:190:MET:HB2	2.19	0.43
1:B:116:VAL:HG12	1:B:193:LYS:HB3	2.01	0.43
1:B:359:ALA:O	1:B:363:LEU:HB2	2.18	0.43
1:B:223:LEU:HB2	1:B:229:TYR:CE2	2.53	0.43
1:A:356:GLU:H	1:A:356:GLU:HG2	1.54	0.43
1:B:332:ILE:O	1:B:336:VAL:HG23	2.19	0.43
1:B:366:ARG:HB3	1:B:367:LYS:HA	2.00	0.42
1:A:158:LYS:HB3	1:A:192:ILE:CD1	2.49	0.42
1:A:299:GLU:H	1:A:299:GLU:HG2	1.48	0.42
1:A:342:GLN:HB3	2:A:387:HOH:O	2.19	0.42
1:B:293:ILE:H	1:B:293:ILE:HG13	1.62	0.42
1:A:84:ILE:HD13	1:A:131:ILE:HG13	2.02	0.42
1:A:137:GLY:N	1:A:186:LEU:O	2.53	0.42
1:B:341:SER:O	1:B:345:ILE:HG13	2.20	0.41
1:B:168:TYR:CE1	1:B:172:LYS:HE2	2.56	0.41
1:B:112:HIS:CB	1:B:115:ILE:HD12	2.50	0.41

All (2) 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:43:GLY:O	1:B:43:GLY:N[3_555]	1.68	0.52
1:A:52:HIS:NE2	1:B:43:GLY:N[3_555]	1.96	0.24

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	312/328 (95%)	291 (93%)	17 (5%)	4 (1%)	9	25
1	B	318/328 (97%)	303 (95%)	13 (4%)	2 (1%)	21	44
All	All	630/656 (96%)	594 (94%)	30 (5%)	6 (1%)	12	32

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	90	THR
1	A	227	LYS
1	A	342	GLN
1	B	66	ASN
1	B	366	ARG
1	A	88	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	265/289 (92%)	234 (88%)	31 (12%)	5	13
1	B	264/289 (91%)	235 (89%)	29 (11%)	6	15
All	All	529/578 (92%)	469 (89%)	60 (11%)	5	14

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	62	ILE
1	A	78	THR
1	A	84	ILE
1	A	90	THR
1	A	118	LEU
1	A	125	GLU
1	A	132	MET
1	A	153	LYS
1	A	175	VAL
1	A	177	ARG
1	A	179	LEU
1	A	192	ILE
1	A	210	ASP
1	A	211	THR
1	A	213	CYS
1	A	227	LYS
1	A	239	LEU
1	A	243	LEU
1	A	258	LEU
1	A	261	LEU
1	A	283	LEU
1	A	299	GLU
1	A	305	ARG
1	A	307	ILE
1	A	326	ILE
1	A	327	SER
1	A	341	SER
1	A	342	GLN
1	A	347	GLU
1	A	349	LEU
1	A	356	GLU
1	B	48	ASP
1	B	49	GLU
1	B	78	THR
1	B	80	ARG
1	B	97	LEU
1	B	116	VAL
1	B	118	LEU
1	B	125	GLU
1	B	131	ILE
1	B	153	LYS
1	B	182	GLU
1	B	215	SER

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Mol	Chain	Res	Type
1	B	227	LYS
1	B	243	LEU
1	B	271	ARG
1	B	278	THR
1	B	283	LEU
1	B	286	ARG
1	B	293	ILE
1	B	307	ILE
1	B	315	GLU
1	B	326	ILE
1	B	331	ARG
1	B	347	GLU
1	B	349	LEU
1	B	351	LYS
1	B	352	MET
1	B	363	LEU
1	B	366	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	75	HIS
1	A	91	GLN
1	A	111	ASN
1	A	161	GLN
1	A	346	GLN
1	B	75	HIS
1	B	111	ASN
1	B	256	GLN
1	B	311	HIS

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 [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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	318/328 (96%)	-0.39	1 (0%) 90 89	25, 36, 44, 54	0
1	B	322/328 (98%)	-0.28	2 (0%) 85 85	13, 35, 44, 57	0
All	All	640/656 (97%)	-0.33	3 (0%) 87 86	13, 36, 44, 57	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	43	GLY	3.4
1	A	43	GLY	2.5
1	B	366	ARG	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.