



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 05:02 PM UTC

PDB ID : 3O0Z / pdb_00003o0z
Title : Crystal structure of a coiled-coil domain from human ROCK I
Authors : Tu, D.; Eck, M.J.
Deposited on : 2010-07-20
Resolution : 2.33 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

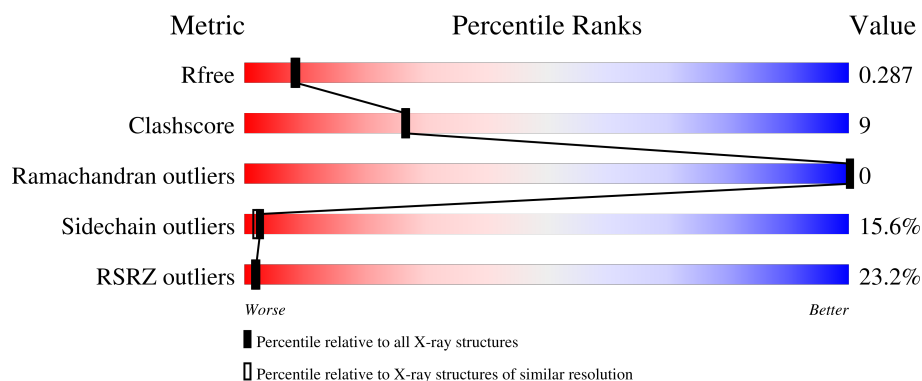
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.33 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	3031 (2.36-2.32)
Clashscore	190562	3127 (2.36-2.32)
Ramachandran outliers	187476	3095 (2.36-2.32)
Sidechain outliers	187428	3095 (2.36-2.32)
RSRZ outliers	180081	3033 (2.36-2.32)

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	168	
1	B	168	
1	C	168	
1	D	168	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5275 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 Rho-associated protein kinase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	152	Total	C	N	O	Se	0	3	0
			1282	778	238	261	5			
1	B	152	Total	C	N	O	Se	0	4	0
			1286	777	242	262	5			
1	C	159	Total	C	N	O	Se	0	3	0
			1335	809	247	272	7			
1	D	160	Total	C	N	O	Se	0	4	0
			1345	815	251	273	6			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	533	GLY	-	expression tag	UNP Q13464
A	534	SER	-	expression tag	UNP Q13464
B	533	GLY	-	expression tag	UNP Q13464
B	534	SER	-	expression tag	UNP Q13464
C	533	GLY	-	expression tag	UNP Q13464
C	534	SER	-	expression tag	UNP Q13464
D	533	GLY	-	expression tag	UNP Q13464
D	534	SER	-	expression tag	UNP Q13464

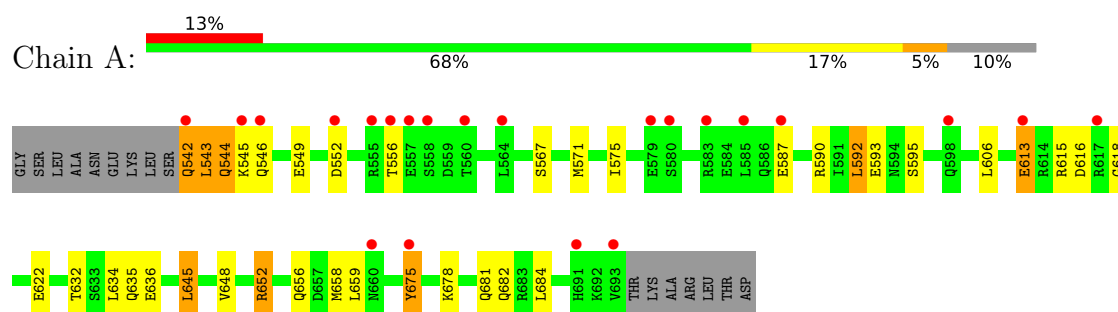
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	7	Total	O	0	0
			7	7		
2	B	7	Total	O	0	0
			7	7		
2	C	9	Total	O	0	0
			9	9		
2	D	4	Total	O	0	0
			4	4		

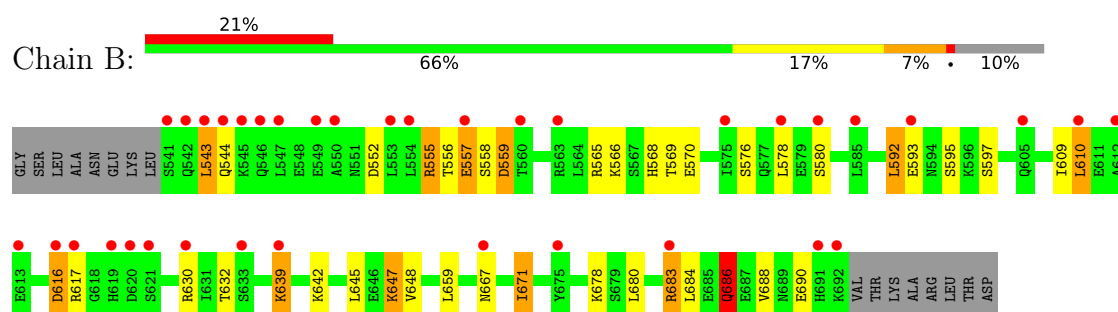
3 Residue-property plots [i](#)

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.

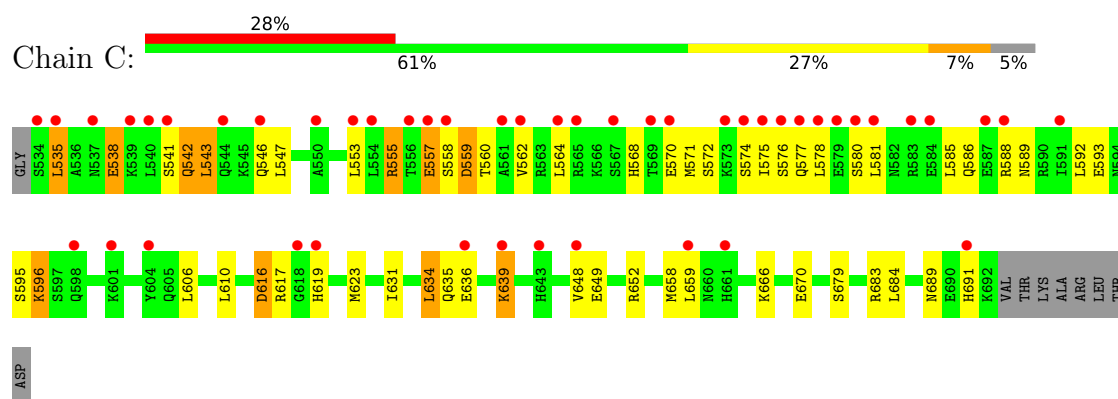
• Molecule 1: Rho-associated protein kinase 1



• Molecule 1: Rho-associated protein kinase 1

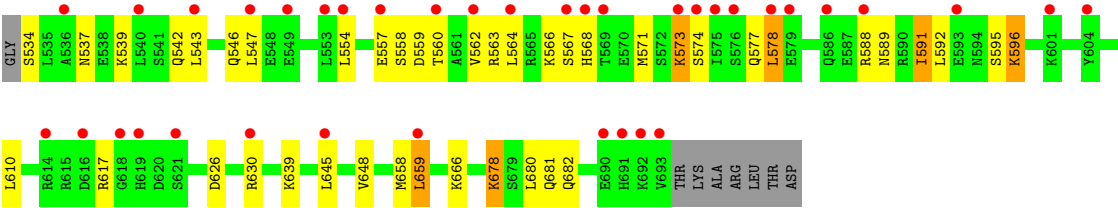


• Molecule 1: Rho-associated protein kinase 1



• Molecule 1: Rho-associated protein kinase 1





4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	84.59Å 84.59Å 340.13Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.13 – 2.33 42.13 – 2.33	Depositor EDS
% Data completeness (in resolution range)	67.9 (42.13-2.33) 69.3 (42.13-2.33)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.31 (at 2.32Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6_289)	Depositor
R, R_{free}	0.239 , 0.286 0.231 , 0.287	Depositor DCC
R_{free} test set	1999 reflections (5.32%)	wwPDB-VP
Wilson B-factor (Å ²)	30.2	Xtriage
Anisotropy	0.981	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 70.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	5275	wwPDB-VP
Average B, all atoms (Å ²)	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.39% 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	0.61	0/1297	0.84	1/1725 (0.1%)
1	B	0.56	0/1303	0.81	2/1731 (0.1%)
1	C	0.54	0/1352	0.86	0/1796
1	D	0.53	0/1362	0.78	1/1810 (0.1%)
All	All	0.56	0/5314	0.82	4/7062 (0.1%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	686	GLN	N-CA-C	-5.42	105.03	111.69
1	D	558	SER	N-CA-C	-5.37	105.86	112.90
1	B	595	SER	N-CA-C	-5.09	105.73	111.28
1	A	622	GLU	N-CA-C	-5.01	105.73	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	1282	0	1282	32	0
1	B	1286	0	1290	28	0
1	C	1335	0	1344	34	0
1	D	1345	0	1357	28	0
2	A	7	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	7	0	0	0	0
2	C	9	0	0	0	0
2	D	4	0	0	0	0
All	All	5275	0	5273	98	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 9.

All (98) 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:C:617:ARG:HD2	1:D:617:ARG:HG3	1.54	0.87
1:D:678:LYS:HA	1:D:678:LYS:HE2	1.67	0.76
1:A:652:ARG:CG	1:A:652:ARG:HH11	2.00	0.75
1:A:652:ARG:HH11	1:A:652:ARG:HG2	1.55	0.72
1:A:552:ASP:O	1:A:556:THR:HG23	1.93	0.69
1:B:565:ARG:O	1:B:569:THR:HG23	1.93	0.69
1:C:666:LYS:HG3	1:D:666:LYS:HB2	1.77	0.66
1:C:658[A]:MSE:HE2	1:D:659:LEU:HD11	1.78	0.65
1:C:593:GLU:OE2	1:D:592:LEU:HD11	1.98	0.63
1:C:535:LEU:HD22	1:C:538:GLU:OE1	2.00	0.62
1:C:559:ASP:O	1:C:562:VAL:HG12	2.00	0.62
1:C:619:HIS:O	1:C:623[A]:MSE:HG3	2.00	0.62
1:A:652:ARG:HH11	1:A:652:ARG:CB	2.13	0.61
1:C:581:LEU:O	1:C:585:LEU:HG	2.01	0.61
1:B:683:ARG:HD2	1:B:683:ARG:C	2.28	0.59
1:C:631:ILE:O	1:C:635:GLN:HG3	2.03	0.58
1:A:635:GLN:HE21	1:B:630[B]:ARG:HH21	1.51	0.57
1:A:635:GLN:HE21	1:B:630[B]:ARG:NH2	2.03	0.57
1:C:617:ARG:HD2	1:D:617:ARG:CG	2.33	0.55
1:A:592:LEU:HD13	1:B:592:LEU:HB3	1.88	0.55
1:C:648:VAL:HG12	1:D:648:VAL:HG12	1.89	0.55
1:A:542:GLN:CD	1:A:544:GLN:HG3	2.31	0.55
1:A:616:ASP:HB3	1:B:617:ARG:HH12	1.71	0.55
1:A:652:ARG:HG2	1:A:652:ARG:NH1	2.19	0.54
1:B:647:LYS:NZ	1:B:647:LYS:HB2	2.22	0.54
1:A:545:LYS:O	1:A:549:GLU:HG3	2.08	0.53
1:A:571:MSE:O	1:A:575:ILE:HD12	2.08	0.53
1:B:543:LEU:HD23	1:B:543:LEU:C	2.34	0.53
1:B:555:ARG:HH11	1:B:555:ARG:HB2	1.74	0.53
1:A:648:VAL:HG12	1:B:648:VAL:HG12	1.90	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:559:ASP:O	1:D:563:ARG:HG2	2.09	0.52
1:B:686:GLN:O	1:B:690:GLU:HG3	2.09	0.52
1:C:542:GLN:O	1:C:546:GLN:HG3	2.09	0.51
1:D:534:SER:HA	1:D:537:ASN:HB2	1.92	0.51
1:C:595:SER:OG	1:D:596:LYS:HD3	2.11	0.51
1:A:543:LEU:HD23	1:A:543:LEU:N	2.26	0.51
1:C:571[B]:MSE:SE	1:D:571[B]:MSE:SE	3.30	0.50
1:C:568:HIS:O	1:C:572:SER:HB2	2.11	0.50
1:B:667:ASN:O	1:B:671:ILE:HD12	2.12	0.49
1:C:652:ARG:NH1	1:C:652:ARG:HG2	2.27	0.49
1:D:626:ASP:O	1:D:630[A]:ARG:HG3	2.12	0.48
1:A:592:LEU:O	1:A:595:SER:HB3	2.13	0.48
1:A:616:ASP:HB3	1:B:617:ARG:NH1	2.28	0.48
1:A:645:LEU:HD23	1:A:645:LEU:HA	1.59	0.48
1:C:588:ARG:O	1:C:592:LEU:HG	2.14	0.48
1:C:617:ARG:HB3	1:D:617:ARG:NH1	2.30	0.47
1:A:542:GLN:NE2	1:A:544:GLN:CG	2.77	0.47
1:A:587:GLU:OE1	1:A:590:ARG:NH1	2.48	0.47
1:A:656:GLN:HE22	1:A:659:LEU:HD23	1.79	0.47
1:D:573:LYS:HD2	1:D:573:LYS:C	2.39	0.47
1:B:557:GLU:CD	1:B:557:GLU:C	2.83	0.46
1:D:539:LYS:HA	1:D:539:LYS:HD2	1.70	0.46
1:D:568:HIS:ND1	1:D:568:HIS:C	2.73	0.46
1:A:606:LEU:HD11	1:B:610:LEU:HD13	1.97	0.46
1:C:570:GLU:O	1:C:574:SER:HB2	2.16	0.46
1:A:658[B]:MSE:HE2	1:B:659:LEU:HD21	1.97	0.46
1:C:596:LYS:HE3	1:D:595:SER:OG	2.16	0.46
1:D:542:GLN:O	1:D:546:GLN:HG3	2.16	0.45
1:D:681:GLN:HE21	1:D:682:GLN:HG3	1.80	0.45
1:A:635:GLN:NE2	1:B:630[B]:ARG:HH21	2.14	0.45
1:B:647:LYS:HG2	1:B:648:VAL:N	2.30	0.45
1:C:616:ASP:O	1:C:617:ARG:C	2.57	0.45
1:C:666:LYS:O	1:C:670:GLU:HG3	2.17	0.45
1:A:592:LEU:HD11	1:B:593:GLU:HG3	1.98	0.45
1:C:553:LEU:O	1:C:557:GLU:HB3	2.16	0.45
1:D:557:GLU:HA	1:D:560:THR:OG1	2.16	0.45
1:C:666:LYS:HB3	1:C:666:LYS:HE2	1.80	0.45
1:A:613:GLU:OE1	1:B:610:LEU:HD23	2.18	0.44
1:B:555:ARG:O	1:B:559:ASP:HB2	2.17	0.44
1:B:568:HIS:ND1	1:B:568:HIS:C	2.76	0.44
1:C:578:LEU:HD21	1:D:578:LEU:HB3	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:617:ARG:O	1:B:617:ARG:HG3	2.18	0.43
1:A:544:GLN:HG3	1:A:544:GLN:H	1.58	0.43
1:B:566:LYS:O	1:B:570:GLU:HG3	2.19	0.43
1:D:568:HIS:HA	1:D:571[B]:MSE:HE2	2.00	0.43
1:C:577:GLN:O	1:C:580:SER:HB2	2.19	0.43
1:B:592:LEU:HD12	1:B:592:LEU:HA	1.70	0.43
1:D:554:LEU:HD23	1:D:554:LEU:HA	1.89	0.42
1:A:652:ARG:HH11	1:A:652:ARG:C	2.28	0.42
1:C:543:LEU:HD23	1:C:543:LEU:HA	1.84	0.42
1:C:555:ARG:HA	1:C:555:ARG:HD3	1.65	0.41
1:C:691:HIS:O	1:C:691:HIS:CG	2.73	0.41
1:C:589:ASN:CB	1:D:589:ASN:HD21	2.33	0.41
1:C:652:ARG:HG2	1:C:652:ARG:HH11	1.86	0.41
1:D:573:LYS:O	1:D:577:GLN:HG3	2.20	0.41
1:C:589:ASN:HB2	1:D:589:ASN:HD21	1.86	0.41
1:A:652:ARG:HH11	1:A:652:ARG:HB3	1.84	0.41
1:C:639:LYS:HE2	1:C:639:LYS:HB3	1.72	0.41
1:A:544:GLN:NE2	1:A:545:LYS:HG3	2.36	0.41
1:D:591:ILE:HG22	1:D:592:LEU:N	2.36	0.41
1:C:634:LEU:HD12	1:C:634:LEU:HA	1.96	0.40
1:B:639:LYS:HD2	1:B:639:LYS:HA	1.59	0.40
1:B:684:LEU:HA	1:B:684:LEU:HD23	1.87	0.40
1:A:616:ASP:C	1:A:618:GLY:N	2.80	0.40
1:B:616:ASP:N	1:B:616:ASP:OD1	2.53	0.40
1:A:678:LYS:HE3	1:A:678:LYS:HB2	1.96	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	153/168 (91%)	151 (99%)	2 (1%)	0	100 100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	154/168 (92%)	151 (98%)	3 (2%)	0	100	100
1	C	161/168 (96%)	156 (97%)	5 (3%)	0	100	100
1	D	162/168 (96%)	160 (99%)	2 (1%)	0	100	100
All	All	630/672 (94%)	618 (98%)	12 (2%)	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	146/153 (95%)	127 (87%)	19 (13%)	4	3
1	B	147/153 (96%)	120 (82%)	27 (18%)	1	1
1	C	153/153 (100%)	125 (82%)	28 (18%)	2	1
1	D	154/153 (101%)	136 (88%)	18 (12%)	5	4
All	All	600/612 (98%)	508 (85%)	92 (15%)	2	2

All (92) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	542	GLN
1	A	543	LEU
1	A	544	GLN
1	A	546	GLN
1	A	567	SER
1	A	592	LEU
1	A	593	GLU
1	A	613	GLU
1	A	615	ARG
1	A	632	THR
1	A	634	LEU
1	A	636	GLU
1	A	645	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	652	ARG
1	A	675[A]	TYR
1	A	675[B]	TYR
1	A	681	GLN
1	A	682	GLN
1	A	684	LEU
1	B	543	LEU
1	B	544	GLN
1	B	552	ASP
1	B	555	ARG
1	B	556	THR
1	B	557	GLU
1	B	558	SER
1	B	559	ASP
1	B	576	SER
1	B	578	LEU
1	B	580	SER
1	B	592	LEU
1	B	597	SER
1	B	609	ILE
1	B	610	LEU
1	B	616	ASP
1	B	632	THR
1	B	639	LYS
1	B	642	LYS
1	B	645	LEU
1	B	647	LYS
1	B	671	ILE
1	B	678	LYS
1	B	680	LEU
1	B	683	ARG
1	B	686	GLN
1	B	688	VAL
1	C	535	LEU
1	C	538	GLU
1	C	541	SER
1	C	542	GLN
1	C	543	LEU
1	C	547	LEU
1	C	555	ARG
1	C	557	GLU
1	C	558	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	559	ASP
1	C	560	THR
1	C	564	LEU
1	C	575	ILE
1	C	576	SER
1	C	586	GLN
1	C	596	LYS
1	C	606	LEU
1	C	610	LEU
1	C	616	ASP
1	C	634	LEU
1	C	636	GLU
1	C	639	LYS
1	C	649	GLU
1	C	659	LEU
1	C	679	SER
1	C	683	ARG
1	C	684	LEU
1	C	689	ASN
1	D	543	LEU
1	D	547	LEU
1	D	562	VAL
1	D	564	LEU
1	D	566	LYS
1	D	567	SER
1	D	573	LYS
1	D	574	SER
1	D	578	LEU
1	D	588	ARG
1	D	591	ILE
1	D	596	LYS
1	D	610	LEU
1	D	639	LYS
1	D	645	LEU
1	D	659	LEU
1	D	678	LYS
1	D	680	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	589	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	628	GLN
1	A	635	GLN
1	A	644	ASN
1	A	656	GLN
1	A	674	ASN
1	A	681	GLN
1	A	689	ASN
1	B	577	GLN
1	B	582	ASN
1	B	586	GLN
1	B	589	ASN
1	B	605	GLN
1	B	661	HIS
1	C	582	ASN
1	C	589	ASN
1	C	598	GLN
1	C	674	ASN
1	D	542	GLN
1	D	551	ASN
1	D	577	GLN
1	D	586	GLN
1	D	589	ASN
1	D	605	GLN
1	D	635	GLN
1	D	644	ASN
1	D	661	HIS
1	D	681	GLN
1	D	686	GLN
1	D	691	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 ⓘ

There are no oligosaccharides 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 [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	149/168 (88%)	1.01	22 (14%)	5 6	27, 63, 113, 140	1 (0%)
1	B	149/168 (88%)	1.33	36 (24%)	2 1	33, 77, 139, 165	2 (1%)
1	C	156/168 (92%)	1.50	47 (30%)	1 1	40, 76, 127, 147	0
1	D	157/168 (93%)	1.38	37 (23%)	2 2	31, 82, 119, 145	1 (0%)
All	All	611/672 (90%)	1.31	142 (23%)	2 2	27, 75, 125, 165	4 (0%)

All (142) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	693	VAL	7.3
1	C	575	ILE	7.0
1	C	581	LEU	6.4
1	A	583	ARG	5.4
1	B	692	LYS	5.2
1	B	544	GLN	5.0
1	A	693	VAL	4.8
1	C	535	LEU	4.4
1	B	630[A]	ARG	4.3
1	C	569	THR	4.2
1	B	691	HIS	4.2
1	C	578	LEU	4.2
1	B	617	ARG	4.1
1	D	574	SER	4.1
1	B	613	GLU	4.0
1	C	534	SER	4.0
1	C	691	HIS	3.9
1	C	591	ILE	3.9
1	D	540	LEU	3.9
1	A	555	ARG	3.9
1	D	575	ILE	3.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	557	GLU	3.8
1	D	553	LEU	3.7
1	D	586	GLN	3.7
1	B	575	ILE	3.6
1	B	560	THR	3.6
1	B	543	LEU	3.5
1	D	692	LYS	3.5
1	C	540	LEU	3.5
1	D	588	ARG	3.4
1	B	553	LEU	3.4
1	B	541	SER	3.4
1	D	619	HIS	3.3
1	B	545	LYS	3.3
1	D	569	THR	3.3
1	B	549	GLU	3.3
1	B	612	ALA	3.2
1	A	691	HIS	3.2
1	B	550	ALA	3.2
1	D	604	TYR	3.2
1	B	547	LEU	3.2
1	D	593	GLU	3.2
1	D	614	ARG	3.1
1	C	562	VAL	3.1
1	D	560	THR	3.1
1	A	580	SER	3.1
1	A	617	ARG	3.1
1	D	621	SER	3.0
1	D	578	LEU	3.0
1	A	587	GLU	3.0
1	A	585	LEU	2.9
1	C	583	ARG	2.9
1	C	537	ASN	2.9
1	C	565	ARG	2.9
1	C	636	GLU	2.9
1	D	564	LEU	2.8
1	C	619	HIS	2.8
1	A	546	GLN	2.8
1	A	557	GLU	2.8
1	C	584	GLU	2.7
1	D	547	LEU	2.7
1	A	598	GLN	2.7
1	A	579	GLU	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	536	ALA	2.7
1	B	546	GLN	2.7
1	A	560	THR	2.7
1	C	618	GLY	2.7
1	C	539	LYS	2.7
1	C	573	LYS	2.7
1	C	574	SER	2.7
1	D	557	GLU	2.7
1	A	556	THR	2.7
1	D	690	GLU	2.7
1	C	588	ARG	2.7
1	B	610	LEU	2.7
1	D	618	GLY	2.6
1	B	542	GLN	2.6
1	B	675	TYR	2.6
1	C	553	LEU	2.6
1	B	563	ARG	2.6
1	C	604	TYR	2.6
1	C	550	ALA	2.6
1	B	557	GLU	2.5
1	C	556	THR	2.5
1	D	691	HIS	2.5
1	D	616	ASP	2.5
1	B	621	SER	2.5
1	D	562	VAL	2.5
1	D	645	LEU	2.4
1	C	661	HIS	2.4
1	C	598	GLN	2.4
1	B	578	LEU	2.4
1	C	577	GLN	2.4
1	C	587	GLU	2.4
1	C	541	SER	2.4
1	C	567	SER	2.4
1	B	554	LEU	2.4
1	D	554	LEU	2.4
1	B	619	HIS	2.4
1	A	613	GLU	2.4
1	C	648	VAL	2.3
1	C	546	GLN	2.3
1	D	543	LEU	2.3
1	B	620	ASP	2.3
1	B	667	ASN	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	675[A]	TYR	2.3
1	B	633	SER	2.3
1	D	630[A]	ARG	2.2
1	B	683	ARG	2.2
1	C	579	GLU	2.2
1	C	576	SER	2.2
1	C	580	SER	2.2
1	A	564	LEU	2.2
1	C	659	LEU	2.2
1	C	570	GLU	2.2
1	D	601	LYS	2.2
1	A	542	GLN	2.2
1	B	605	GLN	2.2
1	C	558	SER	2.2
1	C	561	ALA	2.2
1	B	585	LEU	2.1
1	C	564	LEU	2.1
1	D	549	GLU	2.1
1	C	639	LYS	2.1
1	A	552	ASP	2.1
1	B	616	ASP	2.1
1	B	580	SER	2.1
1	B	639	LYS	2.1
1	D	573	LYS	2.1
1	C	544	GLN	2.1
1	C	643	HIS	2.1
1	A	558	SER	2.1
1	D	576	SER	2.1
1	C	601	LYS	2.1
1	B	593	GLU	2.1
1	D	568	HIS	2.1
1	A	545	LYS	2.0
1	D	567	SER	2.0
1	D	579	GLU	2.0
1	A	660	ASN	2.0
1	D	659	LEU	2.0
1	C	554	LEU	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 [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.