



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 04:48 AM UTC

PDB ID : 5ZQL / pdb_00005zql
Title : crystal structure of human katanin AAA ATPase domain
Authors : Kim, E.E.; Shin, S.C.
Deposited on : 2018-04-19
Resolution : 3.01 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

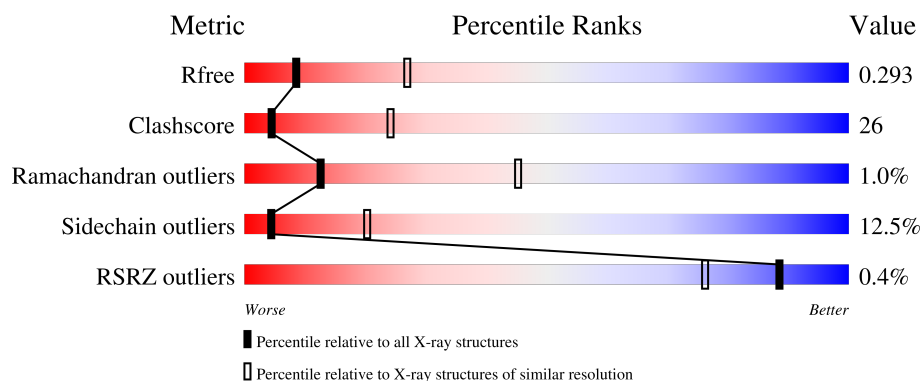
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.01 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	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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	309	 45% 31% 6% 18%
1	B	309	 42% 33% 7% 17%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 4065 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 Katanin p60 ATPase-containing subunit A1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	258	Total	C	N	O	S	0	0	0
			2056	1307	354	379	16			
1	A	252	Total	C	N	O	S	0	0	0
			2009	1280	346	368	15			

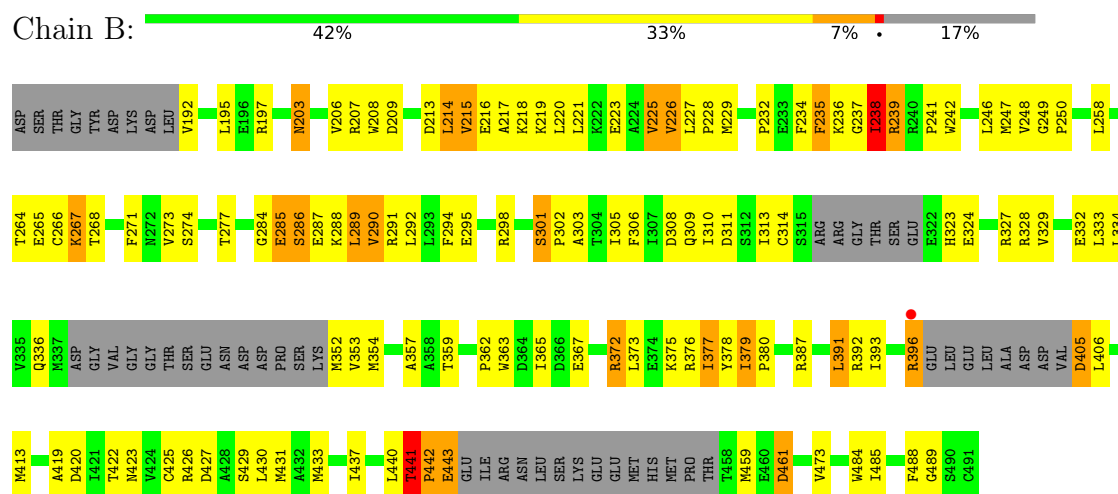
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	309	GLN	GLU	engineered mutation	UNP O75449
A	309	GLN	GLU	engineered mutation	UNP O75449

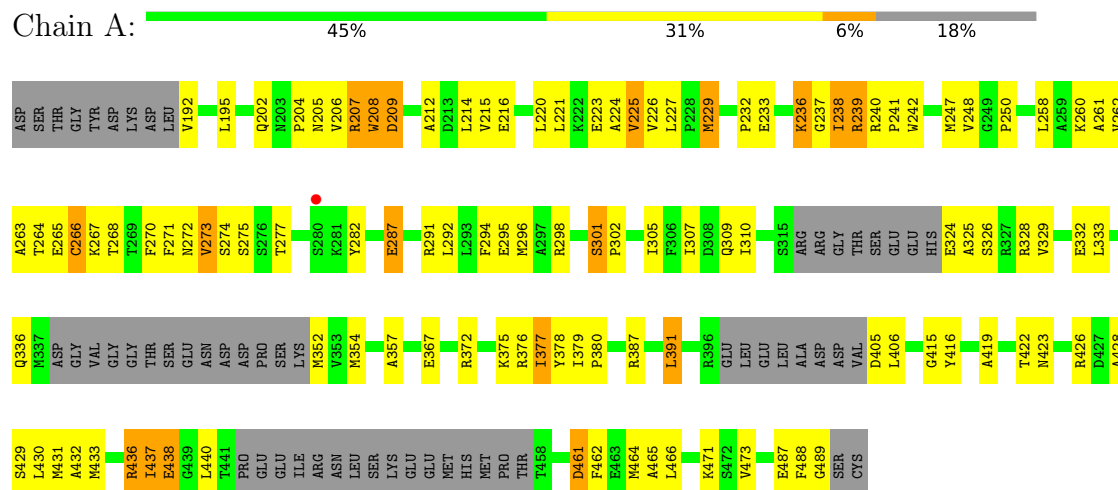
3 Residue-property plots

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: Katanin p60 ATPase-containing subunit A1



• Molecule 1: Katanin p60 ATPase-containing subunit A1



4 Data and refinement statistics

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, α , β , γ	97.81Å 97.81Å 72.71Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.48 – 3.01 37.48 – 3.01	Depositor EDS
% Data completeness (in resolution range)	76.9 (37.48-3.01) 77.1 (37.48-3.01)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.60 (at 3.01Å)	Xtriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, R_{free}	0.275 , 0.285 0.279 , 0.293	Depositor DCC
R_{free} test set	526 reflections (3.81%)	wwPDB-VP
Wilson B-factor (Å ²)	62.7	Xtriage
Anisotropy	0.068	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.19 , 137.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	0.449 for h,-k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	4065	wwPDB-VP
Average B, all atoms (Å ²)	98.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.70% 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	0.37	0/2040	0.92	5/2741 (0.2%)
1	B	0.40	1/2089 (0.0%)	1.02	16/2808 (0.6%)
All	All	0.39	1/4129 (0.0%)	0.97	21/5549 (0.4%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	289	LEU	CA-CB	-6.05	1.44	1.53

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	286	SER	N-CA-C	-9.62	98.69	113.89
1	B	249	GLY	CA-C-N	8.45	125.74	119.66
1	B	249	GLY	C-N-CA	8.45	125.74	119.66
1	B	441	THR	N-CA-C	7.82	118.19	108.11
1	B	290	VAL	N-CA-C	-7.52	102.81	111.00
1	B	301	SER	CA-C-N	-7.09	112.12	120.13
1	B	301	SER	C-N-CA	-7.09	112.12	120.13
1	A	227	LEU	CA-C-N	-6.92	111.20	119.84
1	A	227	LEU	C-N-CA	-6.92	111.20	119.84
1	A	209	ASP	N-CA-C	6.80	120.24	110.24
1	B	203	ASN	CA-C-N	6.40	127.84	119.84
1	B	203	ASN	C-N-CA	6.40	127.84	119.84
1	B	239	ARG	N-CA-C	5.64	117.90	108.02
1	A	212	ALA	CB-CA-C	-5.49	110.22	116.54
1	B	441	THR	CB-CA-C	-5.44	102.53	109.92
1	B	379	ILE	CA-C-N	5.39	125.86	120.52
1	B	379	ILE	C-N-CA	5.39	125.86	120.52
1	A	224	ALA	N-CA-C	-5.27	105.71	111.82
1	B	226	VAL	N-CA-C	5.23	115.44	110.42
1	B	239	ARG	CB-CA-C	-5.23	102.33	110.74
1	B	285	GLU	N-CA-C	-5.15	99.84	110.80

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	2009	0	2054	120	0
1	B	2056	0	2090	100	0
All	All	4065	0	4144	216	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 26.

All (216) 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:237:GLY:O	1:B:238:ILE:HG23	1.18	1.35
1:B:208:TRP:CZ2	1:B:221:LEU:HD12	1.74	1.21
1:A:232:PRO:HB3	1:A:236:LYS:CG	1.73	1.16
1:A:301:SER:HB3	1:A:302:PRO:CD	1.76	1.14
1:A:301:SER:CB	1:A:302:PRO:CD	2.30	1.09
1:A:301:SER:HB3	1:A:302:PRO:HD3	1.10	1.08
1:B:237:GLY:O	1:B:238:ILE:CG2	2.02	1.07
1:A:232:PRO:HB3	1:A:236:LYS:HG2	1.41	0.99
1:A:232:PRO:HB3	1:A:236:LYS:HG3	1.46	0.98
1:A:232:PRO:CB	1:A:236:LYS:CG	2.42	0.96
1:B:208:TRP:HZ2	1:B:221:LEU:HD12	1.27	0.95
1:B:237:GLY:C	1:B:238:ILE:HG23	1.88	0.92
1:B:372:ARG:HA	1:B:372:ARG:HE	1.32	0.92
1:A:301:SER:CB	1:A:302:PRO:HD3	1.95	0.89
1:A:208:TRP:CZ3	1:A:261:ALA:HB1	2.09	0.87
1:A:423:ASN:O	1:A:426:ARG:HG2	1.76	0.85
1:A:428:ALA:HB1	1:A:462:PHE:HA	1.58	0.85
1:A:232:PRO:CA	1:A:236:LYS:HB2	2.07	0.84
1:A:208:TRP:CE3	1:A:261:ALA:HB1	2.13	0.84
1:B:239:ARG:HD2	1:B:239:ARG:O	1.76	0.83
1:A:236:LYS:HB3	1:A:239:ARG:O	1.78	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:290:VAL:HG21	1:B:329:VAL:HG23	1.60	0.81
1:B:208:TRP:CE2	1:B:221:LEU:HD12	2.14	0.81
1:A:232:PRO:O	1:A:236:LYS:HB2	1.81	0.80
1:B:286:SER:O	1:B:289:LEU:HB2	1.85	0.77
1:A:301:SER:HB2	1:A:302:PRO:HD2	1.66	0.77
1:B:207:ARG:HH21	1:A:207:ARG:HG2	1.49	0.75
1:B:291:ARG:HD3	1:B:292:LEU:HD22	1.69	0.75
1:A:232:PRO:CB	1:A:236:LYS:HG2	2.11	0.75
1:B:221:LEU:HD23	1:B:221:LEU:O	1.87	0.75
1:A:301:SER:CB	1:A:302:PRO:HD2	2.15	0.74
1:B:213:ASP:OD2	1:B:216:GLU:HB2	1.88	0.74
1:B:310:ILE:HG13	1:B:357:ALA:HB1	1.71	0.73
1:A:437:ILE:HD13	1:A:437:ILE:O	1.88	0.73
1:A:221:LEU:HD11	1:A:258:LEU:HB3	1.70	0.72
1:B:238:ILE:HG13	1:B:239:ARG:N	2.04	0.72
1:A:232:PRO:C	1:A:236:LYS:HB2	2.15	0.71
1:A:220:LEU:HD21	1:A:377:ILE:HD13	1.72	0.71
1:A:298:ARG:NH1	1:A:336:GLN:OE1	2.23	0.71
1:B:298:ARG:NH1	1:B:336:GLN:OE1	2.23	0.71
1:B:208:TRP:CZ2	1:B:221:LEU:CD1	2.67	0.69
1:B:267:LYS:HB3	1:A:267:LYS:HB3	1.73	0.67
1:B:284:GLY:O	1:B:286:SER:N	2.27	0.67
1:A:301:SER:HB2	1:A:302:PRO:CD	2.20	0.66
1:A:419:ALA:O	1:A:423:ASN:ND2	2.28	0.66
1:A:205:ASN:HD21	1:A:263:ALA:HB3	1.61	0.66
1:A:232:PRO:HA	1:A:236:LYS:HB2	1.77	0.65
1:B:430:LEU:HD13	1:B:433:MET:HB3	1.78	0.65
1:B:207:ARG:HD3	1:B:208:TRP:H	1.62	0.65
1:B:274:SER:HB3	1:B:277:THR:HB	1.79	0.65
1:A:216:GLU:HG3	1:A:380:PRO:HD2	1.77	0.65
1:A:416:TYR:HA	1:A:471:LYS:HG3	1.79	0.64
1:A:232:PRO:CB	1:A:236:LYS:CB	2.76	0.63
1:A:208:TRP:CE3	1:A:261:ALA:O	2.52	0.63
1:A:428:ALA:HA	1:A:465:ALA:HB3	1.81	0.63
1:B:425:CYS:O	1:B:429:SER:N	2.31	0.63
1:B:237:GLY:C	1:B:238:ILE:CG2	2.61	0.63
1:B:237:GLY:O	1:B:238:ILE:HG12	1.98	0.62
1:B:372:ARG:HA	1:B:372:ARG:NE	1.97	0.62
1:A:310:ILE:HG13	1:A:357:ALA:HB1	1.80	0.62
1:B:387:ARG:NH1	1:B:413:MET:O	2.34	0.61
1:B:294:PHE:CD2	1:B:336:GLN:HB3	2.37	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:378:TYR:CE2	1:B:380:PRO:HB3	2.37	0.60
1:A:232:PRO:CB	1:A:236:LYS:HG3	2.20	0.60
1:B:313:ILE:HG13	1:B:314:CYS:H	1.67	0.59
1:B:226:VAL:HG11	1:B:265:GLU:HG2	1.82	0.59
1:A:423:ASN:HA	1:A:426:ARG:HE	1.67	0.59
1:B:287:GLU:O	1:B:290:VAL:HG23	2.01	0.59
1:B:301:SER:HB2	1:B:302:PRO:HD3	1.85	0.59
1:A:208:TRP:CZ3	1:A:261:ALA:CB	2.84	0.58
1:B:237:GLY:O	1:B:238:ILE:CB	2.50	0.58
1:B:220:LEU:CD2	1:B:258:LEU:HB3	2.34	0.58
1:B:241:PRO:HB3	1:B:354:MET:HE1	1.86	0.58
1:B:246:LEU:HB2	1:B:373:LEU:HG	1.86	0.58
1:A:423:ASN:HA	1:A:426:ARG:NE	2.19	0.58
1:A:208:TRP:CG	1:A:209:ASP:H	2.21	0.57
1:B:268:THR:HA	1:B:302:PRO:HB2	1.86	0.57
1:A:205:ASN:ND2	1:A:260:LYS:O	2.38	0.57
1:A:237:GLY:O	1:A:238:ILE:HB	2.03	0.57
1:B:441:THR:HG22	1:B:442:PRO:HD2	1.86	0.57
1:B:311:ASP:H	1:B:359:THR:HG22	1.70	0.56
1:B:359:THR:HG21	1:B:365:ILE:HD11	1.86	0.56
1:A:214:LEU:HD23	1:A:214:LEU:H	1.70	0.56
1:B:236:LYS:HB2	1:B:239:ARG:HH21	1.71	0.55
1:A:220:LEU:HD11	1:A:377:ILE:HB	1.88	0.55
1:B:225:VAL:O	1:B:229:MET:N	2.21	0.55
1:B:207:ARG:HB2	1:A:207:ARG:HH21	1.72	0.55
1:B:391:LEU:HD22	1:B:406:LEU:HD22	1.88	0.55
1:A:432:ALA:O	1:A:436:ARG:N	2.36	0.55
1:A:232:PRO:CA	1:A:236:LYS:HG2	2.36	0.55
1:A:294:PHE:HB3	1:A:298:ARG:HH11	1.71	0.55
1:A:232:PRO:CB	1:A:236:LYS:HB2	2.37	0.55
1:A:367:GLU:OE2	1:A:367:GLU:N	2.37	0.55
1:A:372:ARG:O	1:A:372:ARG:NH1	2.39	0.54
1:A:208:TRP:HZ3	1:A:261:ALA:CB	2.20	0.54
1:A:232:PRO:CA	1:A:236:LYS:CB	2.84	0.54
1:A:430:LEU:HD23	1:A:433:MET:HB3	1.90	0.54
1:B:213:ASP:CG	1:B:216:GLU:OE1	2.51	0.53
1:B:239:ARG:O	1:B:239:ARG:CD	2.53	0.53
1:A:274:SER:O	1:A:277:THR:HG22	2.09	0.53
1:A:236:LYS:HA	1:A:236:LYS:CE	2.39	0.53
1:B:225:VAL:HB	1:B:228:PRO:HB2	1.91	0.53
1:B:405:ASP:N	1:B:405:ASP:OD1	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:266:CYS:HB3	1:A:268:THR:HG23	1.91	0.52
1:A:367:GLU:H	1:A:367:GLU:CD	2.18	0.52
1:B:271:PHE:HB2	1:B:305:ILE:HA	1.92	0.51
1:B:442:PRO:HG2	1:B:443:GLU:H	1.76	0.51
1:A:387:ARG:HH12	1:A:416:TYR:H	1.58	0.50
1:A:236:LYS:HD2	1:A:239:ARG:HB3	1.94	0.50
1:A:250:PRO:HD2	1:A:379:ILE:O	2.11	0.50
1:A:462:PHE:O	1:A:466:LEU:N	2.44	0.49
1:A:324:GLU:OE2	1:A:325:ALA:N	2.44	0.49
1:A:324:GLU:HG3	1:A:326:SER:H	1.76	0.49
1:A:208:TRP:CE3	1:A:208:TRP:HA	2.47	0.49
1:A:216:GLU:CD	1:A:379:ILE:HG23	2.38	0.49
1:A:232:PRO:HA	1:A:236:LYS:HG2	1.94	0.49
1:B:238:ILE:CG1	1:B:239:ARG:N	2.76	0.49
1:B:303:ALA:HB3	1:B:353:VAL:HG12	1.93	0.49
1:A:229:MET:HG3	1:A:241:PRO:HB3	1.94	0.49
1:A:271:PHE:HB2	1:A:305:ILE:HA	1.93	0.49
1:B:227:LEU:HB2	1:B:228:PRO:HD3	1.95	0.49
1:B:376:ARG:HB2	1:B:489:GLY:HA2	1.95	0.49
1:A:208:TRP:CG	1:A:209:ASP:N	2.80	0.49
1:A:208:TRP:HA	1:A:208:TRP:HE3	1.78	0.48
1:A:376:ARG:HB2	1:A:489:GLY:HA2	1.95	0.48
1:B:323:HIS:HE1	1:B:327:ARG:HH21	1.61	0.48
1:B:237:GLY:O	1:B:238:ILE:CG1	2.61	0.48
1:A:206:VAL:HA	1:A:264:THR:OG1	2.14	0.48
1:A:247:MET:HG2	1:A:377:ILE:HD11	1.94	0.48
1:A:270:PHE:CE2	1:A:272:ASN:HB2	2.48	0.47
1:B:216:GLU:HG3	1:B:380:PRO:HD2	1.97	0.47
1:B:392:ARG:O	1:B:396:ARG:HG3	2.13	0.47
1:B:323:HIS:CE1	1:B:327:ARG:HH21	2.31	0.47
1:A:275:SER:HB3	1:A:309:GLN:O	2.15	0.47
1:A:436:ARG:HD2	1:A:436:ARG:HA	1.53	0.47
1:A:232:PRO:HA	1:A:236:LYS:CB	2.45	0.47
1:A:375:LYS:HD2	1:A:377:ILE:HG23	1.97	0.47
1:B:419:ALA:HA	1:B:422:THR:HG22	1.96	0.47
1:A:232:PRO:CA	1:A:236:LYS:CG	2.93	0.46
1:A:372:ARG:HD2	1:A:372:ARG:HA	1.64	0.46
1:B:214:LEU:O	1:B:218:LYS:HG3	2.16	0.46
1:B:376:ARG:HD2	1:B:488:PHE:O	2.16	0.46
1:B:328:ARG:O	1:B:332:GLU:HG2	2.16	0.46
1:A:202:GLN:HG3	1:A:270:PHE:H	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:238:ILE:O	1:A:238:ILE:HG22	2.15	0.46
1:A:387:ARG:NH1	1:A:416:TYR:HB2	2.31	0.46
1:B:207:ARG:O	1:B:264:THR:HG21	2.16	0.45
1:B:234:PHE:HD2	1:B:235:PHE:HB2	1.82	0.45
1:B:461:ASP:N	1:B:461:ASP:OD1	2.50	0.45
1:A:432:ALA:HB2	1:A:464:MET:HE1	1.98	0.45
1:B:229:MET:C	1:B:232:PRO:HD2	2.42	0.45
1:A:247:MET:HA	1:A:377:ILE:HD12	1.98	0.45
1:A:419:ALA:HA	1:A:422:THR:HG22	1.98	0.45
1:A:207:ARG:O	1:A:208:TRP:C	2.59	0.45
1:A:229:MET:C	1:A:232:PRO:HD2	2.42	0.45
1:B:420:ASP:HA	1:B:423:ASN:ND2	2.31	0.44
1:A:223:GLU:O	1:A:225:VAL:HG22	2.18	0.44
1:A:329:VAL:O	1:A:333:LEU:HB2	2.17	0.44
1:B:215:VAL:O	1:B:219:LYS:HG2	2.18	0.44
1:B:220:LEU:HD23	1:B:258:LEU:HB3	1.98	0.44
1:B:363:TRP:HA	1:B:484:TRP:CZ3	2.52	0.44
1:A:471:LYS:HD2	1:A:473:VAL:HB	2.00	0.44
1:A:328:ARG:HG2	1:A:329:VAL:N	2.33	0.44
1:B:250:PRO:HD2	1:B:379:ILE:O	2.17	0.44
1:B:306:PHE:CE2	1:B:308:ASP:HB2	2.53	0.44
1:A:226:VAL:CG1	1:A:266:CYS:HA	2.48	0.44
1:B:289:LEU:HA	1:B:292:LEU:HB2	1.99	0.44
1:A:291:ARG:O	1:A:295:GLU:HG2	2.18	0.44
1:A:487:GLU:HG3	1:A:488:PHE:CD2	2.53	0.44
1:A:242:TRP:CD1	1:A:242:TRP:H	2.35	0.44
1:A:378:TYR:CE2	1:A:380:PRO:HB3	2.53	0.44
1:B:375:LYS:HD2	1:B:377:ILE:HG23	2.00	0.44
1:B:207:ARG:HB2	1:A:207:ARG:NH2	2.33	0.43
1:A:273:VAL:O	1:A:307:ILE:HA	2.18	0.43
1:B:274:SER:O	1:B:277:THR:HG22	2.18	0.43
1:B:376:ARG:HH11	1:B:488:PHE:HB3	1.84	0.43
1:B:427:ASP:O	1:B:431:MET:HB3	2.18	0.43
1:A:207:ARG:HD3	1:A:207:ARG:HA	1.56	0.43
1:A:287:GLU:O	1:A:332:GLU:HG2	2.18	0.43
1:A:429:SER:O	1:A:433:MET:HB2	2.17	0.43
1:A:428:ALA:O	1:A:461:ASP:HB2	2.19	0.43
1:A:391:LEU:HD12	1:A:406:LEU:HD22	2.00	0.43
1:A:325:ALA:HA	1:A:328:ARG:HD3	1.99	0.43
1:B:215:VAL:HG13	1:B:216:GLU:CD	2.43	0.43
1:B:234:PHE:CD2	1:B:235:PHE:HB2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:221:LEU:HD13	1:A:262:VAL:HG23	2.01	0.42
1:B:393:ILE:HA	1:B:396:ARG:HD2	2.00	0.42
1:A:195:LEU:HB3	1:A:282:TYR:OH	2.20	0.42
1:A:208:TRP:CZ3	1:A:261:ALA:O	2.73	0.42
1:B:440:LEU:HD23	1:B:440:LEU:HA	1.77	0.42
1:B:378:TYR:HB2	1:B:485:ILE:HG12	2.02	0.42
1:B:239:ARG:O	1:B:239:ARG:CG	2.68	0.42
1:B:220:LEU:HD11	1:B:247:MET:HE2	2.01	0.42
1:A:226:VAL:HG11	1:A:265:GLU:O	2.20	0.41
1:A:226:VAL:HG11	1:A:266:CYS:HA	2.02	0.41
1:B:217:ALA:O	1:B:221:LEU:HB2	2.20	0.41
1:B:291:ARG:O	1:B:295:GLU:HG2	2.19	0.41
1:B:208:TRP:NE1	1:B:221:LEU:HD12	2.34	0.41
1:B:362:PRO:HB2	1:B:484:TRP:CE2	2.55	0.41
1:B:367:GLU:OE2	1:B:367:GLU:N	2.45	0.41
1:A:202:GLN:HG2	1:A:204:PRO:HA	2.03	0.41
1:A:438:GLU:H	1:A:438:GLU:HG2	1.60	0.41
1:A:292:LEU:O	1:A:296:MET:HG3	2.20	0.41
1:A:237:GLY:O	1:A:238:ILE:CB	2.66	0.41
1:B:288:LYS:O	1:B:291:ARG:HB3	2.21	0.41
1:B:242:TRP:CD1	1:B:242:TRP:H	2.38	0.41
1:B:333:LEU:HD12	1:B:333:LEU:HA	1.89	0.41
1:A:226:VAL:HG22	1:A:266:CYS:SG	2.61	0.41
1:A:236:LYS:HD2	1:A:239:ARG:CB	2.51	0.41
1:A:241:PRO:HB2	1:A:354:MET:HE1	2.02	0.41
1:A:415:GLY:O	1:A:471:LYS:HD3	2.21	0.41
1:B:250:PRO:HD3	1:B:378:TYR:HE1	1.86	0.41
1:B:250:PRO:HD3	1:B:378:TYR:CE1	2.57	0.40
1:A:423:ASN:CA	1:A:426:ARG:HE	2.34	0.40
1:B:208:TRP:CE2	1:B:221:LEU:CD1	2.96	0.40
1:B:433:MET:O	1:B:437:ILE:HG13	2.21	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	242/309 (78%)	217 (90%)	23 (10%)	2 (1%)	16	50
1	B	248/309 (80%)	227 (92%)	18 (7%)	3 (1%)	10	40
All	All	490/618 (79%)	444 (91%)	41 (8%)	5 (1%)	12	45

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	238	ILE
1	B	442	PRO
1	A	238	ILE
1	A	301	SER
1	B	285	GLU

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	217/269 (81%)	193 (89%)	24 (11%)	6	25
1	B	223/269 (83%)	192 (86%)	31 (14%)	3	17
All	All	440/538 (82%)	385 (88%)	55 (12%)	4	20

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	192	VAL
1	B	195	LEU
1	B	197	ARG
1	B	203	ASN
1	B	206	VAL
1	B	209	ASP
1	B	214	LEU
1	B	215	VAL

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Mol	Chain	Res	Type
1	B	223	GLU
1	B	225	VAL
1	B	235	PHE
1	B	238	ILE
1	B	248	VAL
1	B	266	CYS
1	B	267	LYS
1	B	273	VAL
1	B	309	GLN
1	B	324	GLU
1	B	334	LEU
1	B	352	MET
1	B	372	ARG
1	B	377	ILE
1	B	391	LEU
1	B	396	ARG
1	B	405	ASP
1	B	426	ARG
1	B	441	THR
1	B	443	GLU
1	B	459	MET
1	B	461	ASP
1	B	473	VAL
1	A	192	VAL
1	A	207	ARG
1	A	208	TRP
1	A	215	VAL
1	A	225	VAL
1	A	229	MET
1	A	233	GLU
1	A	236	LYS
1	A	239	ARG
1	A	240	ARG
1	A	248	VAL
1	A	266	CYS
1	A	273	VAL
1	A	287	GLU
1	A	352	MET
1	A	377	ILE
1	A	391	LEU
1	A	405	ASP
1	A	431	MET

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Mol	Chain	Res	Type
1	A	436	ARG
1	A	437	ILE
1	A	438	GLU
1	A	440	LEU
1	A	461	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	309	GLN
1	B	323	HIS
1	A	309	GLN

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 [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	252/309 (81%)	-1.03	1 (0%) 88 76	24, 80, 224, 394	0
1	B	258/309 (83%)	-1.02	1 (0%) 88 76	25, 83, 229, 351	0
All	All	510/618 (82%)	-1.02	2 (0%) 88 76	24, 82, 229, 394	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	280	SER	3.6
1	B	396	ARG	2.6

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.