



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:17 PM UTC

PDB ID : 3UIU / pdb_00003uiu
Title : Crystal structure of Apo-PKR kinase domain
Authors : Li, F.; Li, S.; Yang, X.; Shen, Y.; Zhang, T.
Deposited on : 2011-11-06
Resolution : 2.90 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

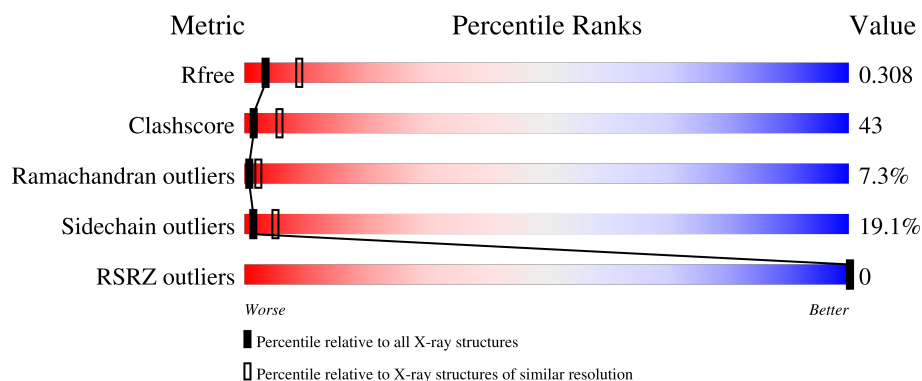
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

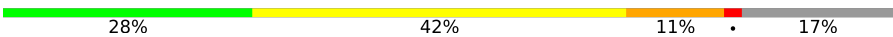
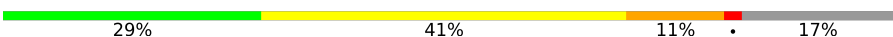
The reported resolution of this entry is 2.90 Å.

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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	306	 28% 42% 11% • 17%
1	B	306	 29% 41% 11% • 17%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4102 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 Interferon-induced, double-stranded RNA-activated protein kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	255	Total	C	N	O	S	0	0	0
			2039	1311	350	372	6			
1	B	255	Total	C	N	O	S	0	0	0
			2039	1311	350	372	6			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	296	ARG	LYS	SEE REMARK 999	UNP P19525
A	552	VAL	-	expression tag	UNP P19525
A	553	LEU	-	expression tag	UNP P19525
A	554	HIS	-	expression tag	UNP P19525
A	555	HIS	-	expression tag	UNP P19525
A	556	HIS	-	expression tag	UNP P19525
A	557	HIS	-	expression tag	UNP P19525
A	558	HIS	-	expression tag	UNP P19525
A	559	HIS	-	expression tag	UNP P19525
B	296	ARG	LYS	SEE REMARK 999	UNP P19525
B	552	VAL	-	expression tag	UNP P19525
B	553	LEU	-	expression tag	UNP P19525
B	554	HIS	-	expression tag	UNP P19525
B	555	HIS	-	expression tag	UNP P19525
B	556	HIS	-	expression tag	UNP P19525
B	557	HIS	-	expression tag	UNP P19525
B	558	HIS	-	expression tag	UNP P19525
B	559	HIS	-	expression tag	UNP P19525

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	13	Total	O	0	0
			13	13		

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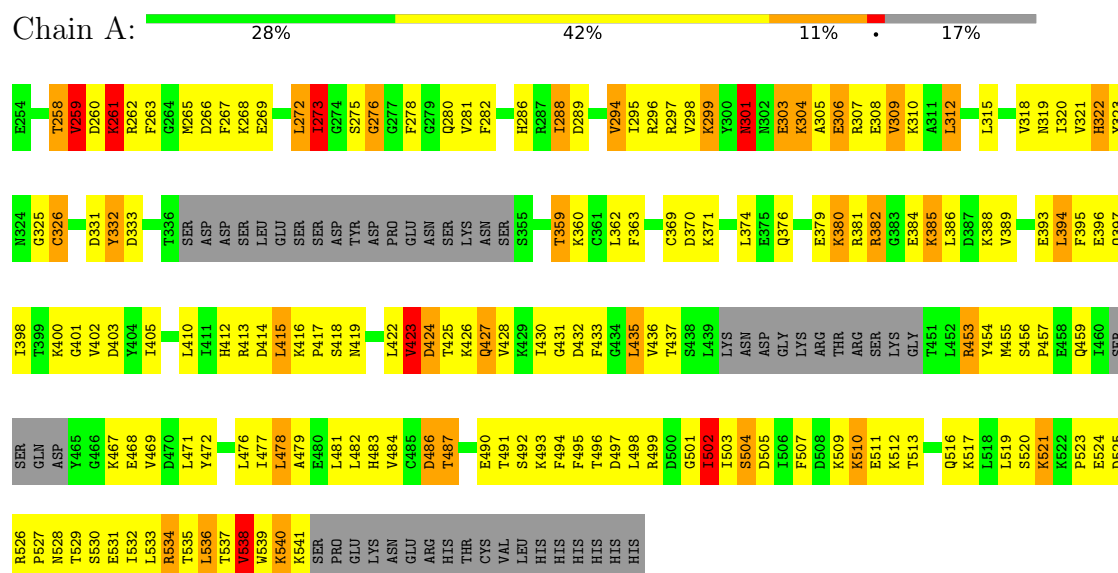
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	11	Total	O	0	0
			11	11		

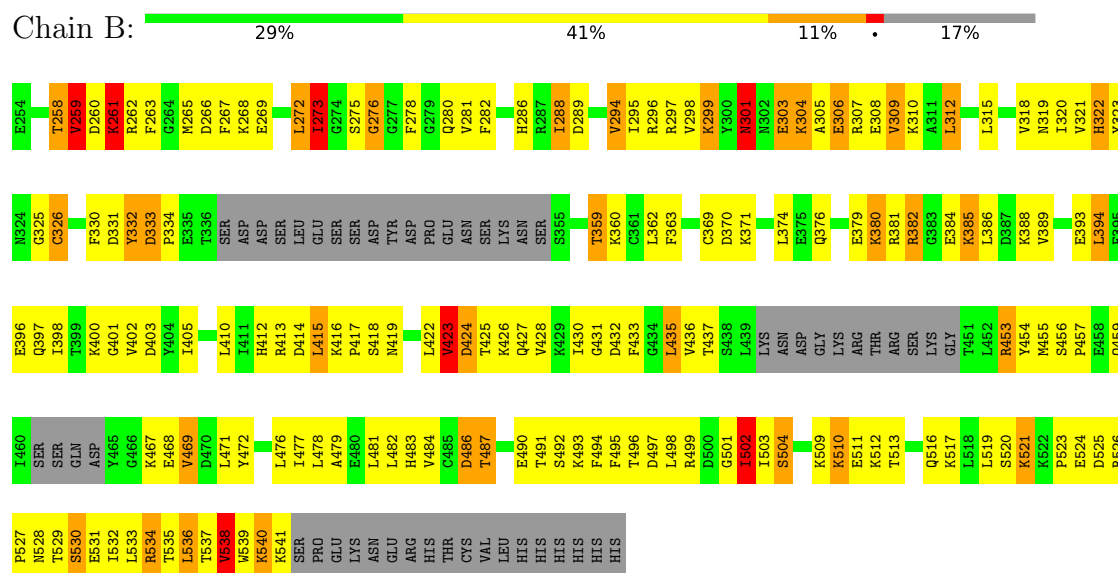
3 Residue-property plots

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: Interferon-induced, double-stranded RNA-activated protein kinase



- Molecule 1: Interferon-induced, double-stranded RNA-activated protein kinase



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 1 2	Depositor
Cell constants a, b, c, α , β , γ	95.41Å 95.41Å 122.02Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	27.80 – 2.90 27.80 – 2.90	Depositor EDS
% Data completeness (in resolution range)	95.7 (27.80-2.90) 95.3 (27.80-2.90)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.61 (at 2.90Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.4_486)	Depositor
R, R_{free}	0.240 , 0.305 0.248 , 0.308	Depositor DCC
R_{free} test set	1418 reflections (10.00%)	wwPDB-VP
Wilson B-factor (Å ²)	88.0	Xtriage
Anisotropy	0.005	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 111.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.490 for -h,-k,l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	4102	wwPDB-VP
Average B, all atoms (Å ²)	97.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.81% 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	0.64	0/2074	1.05	10/2784 (0.4%)
1	B	0.64	0/2074	1.05	9/2784 (0.3%)
All	All	0.64	0/4148	1.05	19/5568 (0.3%)

There are no bond length outliers.

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	304	LYS	N-CA-C	-7.04	106.59	114.62
1	B	304	LYS	N-CA-C	-7.04	106.60	114.62
1	B	309	VAL	N-CA-C	6.43	117.53	111.48
1	A	309	VAL	N-CA-C	6.28	117.39	111.48
1	A	333	ASP	CA-C-N	5.88	125.50	119.56
1	A	333	ASP	C-N-CA	5.88	125.50	119.56
1	B	333	ASP	CA-C-N	5.72	125.34	119.56
1	B	333	ASP	C-N-CA	5.72	125.34	119.56
1	B	322	HIS	N-CA-C	5.55	118.49	110.28
1	A	301	ASN	N-CA-C	5.50	113.29	108.78
1	B	301	ASN	N-CA-C	5.47	113.27	108.78
1	B	331	ASP	N-CA-C	5.46	116.28	108.74
1	A	322	HIS	N-CA-C	5.39	118.26	110.28
1	A	423	VAL	N-CA-C	-5.37	106.46	111.45
1	A	331	ASP	N-CA-C	5.30	116.06	108.74
1	B	423	VAL	N-CA-C	-5.28	106.54	111.45
1	A	326	CYS	N-CA-C	5.21	116.06	108.14
1	B	326	CYS	N-CA-C	5.21	116.05	108.14
1	A	427	GLN	N-CA-C	5.08	116.69	108.26

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	2039	0	2033	175	0
1	B	2039	0	2033	175	0
2	A	13	0	0	0	0
2	B	11	0	0	0	0
All	All	4102	0	4066	349	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 43.

All (349) 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:412:HIS:NE2	1:B:432:ASP:HB3	1.30	1.42
1:A:412:HIS:NE2	1:A:432:ASP:HB3	1.30	1.40
1:B:453:ARG:HG2	1:B:454:TYR:H	1.12	1.08
1:A:453:ARG:HG2	1:A:454:TYR:H	1.13	1.03
1:A:412:HIS:NE2	1:A:432:ASP:CB	2.26	0.98
1:B:412:HIS:NE2	1:B:432:ASP:CB	2.27	0.97
1:B:433:PHE:HA	1:B:436:VAL:HG23	1.53	0.91
1:B:381:ARG:HG3	1:B:384:GLU:OE2	1.72	0.89
1:A:433:PHE:HA	1:A:436:VAL:HG23	1.54	0.89
1:A:381:ARG:HG3	1:A:384:GLU:OE2	1.71	0.89
1:B:301:ASN:HD22	1:B:301:ASN:H	1.26	0.84
1:B:453:ARG:HG2	1:B:454:TYR:N	1.92	0.84
1:B:312:LEU:HA	1:B:315:LEU:HD13	1.59	0.83
1:A:301:ASN:H	1:A:301:ASN:HD22	1.26	0.83
1:A:312:LEU:HA	1:A:315:LEU:HD13	1.57	0.83
1:A:322:HIS:CE1	1:B:322:HIS:CE1	2.65	0.83
1:A:308:GLU:O	1:A:312:LEU:HB2	1.80	0.81
1:A:309:VAL:HG21	1:A:362:LEU:HD21	1.63	0.81
1:A:433:PHE:HA	1:A:436:VAL:CG2	2.11	0.81
1:B:308:GLU:O	1:B:312:LEU:HB2	1.80	0.81
1:B:433:PHE:HA	1:B:436:VAL:CG2	2.11	0.81
1:A:513:THR:O	1:A:517:LYS:HG3	1.80	0.80
1:B:513:THR:O	1:B:517:LYS:HG3	1.81	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:309:VAL:HG21	1:B:362:LEU:HD21	1.62	0.78
1:B:374:LEU:HB3	1:B:417:PRO:HB3	1.65	0.77
1:A:496:THR:HA	1:A:499:ARG:HB2	1.66	0.77
1:B:393:GLU:HA	1:B:393:GLU:OE1	1.85	0.77
1:B:496:THR:HA	1:B:499:ARG:HB2	1.66	0.76
1:A:261:LYS:H	1:A:261:LYS:HD2	1.49	0.76
1:A:453:ARG:CG	1:A:454:TYR:H	1.97	0.76
1:A:374:LEU:HB3	1:A:417:PRO:HB3	1.66	0.76
1:B:455:MET:H	1:B:499:ARG:HH22	1.34	0.76
1:B:261:LYS:H	1:B:261:LYS:HD2	1.51	0.76
1:A:422:LEU:HD23	1:A:428:VAL:HG12	1.68	0.75
1:A:412:HIS:CE1	1:A:432:ASP:HB3	2.20	0.75
1:A:455:MET:H	1:A:499:ARG:HH22	1.34	0.75
1:B:422:LEU:HD23	1:B:428:VAL:HG12	1.67	0.74
1:A:393:GLU:OE1	1:A:393:GLU:HA	1.85	0.74
1:A:525:ASP:O	1:A:527:PRO:HD3	1.90	0.72
1:A:453:ARG:HG2	1:A:454:TYR:N	1.93	0.71
1:B:471:LEU:HD21	1:B:528:ASN:HA	1.73	0.71
1:A:273:ILE:HG13	1:A:281:VAL:O	1.90	0.71
1:B:412:HIS:CE1	1:B:432:ASP:HB3	2.21	0.71
1:A:510:LYS:HD2	1:A:511:GLU:H	1.56	0.70
1:A:534:ARG:HG3	1:A:535:THR:N	2.07	0.70
1:B:510:LYS:HD2	1:B:511:GLU:H	1.56	0.70
1:B:273:ILE:HG13	1:B:281:VAL:O	1.91	0.70
1:B:525:ASP:O	1:B:527:PRO:HD3	1.91	0.69
1:A:471:LEU:HD21	1:A:528:ASN:HA	1.73	0.69
1:B:534:ARG:HG3	1:B:535:THR:N	2.07	0.69
1:A:510:LYS:CD	1:A:511:GLU:H	2.07	0.68
1:A:301:ASN:HD22	1:A:301:ASN:N	1.92	0.68
1:A:385:LYS:HD2	1:A:385:LYS:H	1.57	0.67
1:B:385:LYS:H	1:B:385:LYS:HD2	1.57	0.67
1:A:306:GLU:HB3	1:A:310:LYS:HG3	1.77	0.67
1:A:512:LYS:O	1:A:516:GLN:HG2	1.95	0.67
1:B:453:ARG:CG	1:B:454:TYR:H	1.96	0.67
1:A:503:ILE:O	1:A:504:SER:O	2.13	0.66
1:B:512:LYS:O	1:B:516:GLN:HG2	1.95	0.66
1:A:396:GLU:HG2	1:A:400:LYS:HE2	1.78	0.66
1:B:503:ILE:O	1:B:504:SER:O	2.13	0.66
1:A:301:ASN:H	1:A:301:ASN:ND2	1.93	0.66
1:B:510:LYS:CD	1:B:511:GLU:H	2.07	0.66
1:B:295:ILE:N	1:B:295:ILE:HD12	2.13	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:306:GLU:HB3	1:B:310:LYS:HG3	1.78	0.64
1:A:281:VAL:HG22	1:A:296:ARG:HG2	1.79	0.64
1:A:320:ILE:HG23	1:A:433:PHE:HZ	1.64	0.64
1:B:301:ASN:H	1:B:301:ASN:ND2	1.93	0.63
1:B:304:LYS:O	1:B:307:ARG:HB3	1.99	0.63
1:B:320:ILE:HG23	1:B:433:PHE:HZ	1.63	0.63
1:A:453:ARG:HG2	1:A:499:ARG:HH21	1.64	0.63
1:B:453:ARG:HG2	1:B:499:ARG:HH21	1.64	0.63
1:A:295:ILE:HD12	1:A:295:ILE:N	2.13	0.63
1:A:260:ASP:HB3	1:A:263:PHE:HB3	1.81	0.63
1:B:281:VAL:HG22	1:B:296:ARG:HG2	1.80	0.63
1:B:396:GLU:HG2	1:B:400:LYS:HE2	1.80	0.62
1:A:401:GLY:O	1:A:405:ILE:HG13	1.99	0.61
1:B:503:ILE:HG21	1:B:512:LYS:HG2	1.82	0.61
1:B:260:ASP:HB3	1:B:263:PHE:HB3	1.83	0.61
1:B:401:GLY:O	1:B:405:ILE:HG13	2.01	0.61
1:A:304:LYS:O	1:A:307:ARG:HB3	1.99	0.60
1:A:503:ILE:HG21	1:A:512:LYS:HG2	1.83	0.60
1:A:315:LEU:H	1:A:315:LEU:HD12	1.67	0.60
1:B:503:ILE:HD13	1:B:516:GLN:HB3	1.84	0.60
1:B:537:THR:C	1:B:539:TRP:H	2.09	0.60
1:A:272:LEU:O	1:A:273:ILE:HG23	2.02	0.60
1:A:503:ILE:HD13	1:A:516:GLN:HB3	1.84	0.59
1:B:319:ASN:C	1:B:320:ILE:HD12	2.26	0.59
1:A:423:VAL:HG13	1:A:427:GLN:O	2.03	0.59
1:B:312:LEU:CA	1:B:315:LEU:HD13	2.32	0.59
1:A:454:TYR:HA	1:A:476:LEU:HD12	1.85	0.59
1:B:454:TYR:HA	1:B:476:LEU:HD12	1.84	0.59
1:B:510:LYS:HD3	1:B:511:GLU:HG3	1.85	0.59
1:A:312:LEU:CA	1:A:315:LEU:HD13	2.31	0.59
1:A:497:ASP:O	1:A:502:ILE:HG13	2.03	0.59
1:B:301:ASN:HD22	1:B:301:ASN:N	1.92	0.59
1:B:497:ASP:O	1:B:502:ILE:HG13	2.03	0.59
1:B:315:LEU:HD12	1:B:315:LEU:H	1.69	0.58
1:A:319:ASN:C	1:A:320:ILE:HD12	2.29	0.58
1:A:326:CYS:HB2	1:A:363:PHE:O	2.03	0.58
1:B:294:VAL:C	1:B:295:ILE:HD12	2.29	0.58
1:B:326:CYS:HB2	1:B:363:PHE:O	2.04	0.58
1:A:537:THR:C	1:A:539:TRP:H	2.10	0.57
1:B:272:LEU:O	1:B:273:ILE:HG23	2.02	0.57
1:B:423:VAL:HG13	1:B:427:GLN:O	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:381:ARG:CZ	1:B:484:VAL:HG12	2.34	0.57
1:A:294:VAL:C	1:A:295:ILE:HD12	2.29	0.57
1:A:510:LYS:HD3	1:A:511:GLU:HG3	1.85	0.57
1:A:413:ARG:NH2	1:A:437:THR:HB	2.20	0.57
1:A:537:THR:C	1:A:539:TRP:N	2.63	0.57
1:B:472:TYR:HB2	1:B:526:ARG:NH1	2.20	0.57
1:A:394:LEU:O	1:A:398:ILE:HD12	2.05	0.57
1:B:413:ARG:NH2	1:B:437:THR:HB	2.20	0.57
1:A:381:ARG:HG3	1:A:384:GLU:CD	2.30	0.57
1:A:258:THR:OG1	1:A:259:VAL:N	2.38	0.56
1:A:381:ARG:CZ	1:A:484:VAL:HG12	2.34	0.56
1:A:472:TYR:HB2	1:A:526:ARG:NH1	2.20	0.56
1:B:419:ASN:CG	1:B:432:ASP:HB2	2.30	0.56
1:B:457:PRO:HD3	1:B:526:ARG:HH22	1.70	0.56
1:A:419:ASN:CG	1:A:432:ASP:HB2	2.31	0.56
1:A:510:LYS:CD	1:A:511:GLU:HG3	2.35	0.56
1:A:523:PRO:O	1:A:526:ARG:HB2	2.05	0.56
1:B:510:LYS:CD	1:B:511:GLU:HG3	2.35	0.56
1:B:394:LEU:O	1:B:398:ILE:HD12	2.06	0.56
1:B:309:VAL:HG12	1:B:310:LYS:N	2.21	0.56
1:A:457:PRO:HD3	1:A:526:ARG:HH22	1.70	0.56
1:B:456:SER:HB3	1:B:526:ARG:HH22	1.70	0.56
1:B:483:HIS:HD2	1:B:494:PHE:CE2	2.24	0.56
1:A:386:LEU:H	1:A:386:LEU:HD12	1.71	0.55
1:A:483:HIS:HD2	1:A:494:PHE:CE2	2.24	0.55
1:B:433:PHE:HD2	1:B:436:VAL:HG21	1.71	0.55
1:B:503:ILE:CG2	1:B:512:LYS:HG2	2.37	0.55
1:B:523:PRO:O	1:B:526:ARG:HB2	2.05	0.55
1:A:456:SER:HB3	1:A:457:PRO:HD3	1.87	0.55
1:B:456:SER:HB3	1:B:457:PRO:HD3	1.87	0.55
1:A:323:TYR:CZ	1:A:325:GLY:HA2	2.41	0.55
1:B:381:ARG:HG3	1:B:384:GLU:CD	2.30	0.55
1:A:433:PHE:HD2	1:A:436:VAL:HG21	1.71	0.55
1:B:400:LYS:O	1:B:403:ASP:HB3	2.07	0.55
1:B:491:THR:O	1:B:495:PHE:HB2	2.07	0.55
1:A:309:VAL:HG12	1:A:310:LYS:N	2.21	0.55
1:B:258:THR:OG1	1:B:259:VAL:N	2.38	0.55
1:A:413:ARG:HH21	1:A:437:THR:HB	1.72	0.55
1:A:456:SER:HB3	1:A:526:ARG:HH22	1.70	0.55
1:A:491:THR:O	1:A:495:PHE:HB2	2.07	0.55
1:A:519:LEU:O	1:A:520:SER:C	2.49	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:537:THR:C	1:B:539:TRP:N	2.62	0.55
1:A:413:ARG:HD3	1:A:435:LEU:O	2.07	0.54
1:B:413:ARG:HH21	1:B:437:THR:HB	1.72	0.54
1:B:258:THR:HB	1:B:297:ARG:NH1	2.22	0.54
1:B:413:ARG:HD3	1:B:435:LEU:O	2.07	0.54
1:B:323:TYR:CZ	1:B:325:GLY:HA2	2.43	0.54
1:A:400:LYS:O	1:A:403:ASP:HB3	2.08	0.54
1:B:386:LEU:HD12	1:B:386:LEU:H	1.71	0.54
1:B:261:LYS:HD2	1:B:261:LYS:N	2.21	0.54
1:B:374:LEU:HB3	1:B:417:PRO:CB	2.37	0.54
1:B:503:ILE:O	1:B:503:ILE:HG22	2.07	0.54
1:B:519:LEU:O	1:B:520:SER:C	2.48	0.53
1:B:398:ILE:HG23	1:B:430:ILE:HD11	1.90	0.53
1:B:454:TYR:HA	1:B:476:LEU:CD1	2.39	0.53
1:A:261:LYS:HD2	1:A:261:LYS:N	2.20	0.53
1:A:503:ILE:CG2	1:A:512:LYS:HG2	2.37	0.53
1:A:487:THR:HG23	1:A:490:GLU:HB2	1.91	0.53
1:A:258:THR:HB	1:A:297:ARG:NH1	2.23	0.53
1:A:306:GLU:OE2	1:A:306:GLU:N	2.41	0.53
1:B:306:GLU:OE2	1:B:306:GLU:N	2.42	0.53
1:A:402:VAL:HG12	1:A:529:THR:HG21	1.92	0.52
1:A:513:THR:C	1:A:517:LYS:HZ3	2.18	0.52
1:B:402:VAL:HG12	1:B:529:THR:HG21	1.90	0.52
1:A:423:VAL:CG2	1:A:424:ASP:N	2.72	0.52
1:A:398:ILE:HG23	1:A:430:ILE:HD11	1.90	0.52
1:A:410:LEU:HD23	1:A:437:THR:O	2.09	0.52
1:A:454:TYR:HA	1:A:476:LEU:CD1	2.39	0.52
1:B:487:THR:HG23	1:B:490:GLU:HB2	1.91	0.52
1:A:503:ILE:O	1:A:503:ILE:HG22	2.08	0.52
1:B:410:LEU:HD23	1:B:437:THR:O	2.10	0.52
1:A:412:HIS:HB3	1:A:415:LEU:HD12	1.92	0.52
1:B:386:LEU:HG	1:B:484:VAL:HG22	1.92	0.52
1:B:288:ILE:HD12	1:B:288:ILE:N	2.25	0.51
1:A:261:LYS:O	1:A:262:ARG:C	2.53	0.51
1:B:278:PHE:O	1:B:298:VAL:HG23	2.10	0.51
1:B:423:VAL:CG2	1:B:424:ASP:N	2.72	0.51
1:A:288:ILE:HD12	1:A:288:ILE:N	2.26	0.51
1:B:412:HIS:HB3	1:B:415:LEU:HD12	1.91	0.51
1:B:483:HIS:HB3	1:B:494:PHE:CZ	2.46	0.51
1:A:386:LEU:HG	1:A:484:VAL:HG22	1.92	0.51
1:B:513:THR:C	1:B:517:LYS:HZ3	2.19	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:397:GLN:O	1:A:400:LYS:HB2	2.10	0.51
1:B:261:LYS:O	1:B:262:ARG:C	2.53	0.51
1:B:369:CYS:HB3	1:B:422:LEU:O	2.11	0.51
1:B:389:VAL:HA	1:B:540:LYS:HZ1	1.76	0.51
1:A:369:CYS:HB3	1:A:422:LEU:O	2.11	0.50
1:A:296:ARG:HH12	1:A:433:PHE:H	1.58	0.50
1:A:312:LEU:HD22	1:A:323:TYR:HB2	1.94	0.50
1:B:315:LEU:HD12	1:B:315:LEU:N	2.26	0.50
1:B:503:ILE:C	1:B:504:SER:O	2.54	0.50
1:A:278:PHE:O	1:A:298:VAL:HG23	2.11	0.50
1:B:388:LYS:O	1:B:388:LYS:HG2	2.12	0.50
1:B:397:GLN:O	1:B:400:LYS:HB2	2.11	0.50
1:A:389:VAL:HA	1:A:540:LYS:HZ1	1.76	0.50
1:A:497:ASP:HA	1:A:502:ILE:CD1	2.42	0.50
1:A:388:LYS:O	1:A:388:LYS:HG2	2.12	0.50
1:B:312:LEU:HD22	1:B:323:TYR:HB2	1.94	0.50
1:B:497:ASP:HA	1:B:502:ILE:CD1	2.42	0.50
1:A:483:HIS:HB3	1:A:494:PHE:CZ	2.46	0.49
1:B:296:ARG:HH12	1:B:433:PHE:H	1.58	0.49
1:B:286:HIS:HB3	1:B:289:ASP:OD1	2.12	0.49
1:B:424:ASP:OD1	1:B:425:THR:HG23	2.12	0.49
1:A:456:SER:HB3	1:A:526:ARG:NH2	2.28	0.49
1:A:374:LEU:HB3	1:A:417:PRO:CB	2.38	0.49
1:B:379:GLU:HG3	1:B:382:ARG:NH1	2.28	0.49
1:A:424:ASP:OD1	1:A:425:THR:HG23	2.12	0.48
1:A:503:ILE:HG22	1:A:504:SER:O	2.13	0.48
1:A:503:ILE:C	1:A:504:SER:O	2.54	0.48
1:B:273:ILE:HD11	1:B:282:PHE:O	2.13	0.48
1:B:381:ARG:CG	1:B:384:GLU:HB2	2.44	0.48
1:A:381:ARG:O	1:A:381:ARG:HG2	2.12	0.48
1:B:312:LEU:HA	1:B:315:LEU:CD1	2.37	0.48
1:A:273:ILE:HD11	1:A:282:PHE:O	2.12	0.48
1:B:503:ILE:HG22	1:B:504:SER:O	2.13	0.48
1:A:381:ARG:CG	1:A:384:GLU:HB2	2.43	0.48
1:A:379:GLU:HA	1:A:382:ARG:HD3	1.96	0.48
1:A:541:LYS:NZ	1:A:541:LYS:HB3	2.29	0.48
1:A:379:GLU:HG3	1:A:382:ARG:NH1	2.28	0.48
1:A:528:ASN:N	1:A:531:GLU:OE2	2.46	0.48
1:B:528:ASN:N	1:B:531:GLU:OE2	2.47	0.48
1:B:534:ARG:O	1:B:538:VAL:HG23	2.14	0.48
1:A:312:LEU:HA	1:A:315:LEU:CD1	2.36	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:286:HIS:HB3	1:A:289:ASP:OD1	2.14	0.47
1:A:315:LEU:HD12	1:A:315:LEU:N	2.28	0.47
1:B:456:SER:HB3	1:B:526:ARG:NH2	2.28	0.47
1:A:490:GLU:O	1:A:493:LYS:N	2.47	0.47
1:B:381:ARG:HG2	1:B:381:ARG:O	2.13	0.47
1:B:493:LYS:O	1:B:494:PHE:C	2.57	0.47
1:B:490:GLU:O	1:B:493:LYS:N	2.48	0.47
1:B:521:LYS:O	1:B:523:PRO:HD3	2.14	0.47
1:A:493:LYS:O	1:A:494:PHE:C	2.57	0.47
1:B:541:LYS:HB3	1:B:541:LYS:NZ	2.29	0.47
1:A:534:ARG:O	1:A:538:VAL:HG23	2.14	0.47
1:A:268:LYS:HE3	1:A:269:GLU:OE2	2.14	0.47
1:B:268:LYS:HE3	1:B:269:GLU:OE2	2.15	0.47
1:B:381:ARG:HG2	1:B:384:GLU:HB2	1.98	0.46
1:B:482:LEU:HD23	1:B:482:LEU:HA	1.73	0.46
1:A:521:LYS:O	1:A:523:PRO:HD3	2.14	0.46
1:B:379:GLU:HA	1:B:382:ARG:HD3	1.96	0.46
1:A:258:THR:HG22	1:A:282:PHE:CE2	2.51	0.46
1:B:479:ALA:C	1:B:481:LEU:H	2.23	0.46
1:A:263:PHE:O	1:A:267:PHE:HB2	2.15	0.46
1:A:299:LYS:HB3	1:A:299:LYS:HE2	1.82	0.46
1:A:381:ARG:HG2	1:A:384:GLU:HB2	1.98	0.46
1:A:386:LEU:HD21	1:A:483:HIS:HA	1.97	0.46
1:B:258:THR:HG22	1:B:282:PHE:CE2	2.51	0.46
1:A:412:HIS:CD2	1:A:432:ASP:O	2.69	0.46
1:A:479:ALA:C	1:A:481:LEU:H	2.23	0.46
1:A:261:LYS:N	1:A:261:LYS:CD	2.79	0.45
1:A:413:ARG:HD2	1:A:437:THR:HG22	1.97	0.45
1:A:410:LEU:HD23	1:A:437:THR:C	2.42	0.45
1:B:433:PHE:HA	1:B:436:VAL:HG21	1.96	0.45
1:A:376:GLN:O	1:A:380:LYS:HB2	2.17	0.45
1:A:413:ARG:NH1	1:A:435:LEU:HD22	2.31	0.45
1:B:263:PHE:O	1:B:267:PHE:HB2	2.15	0.45
1:B:374:LEU:HD12	1:B:374:LEU:HA	1.74	0.45
1:B:295:ILE:N	1:B:295:ILE:CD1	2.79	0.45
1:B:376:GLN:O	1:B:380:LYS:HB2	2.17	0.45
1:B:386:LEU:HD21	1:B:483:HIS:HA	1.97	0.45
1:B:412:HIS:CD2	1:B:432:ASP:O	2.69	0.45
1:B:528:ASN:OD1	1:B:528:ASN:C	2.60	0.45
1:A:494:PHE:O	1:A:498:LEU:HG	2.16	0.45
1:B:410:LEU:HD23	1:B:437:THR:C	2.42	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:413:ARG:NH1	1:B:435:LEU:HD22	2.32	0.45
1:B:494:PHE:O	1:B:498:LEU:HG	2.16	0.45
1:A:359:THR:HB	1:A:360:LYS:H	1.59	0.45
1:A:535:THR:O	1:A:536:LEU:C	2.60	0.45
1:A:455:MET:N	1:A:499:ARG:HH22	2.10	0.44
1:A:482:LEU:HD23	1:A:482:LEU:HA	1.71	0.44
1:B:413:ARG:HD2	1:B:437:THR:HG22	1.98	0.44
1:A:275:SER:OG	1:A:280:GLN:HG3	2.18	0.44
1:B:275:SER:OG	1:B:280:GLN:HG3	2.18	0.44
1:B:381:ARG:CZ	1:B:484:VAL:CG1	2.96	0.44
1:A:528:ASN:C	1:A:528:ASN:OD1	2.60	0.44
1:B:260:ASP:HB3	1:B:263:PHE:CB	2.48	0.44
1:B:261:LYS:N	1:B:261:LYS:CD	2.80	0.44
1:B:535:THR:O	1:B:536:LEU:C	2.61	0.44
1:A:423:VAL:HG22	1:A:424:ASP:N	2.33	0.44
1:B:423:VAL:HG22	1:B:424:ASP:N	2.33	0.43
1:B:453:ARG:CG	1:B:454:TYR:N	2.66	0.43
1:A:385:LYS:H	1:A:385:LYS:CD	2.28	0.43
1:A:389:VAL:HA	1:A:540:LYS:NZ	2.32	0.43
1:A:505:ASP:C	1:A:507:PHE:N	2.75	0.43
1:A:278:PHE:CD1	1:A:278:PHE:N	2.87	0.43
1:A:295:ILE:N	1:A:295:ILE:CD1	2.80	0.43
1:B:389:VAL:HA	1:B:540:LYS:NZ	2.33	0.43
1:B:476:LEU:O	1:B:479:ALA:HB3	2.18	0.43
1:A:433:PHE:HA	1:A:436:VAL:HG21	1.96	0.43
1:A:398:ILE:HG13	1:A:428:VAL:HG21	2.00	0.43
1:A:426:LYS:C	1:A:427:GLN:HG2	2.43	0.43
1:B:398:ILE:HG13	1:B:428:VAL:HG21	2.01	0.43
1:B:523:PRO:HB2	1:B:524:GLU:OE2	2.19	0.43
1:B:469:VAL:HG22	1:B:469:VAL:O	2.18	0.42
1:A:381:ARG:CZ	1:A:484:VAL:CG1	2.96	0.42
1:B:333:ASP:HA	1:B:334:PRO:HD2	1.88	0.42
1:A:275:SER:C	1:A:276:GLY:O	2.61	0.42
1:B:278:PHE:N	1:B:278:PHE:CD1	2.87	0.42
1:B:486:ASP:N	1:B:486:ASP:OD2	2.52	0.42
1:B:509:LYS:O	1:B:510:LYS:C	2.62	0.42
1:A:509:LYS:O	1:A:510:LYS:C	2.62	0.42
1:B:275:SER:C	1:B:276:GLY:O	2.62	0.42
1:A:476:LEU:O	1:A:479:ALA:HB3	2.19	0.42
1:A:374:LEU:HD12	1:A:374:LEU:HA	1.75	0.42
1:A:435:LEU:HD23	1:A:435:LEU:HA	1.93	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:320:ILE:HG23	1:B:433:PHE:CZ	2.50	0.42
1:B:359:THR:HB	1:B:360:LYS:H	1.59	0.42
1:A:385:LYS:HD2	1:A:385:LYS:N	2.30	0.42
1:A:523:PRO:HB2	1:A:524:GLU:OE2	2.19	0.42
1:B:319:ASN:O	1:B:320:ILE:HD12	2.19	0.42
1:B:493:LYS:O	1:B:496:THR:N	2.52	0.42
1:B:530:SER:O	1:B:531:GLU:C	2.63	0.42
1:A:260:ASP:HB3	1:A:263:PHE:CB	2.47	0.41
1:B:426:LYS:C	1:B:427:GLN:HG2	2.44	0.41
1:B:455:MET:N	1:B:499:ARG:HH22	2.09	0.41
1:A:315:LEU:H	1:A:315:LEU:CD1	2.31	0.41
1:A:305:ALA:HB1	1:A:362:LEU:HD22	2.02	0.41
1:A:320:ILE:HG23	1:A:433:PHE:CZ	2.50	0.41
1:A:326:CYS:CB	1:A:363:PHE:O	2.69	0.41
1:A:490:GLU:C	1:A:492:SER:N	2.78	0.41
1:A:487:THR:HG23	1:A:490:GLU:CB	2.49	0.41
1:B:479:ALA:O	1:B:481:LEU:N	2.53	0.41
1:B:288:ILE:HD12	1:B:288:ILE:H	1.86	0.41
1:B:497:ASP:HA	1:B:502:ILE:HD12	2.02	0.41
1:A:479:ALA:O	1:A:481:LEU:N	2.54	0.41
1:A:486:ASP:OD2	1:A:486:ASP:N	2.52	0.41
1:B:305:ALA:HB1	1:B:362:LEU:HD22	2.02	0.41
1:B:491:THR:O	1:B:495:PHE:CD1	2.74	0.41
1:A:477:ILE:O	1:A:481:LEU:HG	2.20	0.41
1:B:330:PHE:CD2	1:B:359:THR:O	2.74	0.41
1:A:479:ALA:C	1:A:481:LEU:N	2.80	0.40
1:A:497:ASP:HA	1:A:502:ILE:HD12	2.02	0.40
1:A:497:ASP:HA	1:A:502:ILE:HG13	2.03	0.40
1:A:535:THR:HG22	1:A:539:TRP:NE1	2.36	0.40
1:B:371:LYS:HG3	1:B:424:ASP:HA	2.03	0.40
1:B:483:HIS:CD2	1:B:494:PHE:CE2	3.08	0.40
1:B:490:GLU:C	1:B:492:SER:N	2.78	0.40
1:B:535:THR:HG22	1:B:539:TRP:NE1	2.36	0.40
1:A:395:PHE:CE2	1:A:478:LEU:HG	2.56	0.40
1:B:299:LYS:HE2	1:B:299:LYS:HB3	1.82	0.40
1:B:479:ALA:C	1:B:481:LEU:N	2.79	0.40
1:A:371:LYS:HG3	1:A:424:ASP:HA	2.03	0.40
1:A:423:VAL:HG22	1:A:424:ASP:H	1.87	0.40
1:B:477:ILE:O	1:B:481:LEU:HG	2.20	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	247/306 (81%)	175 (71%)	54 (22%)	18 (7%)	1	2
1	B	247/306 (81%)	175 (71%)	54 (22%)	18 (7%)	1	2
All	All	494/612 (81%)	350 (71%)	108 (22%)	36 (7%)	1	2

All (36) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	504	SER
1	A	540	LYS
1	B	504	SER
1	B	540	LYS
1	A	261	LYS
1	A	303	GLU
1	A	414	ASP
1	A	424	ASP
1	A	467	LYS
1	A	538	VAL
1	B	261	LYS
1	B	303	GLU
1	B	414	ASP
1	B	424	ASP
1	B	467	LYS
1	B	538	VAL
1	A	273	ILE
1	B	273	ILE
1	A	259	VAL
1	A	332	TYR
1	A	435	LEU
1	A	459	GLN
1	A	530	SER
1	B	259	VAL
1	B	435	LEU

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Mol	Chain	Res	Type
1	B	459	GLN
1	B	530	SER
1	A	501	GLY
1	B	332	TYR
1	B	501	GLY
1	A	276	GLY
1	B	276	GLY
1	A	431	GLY
1	B	431	GLY
1	B	502	ILE
1	A	502	ILE

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	215/280 (77%)	174 (81%)	41 (19%)	1	5
1	B	215/280 (77%)	174 (81%)	41 (19%)	1	5
All	All	430/560 (77%)	348 (81%)	82 (19%)	1	5

All (82) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	258	THR
1	A	259	VAL
1	A	261	LYS
1	A	265	MET
1	A	266	ASP
1	A	272	LEU
1	A	273	ILE
1	A	288	ILE
1	A	294	VAL
1	A	299	LYS
1	A	301	ASN
1	A	303	GLU

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Mol	Chain	Res	Type
1	A	306	GLU
1	A	312	LEU
1	A	318	VAL
1	A	321	VAL
1	A	332	TYR
1	A	359	THR
1	A	370	ASP
1	A	380	LYS
1	A	382	ARG
1	A	385	LYS
1	A	394	LEU
1	A	415	LEU
1	A	416	LYS
1	A	418	SER
1	A	423	VAL
1	A	453	ARG
1	A	468	GLU
1	A	469	VAL
1	A	478	LEU
1	A	486	ASP
1	A	487	THR
1	A	502	ILE
1	A	510	LYS
1	A	521	LYS
1	A	532	ILE
1	A	533	LEU
1	A	534	ARG
1	A	536	LEU
1	A	538	VAL
1	B	258	THR
1	B	259	VAL
1	B	261	LYS
1	B	265	MET
1	B	266	ASP
1	B	272	LEU
1	B	273	ILE
1	B	288	ILE
1	B	294	VAL
1	B	299	LYS
1	B	301	ASN
1	B	303	GLU
1	B	306	GLU

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Mol	Chain	Res	Type
1	B	312	LEU
1	B	318	VAL
1	B	321	VAL
1	B	332	TYR
1	B	359	THR
1	B	370	ASP
1	B	380	LYS
1	B	382	ARG
1	B	385	LYS
1	B	394	LEU
1	B	415	LEU
1	B	416	LYS
1	B	418	SER
1	B	423	VAL
1	B	453	ARG
1	B	468	GLU
1	B	469	VAL
1	B	478	LEU
1	B	486	ASP
1	B	487	THR
1	B	502	ILE
1	B	510	LYS
1	B	521	LYS
1	B	532	ILE
1	B	533	LEU
1	B	534	ARG
1	B	536	LEU
1	B	538	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	301	ASN
1	A	322	HIS
1	A	406	HIS
1	A	419	ASN
1	A	427	GLN
1	A	483	HIS
1	B	301	ASN
1	B	322	HIS
1	B	406	HIS
1	B	419	ASN

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Mol	Chain	Res	Type
1	B	427	GLN
1	B	483	HIS

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	255/306 (83%)	-1.14	0 100 100	40, 98, 133, 146	0
1	B	255/306 (83%)	-1.15	0 100 100	40, 98, 133, 146	0
All	All	510/612 (83%)	-1.14	0 100 100	40, 98, 133, 146	0

There are no RSRZ outliers to report.

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.