



Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 05:20 am BST

PDB ID : 4LK2
Title : Crystal structure of RNA splicing effector Prp5
Authors : Zhang, Z.-M.; Li, J.; Yang, F.; Xu, Y.; Zhou, J.
Deposited on : 2013-07-05
Resolution : 2.12 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.11
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

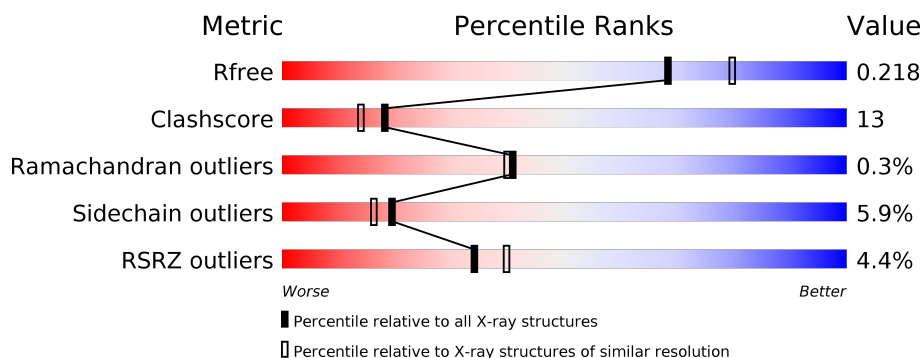
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.12 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}	130704	6241 (2.14-2.10)
Clashscore	141614	6778 (2.14-2.10)
Ramachandran outliers	138981	6705 (2.14-2.10)
Sidechain outliers	138945	6706 (2.14-2.10)
RSRZ outliers	127900	6112 (2.14-2.10)

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 on 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	493	<div> <div>3%</div> <div> <div></div> <div>66%</div> <div>23%</div> <div>• 10%</div> </div> </div>
1	B	493	<div> <div>4%</div> <div> <div></div> <div>65%</div> <div>21%</div> <div>• 12%</div> </div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7012 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 Pre-mRNA-processing ATP-dependent RNA helicase PRP5.

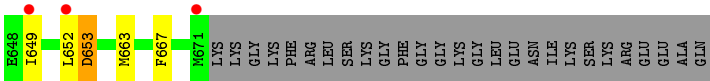
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	444	Total	C	N	O	S	0	5	0
			3436	2175	591	648	22			
1	B	436	Total	C	N	O	S	0	1	0
			3338	2114	571	632	21			

- Molecule 2 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Ni	0	0
			1	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	109	Total	O	0	0
			109	109		
3	B	128	Total	O	0	0
			128	128		



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	87.16 Å 86.08 Å 127.99 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.88 – 2.12 38.88 – 2.05	Depositor EDS
% Data completeness (in resolution range)	93.1 (38.88-2.12) 97.3 (38.88-2.05)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.98 (at 2.05 Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.2_432)	Depositor
R, R_{free}	0.212 , 0.255 0.208 , 0.218	Depositor DCC
R_{free} test set	2946 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	33.3	Xtriage
Anisotropy	0.753	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 56.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.033 for k,h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7012	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.47% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NI

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	0.53	1/3502 (0.0%)	0.63	3/4728 (0.1%)
1	B	0.39	0/3388	0.56	0/4576
All	All	0.46	1/6890 (0.0%)	0.60	3/9304 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	271	THR	C-N	20.20	1.80	1.34

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	271	THR	O-C-N	-18.60	92.94	122.70
1	A	271	THR	CA-C-N	6.33	131.12	117.20
1	A	273	LYS	N-CA-C	5.46	125.75	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	3436	0	3485	93	0
1	B	3338	0	3371	90	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	1	0	0	0	0
3	A	109	0	0	4	0
3	B	128	0	0	5	0
All	All	7012	0	6856	183	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 13.

All (183) 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:A:271:THR:C	1:A:273:LYS:N	1.80	1.32
1:A:485:ILE:H	1:A:656:GLN:HE22	1.03	0.94
1:A:484:ARG:HD3	1:A:626:ILE:HD11	1.51	0.91
1:B:555:ILE:HD11	1:B:564:ARG:HA	1.58	0.86
1:A:560:PRO:HG2	1:A:563:GLU:HG2	1.58	0.85
1:A:256:LYS:HG3	1:A:258:SER:H	1.43	0.83
1:B:449:PHE:CE2	1:B:454:ARG:HG2	2.13	0.83
1:B:449:PHE:CZ	1:B:454:ARG:HG2	2.12	0.83
1:B:484[A]:ARG:HH11	1:B:484[A]:ARG:HG2	1.46	0.80
1:B:406:THR:HG21	1:B:435:THR:HG22	1.61	0.79
1:B:526:ALA:H	1:B:576:ASN:ND2	1.80	0.78
1:B:569:GLU:HG3	1:B:573:ARG:NH1	1.98	0.77
1:A:485:ILE:H	1:A:656:GLN:NE2	1.80	0.76
1:B:236:LEU:HD23	1:B:253:PRO:HG2	1.68	0.74
1:B:480:LYS:HE2	1:B:482:LYS:NZ	2.01	0.74
1:A:291[A]:MET:HG2	1:A:313:PRO:HG3	1.68	0.74
1:A:658:LYS:O	1:A:658:LYS:HD2	1.87	0.73
1:A:257:TRP:HH2	1:A:308:ILE:HD13	1.53	0.72
1:B:468:THR:HG23	3:B:766:HOH:O	1.88	0.72
1:A:485:ILE:N	1:A:656:GLN:HE22	1.85	0.71
1:B:451:ASN:H	1:B:451:ASN:HD22	1.36	0.71
1:A:271:THR:O	1:A:273:LYS:N	2.22	0.71
1:B:484[A]:ARG:HH11	1:B:484[A]:ARG:CG	2.05	0.69
1:B:412:VAL:HG11	1:B:433:MET:HE3	1.74	0.68
1:B:503:ARG:HH12	1:B:576:ASN:HB3	1.59	0.67
1:B:477:GLU:H	1:B:477:GLU:CD	1.99	0.66
1:B:451:ASN:H	1:B:451:ASN:ND2	1.93	0.65
1:A:306:LYS:HB2	1:A:445:PHE:CD1	2.31	0.65
1:B:526:ALA:H	1:B:576:ASN:HD22	1.42	0.65
1:B:478:ASN:O	1:B:622:SER:HB2	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:613:THR:O	1:A:616:THR:HG22	1.97	0.65
1:A:347:HIS:O	1:A:351:THR:HG23	1.95	0.64
1:B:480:LYS:HE2	1:B:482:LYS:HZ2	1.62	0.64
1:B:375:ILE:HG22	1:B:379:LYS:HE3	1.79	0.64
1:A:395:ILE:O	1:A:403:LEU:HD21	1.98	0.64
1:B:316:ARG:HD2	3:B:770:HOH:O	1.97	0.63
1:B:503:ARG:HD3	1:B:528:ALA:HB2	1.80	0.63
1:A:584:VAL:HG13	3:A:908:HOH:O	1.97	0.63
1:A:354:THR:HG22	1:A:360:ILE:HG22	1.80	0.63
1:A:264:THR:O	1:A:268:VAL:HG23	1.98	0.63
1:B:535:GLN:HG3	3:B:751:HOH:O	2.00	0.61
1:B:630:LEU:HB2	1:B:633:GLU:HG3	1.82	0.61
1:A:312:LEU:HB2	1:A:313:PRO:HD3	1.83	0.60
1:B:265:ASP:OD1	1:B:266:THR:N	2.35	0.58
1:B:593:GLU:H	1:B:593:GLU:CD	2.06	0.58
1:A:374:GLN:OE1	1:A:391:ARG:HD2	2.04	0.56
1:A:526:ALA:O	1:A:576:ASN:HA	2.05	0.56
1:B:316:ARG:HA	1:B:319:LYS:HE3	1.87	0.56
1:A:265:ASP:OD1	1:A:266:THR:N	2.34	0.56
1:A:484:ARG:CD	1:A:626:ILE:HD11	2.29	0.56
1:B:312:LEU:HB2	1:B:313:PRO:HD3	1.86	0.56
1:B:348:GLU:O	1:B:352:LYS:HG2	2.06	0.56
1:A:340:ARG:HD2	1:A:367:GLY:O	2.06	0.56
1:A:504:SER:HA	1:A:507:PHE:CE2	2.41	0.56
1:A:455:SER:O	1:A:459[B]:ARG:HG3	2.06	0.56
1:B:646:ASP:OD2	1:B:646:ASP:N	2.38	0.55
1:A:351:THR:HA	1:A:354:THR:OG1	2.07	0.55
1:A:314:LEU:O	1:A:318:VAL:HG22	2.07	0.55
1:A:218:PHE:HB2	1:A:291[A]:MET:HE1	1.88	0.55
1:A:372:LYS:O	1:A:376:THR:HG23	2.06	0.54
1:B:555:ILE:HD11	1:B:564:ARG:CA	2.36	0.54
1:B:426:GLU:N	1:B:427:PRO:HD2	2.23	0.54
1:A:634:LEU:HB3	1:A:667:PHE:HB2	1.90	0.54
1:B:456:PHE:O	1:B:460:VAL:HG12	2.07	0.54
1:A:569:GLU:O	1:A:573:ARG:HB2	2.07	0.54
1:A:269:LEU:O	1:A:273:LYS:CB	2.56	0.54
1:A:256:LYS:HG2	1:A:258:SER:OG	2.08	0.53
1:A:332:MET:HE3	1:A:383:GLU:HA	1.90	0.53
1:B:555:ILE:CD1	1:B:564:ARG:HA	2.37	0.52
1:A:553:CYS:O	1:A:579:LEU:HD12	2.09	0.52
1:A:414:MET:HB2	1:A:444:LEU:HD12	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:484:ARG:HH22	1:A:498:GLN:NE2	2.08	0.52
1:B:545:LEU:O	1:B:550:ILE:HB	2.10	0.52
1:B:593:GLU:CD	1:B:593:GLU:N	2.64	0.52
1:B:504:SER:C	1:B:505:GLU:HG3	2.30	0.51
1:B:503:ARG:NH1	1:B:576:ASN:HB3	2.25	0.51
1:B:347:HIS:O	1:B:351:THR:HG23	2.10	0.51
1:B:637:ALA:HB2	1:B:663:MET:HE3	1.93	0.51
1:B:554:ALA:O	1:B:555:ILE:HD12	2.10	0.51
1:A:527:LYS:HE2	1:A:577:SER:OG	2.12	0.50
1:A:283:GLN:NE2	1:A:308:ILE:HD11	2.26	0.50
1:A:218:PHE:HB2	1:A:291[A]:MET:CE	2.41	0.50
1:A:306:LYS:HB2	1:A:445:PHE:CE1	2.47	0.49
1:A:631:HIS:HA	1:A:663:MET:HE1	1.93	0.49
1:B:359:SER:C	1:B:360:ILE:HD12	2.33	0.49
1:B:629:LEU:HD21	1:B:663:MET:HE3	1.93	0.49
1:B:404:LEU:HD13	1:B:405:SER:N	2.28	0.49
1:B:260:LEU:HB3	1:B:262:LEU:HD13	1.94	0.49
1:A:257:TRP:CH2	1:A:308:ILE:HD13	2.39	0.49
1:B:412:VAL:HG11	1:B:433:MET:CE	2.41	0.49
1:A:332:MET:CE	1:A:383:GLU:HG3	2.43	0.49
1:A:419:ARG:HD2	3:A:902:HOH:O	2.13	0.48
1:A:270:ILE:C	1:A:274:LEU:H	2.17	0.48
1:B:634:LEU:HB3	1:B:667:PHE:HB2	1.96	0.48
1:A:241:ASP:O	1:A:470:ASN:HB2	2.13	0.48
1:B:404:LEU:HD13	1:B:405:SER:H	1.79	0.48
1:A:371:MET:O	1:A:375:ILE:HG13	2.14	0.48
1:B:331:PRO:HD3	1:B:404:LEU:HD11	1.94	0.48
1:A:240:LEU:O	1:A:241:ASP:HB2	2.14	0.48
1:B:211:LEU:HD23	1:B:437:ARG:HB2	1.95	0.47
1:B:555:ILE:CD1	1:B:567:ASN:HB2	2.45	0.47
1:B:500:ILE:HD11	1:B:530:ILE:HD11	1.96	0.47
1:A:287:LEU:O	1:A:291[B]:MET:HB2	2.14	0.47
1:A:263:SER:HB3	1:A:265:ASP:OD1	2.15	0.47
1:A:371:MET:O	1:A:374:GLN:HG2	2.15	0.47
1:B:352:LYS:N	1:B:352:LYS:HD3	2.30	0.46
1:A:396:LEU:O	1:A:401:GLY:HA2	2.15	0.46
1:A:324:LEU:HG	1:A:332:MET:HE1	1.96	0.46
1:A:273:LYS:O	1:A:276:PHE:CE2	2.68	0.46
1:B:526:ALA:N	1:B:576:ASN:HD22	2.12	0.46
1:A:257:TRP:HH2	1:A:308:ILE:CD1	2.25	0.45
1:A:540:PHE:CE2	1:A:544:LYS:HG3	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:287:LEU:O	1:B:291:MET:HG3	2.16	0.45
1:B:332:MET:CE	1:B:383:GLU:HG3	2.45	0.45
1:B:449:PHE:CE1	1:B:454:ARG:HG2	2.48	0.45
1:B:484[A]:ARG:HG3	1:B:626:ILE:HD11	1.99	0.45
1:B:451:ASN:ND2	1:B:451:ASN:N	2.64	0.45
1:A:398:LEU:HD23	1:A:399:ASN:HB2	1.99	0.45
1:B:331:PRO:HA	1:B:382:THR:O	2.17	0.45
1:A:338:PRO:HG3	1:A:419:ARG:HB2	1.98	0.45
1:A:440:LYS:HD3	1:A:440:LYS:N	2.32	0.45
1:B:211:LEU:CD2	1:B:437:ARG:HB2	2.47	0.45
1:B:584:VAL:HG13	3:B:735:HOH:O	2.17	0.45
1:A:615:ARG:HD3	3:A:888:HOH:O	2.17	0.44
1:A:403:LEU:HD23	1:A:403:LEU:H	1.82	0.44
1:B:362:SER:HA	1:B:384:ILE:O	2.17	0.44
1:B:413:VAL:HG22	1:B:443:VAL:CG2	2.46	0.44
1:A:306:LYS:O	1:A:309:SER:HB2	2.17	0.44
1:B:449:PHE:CD2	1:B:454:ARG:HG2	2.51	0.44
1:A:307:THR:HG22	1:A:311:LEU:HD11	2.00	0.44
1:A:398:LEU:HD22	1:A:403:LEU:HD22	1.99	0.44
1:A:668:GLU:O	1:A:671:MET:HG2	2.17	0.44
1:B:653:ASP:OD1	1:B:653:ASP:N	2.36	0.44
1:B:663:MET:HE2	1:B:663:MET:HB2	1.78	0.44
1:B:306:LYS:O	1:B:309:SER:HB2	2.18	0.44
1:B:638:TYR:CZ	1:B:642:LYS:HD2	2.53	0.44
1:B:649:ILE:HA	1:B:652:LEU:CD1	2.48	0.44
1:A:332:MET:HE3	1:A:383:GLU:HG3	2.00	0.43
1:A:449:PHE:CD2	1:A:454:ARG:NH2	2.86	0.43
1:B:354:THR:HG21	1:B:360:ILE:HG22	2.00	0.43
1:B:332:MET:HE1	1:B:383:GLU:HG3	2.00	0.43
1:A:270:ILE:HG22	1:A:270:ILE:O	2.17	0.43
1:A:307:THR:O	1:A:311:LEU:HG	2.19	0.43
1:B:211:LEU:HD12	1:B:211:LEU:N	2.33	0.43
1:A:265:ASP:CG	1:A:266:THR:N	2.72	0.43
1:A:275:HIS:CD2	1:A:283:GLN:HE22	2.37	0.43
1:A:346:ILE:O	1:A:350:VAL:HG23	2.18	0.43
1:A:504:SER:HA	1:A:507:PHE:CD2	2.54	0.43
1:B:484[B]:ARG:HG3	1:B:626:ILE:HD11	2.01	0.43
1:A:459[B]:ARG:HB3	1:A:459[B]:ARG:CZ	2.49	0.43
1:B:570:LYS:O	1:B:574:GLU:HG3	2.18	0.43
1:A:430:THR:O	1:A:434:LYS:HG3	2.19	0.42
1:A:658:LYS:HD3	1:A:658:LYS:HA	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:265:ASP:CG	1:A:266:THR:H	2.20	0.42
1:A:354:THR:CG2	1:A:360:ILE:HG22	2.48	0.42
1:B:480:LYS:HB2	1:B:480:LYS:HE3	1.74	0.42
1:B:614:GLY:O	1:B:615:ARG:NH1	2.53	0.42
1:A:332:MET:HE3	1:A:383:GLU:CB	2.50	0.42
1:A:631:HIS:HA	1:A:663:MET:CE	2.49	0.42
1:B:314:LEU:C	1:B:314:LEU:HD23	2.40	0.42
1:B:571:PHE:CD1	1:B:579:LEU:HB2	2.54	0.42
1:B:611:HIS:HD2	3:B:761:HOH:O	2.02	0.42
1:A:398:LEU:HD23	1:A:399:ASN:CB	2.49	0.42
1:A:462:HIS:O	1:A:463:SER:C	2.58	0.42
1:B:332:MET:HA	1:B:408:ARG:O	2.20	0.42
1:A:345:GLN:O	1:A:349:GLU:OE1	2.37	0.42
1:B:375:ILE:O	1:B:379:LYS:HG3	2.20	0.41
1:A:218:PHE:CB	1:A:291[A]:MET:HE1	2.50	0.41
1:B:380:ARG:HA	1:B:380:ARG:HD3	1.82	0.41
1:B:449:PHE:CZ	1:B:454:ARG:HA	2.55	0.41
1:A:302:THR:HG21	3:A:897:HOH:O	2.19	0.41
1:A:469:ILE:O	1:A:470:ASN:C	2.59	0.41
1:A:374:GLN:HB3	1:A:374:GLN:HE21	1.59	0.41
1:B:392:PHE:CE2	1:B:396:LEU:HD11	2.56	0.41
1:A:257:TRP:CD1	1:A:279:LEU:HD11	2.56	0.40
1:B:260:LEU:CB	1:B:262:LEU:HD13	2.52	0.40
1:B:470:ASN:HA	1:B:470:ASN:HD22	1.70	0.40
1:A:214:PHE:CE1	1:A:410:THR:HB	2.57	0.40
1:A:393:ILE:HD13	1:A:393:ILE:HA	1.87	0.40
1:B:250:CYS:HA	1:B:251:PRO:HD3	1.95	0.40
1:B:308:ILE:HD12	1:B:353:PHE:HZ	1.86	0.40
1:B:546:LEU:HA	1:B:550:ILE:O	2.22	0.40
1:A:530:ILE:HA	1:A:598:ILE:O	2.22	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	445/493 (90%)	431 (97%)	13 (3%)	1 (0%)	47	48
1	B	427/493 (87%)	415 (97%)	10 (2%)	2 (0%)	29	25
All	All	872/986 (88%)	846 (97%)	23 (3%)	3 (0%)	41	40

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	272	GLU
1	A	273	LYS
1	B	274	LEU

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	380/437 (87%)	360 (95%)	20 (5%)	22	20
1	B	369/437 (84%)	342 (93%)	27 (7%)	14	10
All	All	749/874 (86%)	702 (94%)	47 (6%)	19	14

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	211	LEU
1	A	224	THR
1	A	234[A]	GLU
1	A	234[B]	GLU
1	A	256	LYS
1	A	262	LEU
1	A	315	LEU
1	A	352[A]	LYS
1	A	352[B]	LYS
1	A	374	GLN

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Mol	Chain	Res	Type
1	A	380	ARG
1	A	404	LEU
1	A	411	PHE
1	A	440	LYS
1	A	443	VAL
1	A	444	LEU
1	A	480	LYS
1	A	527	LYS
1	A	566	MET
1	A	618	ARG
1	B	224	THR
1	B	240	LEU
1	B	262	LEU
1	B	263	SER
1	B	316	ARG
1	B	342	LEU
1	B	404	LEU
1	B	406	THR
1	B	411	PHE
1	B	426	GLU
1	B	440	LYS
1	B	444	LEU
1	B	449	PHE
1	B	451	ASN
1	B	470	ASN
1	B	484[A]	ARG
1	B	484[B]	ARG
1	B	498	GLN
1	B	505	GLU
1	B	551	VAL
1	B	555	ILE
1	B	580	LEU
1	B	589	LEU
1	B	615	ARG
1	B	616	THR
1	B	646	ASP
1	B	653	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	275	HIS

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Mol	Chain	Res	Type
1	A	498	GLN
1	A	576	ASN
1	A	656	GLN
1	B	451	ASN
1	B	470	ASN
1	B	535	GLN
1	B	547	ASN
1	B	576	ASN
1	B	656	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

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 ⓘ

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	444/493 (90%)	0.24	17 (3%) 40 46	23, 40, 64, 73	0
1	B	436/493 (88%)	0.23	22 (5%) 28 34	28, 43, 68, 82	0
All	All	880/986 (89%)	0.24	39 (4%) 34 40	23, 42, 65, 82	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	277	GLY	5.4
1	A	620	SER	4.2
1	A	262	LEU	3.6
1	A	327	HIS	3.4
1	A	274	LEU	3.3
1	B	276	PHE	3.2
1	B	275	HIS	3.2
1	B	649	ILE	3.1
1	B	623	GLY	3.1
1	A	264	THR	3.1
1	A	619	GLY	3.0
1	A	618	ARG	3.0
1	B	371	MET	2.9
1	B	524	VAL	2.9
1	B	344	LEU	2.9
1	B	401	GLY	2.8
1	A	370	GLU	2.7
1	A	506	PHE	2.7
1	B	671	MET	2.7
1	B	265	ASP	2.6
1	B	504	SER	2.5
1	A	617	ALA	2.5
1	B	617	ALA	2.4
1	A	270	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	353	PHE	2.3
1	B	400	ASP	2.3
1	A	477	GLU	2.2
1	B	397	THR	2.2
1	A	525	ASP	2.2
1	A	267	MET	2.1
1	A	478	ASN	2.1
1	B	270	ILE	2.1
1	B	262	LEU	2.1
1	B	621	ARG	2.1
1	B	622	SER	2.0
1	B	652	LEU	2.0
1	A	225	VAL	2.0
1	A	622	SER	2.0
1	B	647	GLU	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 carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	NI	A	701	1/1	0.99	0.13	32,32,32,32	0

6.5 Other polymers [i](#)

There are no such residues in this entry.