



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 09:56 AM UTC

PDB ID : 5DCA / pdb_00005dca
Title : Crystal structure of yeast full length Brr2 in complex with Prp8 Jab1 domain
Authors : Absmeier, E.; Wollenhaupt, J.; Santos, K.F.; Wahl, M.C.
Deposited on : 2015-08-23
Resolution : 2.80 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
Xtrriage (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

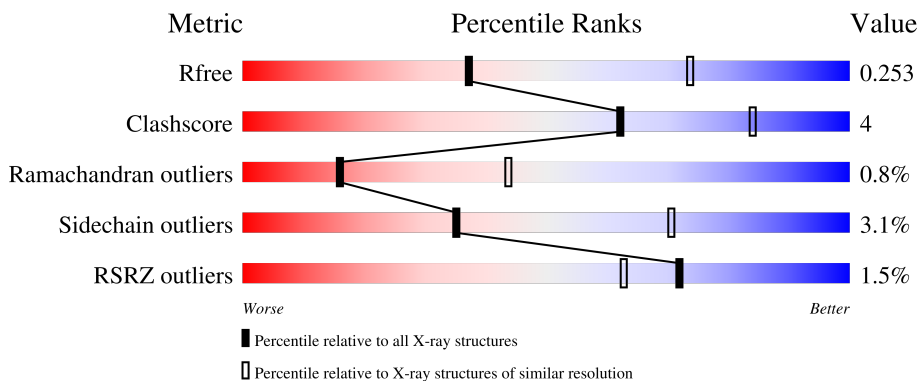
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	1948	
2	J	251	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 17842 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-splicing helicase BRR2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	1948	15639	10006	2602	2973	58	0	0	0

There are 103 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	THR	deletion	UNP P32639
A	?	-	ASP	deletion	UNP P32639
A	?	-	TYR	deletion	UNP P32639
A	?	-	GLU	deletion	UNP P32639
A	?	-	THR	deletion	UNP P32639
A	?	-	HIS	deletion	UNP P32639
A	?	-	PRO	deletion	UNP P32639
A	?	-	ASP	deletion	UNP P32639
A	?	-	ASN	deletion	UNP P32639
A	?	-	SER	deletion	UNP P32639
A	?	-	ASN	deletion	UNP P32639
A	?	-	LYS	deletion	UNP P32639
A	?	-	GLN	deletion	UNP P32639
A	?	-	ALA	deletion	UNP P32639
A	?	-	VAL	deletion	UNP P32639
A	?	-	ALA	deletion	UNP P32639
A	?	-	ILE	deletion	UNP P32639
A	?	-	LEU	deletion	UNP P32639
A	?	-	ALA	deletion	UNP P32639
A	?	-	ASP	deletion	UNP P32639
A	?	-	ASP	deletion	UNP P32639
A	?	-	GLU	deletion	UNP P32639
A	?	-	LYS	deletion	UNP P32639
A	?	-	SER	deletion	UNP P32639
A	?	-	ASP	deletion	UNP P32639
A	?	-	GLU	deletion	UNP P32639
A	?	-	GLU	deletion	UNP P32639

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	GLU	deletion	UNP P32639
A	?	-	VAL	deletion	UNP P32639
A	?	-	THR	deletion	UNP P32639
A	?	-	GLU	deletion	UNP P32639
A	?	-	MET	deletion	UNP P32639
A	?	-	SER	deletion	UNP P32639
A	?	-	ASN	deletion	UNP P32639
A	?	-	ASN	deletion	UNP P32639
A	?	-	ALA	deletion	UNP P32639
A	?	-	ASN	deletion	UNP P32639
A	?	-	VAL	deletion	UNP P32639
A	?	-	LEU	deletion	UNP P32639
A	?	-	GLY	deletion	UNP P32639
A	?	-	GLY	deletion	UNP P32639
A	?	-	GLU	deletion	UNP P32639
A	?	-	ILE	deletion	UNP P32639
A	?	-	ASN	deletion	UNP P32639
A	?	-	ASP	deletion	UNP P32639
A	?	-	ASN	deletion	UNP P32639
A	?	-	GLU	deletion	UNP P32639
A	?	-	ASP	deletion	UNP P32639
A	?	-	ASP	deletion	UNP P32639
A	?	-	ASP	deletion	UNP P32639
A	?	-	GLU	deletion	UNP P32639
A	?	-	GLU	deletion	UNP P32639
A	?	-	TYR	deletion	UNP P32639
A	?	-	ASP	deletion	UNP P32639
A	?	-	TYR	deletion	UNP P32639
A	?	-	ASN	deletion	UNP P32639
A	?	-	ASP	deletion	UNP P32639
A	?	-	VAL	deletion	UNP P32639
A	?	-	GLU	deletion	UNP P32639
A	?	-	VAL	deletion	UNP P32639
A	?	-	ASN	deletion	UNP P32639
A	?	-	SER	deletion	UNP P32639
A	?	-	LYS	deletion	UNP P32639
A	?	-	LYS	deletion	UNP P32639
A	?	-	LYS	deletion	UNP P32639
A	?	-	THR	deletion	UNP P32639
A	?	-	THR	deletion	UNP P32639
A	?	-	HIS	deletion	UNP P32639
A	?	-	SER	deletion	UNP P32639

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	LYS	deletion	UNP P32639
A	?	-	ARG	deletion	UNP P32639
A	?	-	GLU	deletion	UNP P32639
A	?	-	LEU	deletion	UNP P32639
A	?	-	ASP	deletion	UNP P32639
A	?	-	SER	deletion	UNP P32639
A	?	-	GLY	deletion	UNP P32639
A	?	-	ASP	deletion	UNP P32639
A	?	-	ASP	deletion	UNP P32639
A	?	-	GLN	deletion	UNP P32639
A	?	-	PRO	deletion	UNP P32639
A	?	-	GLN	deletion	UNP P32639
A	?	-	SER	deletion	UNP P32639
A	?	-	SER	deletion	UNP P32639
A	?	-	GLU	deletion	UNP P32639
A	?	-	ALA	deletion	UNP P32639
A	?	-	LYS	deletion	UNP P32639
A	?	-	ARG	deletion	UNP P32639
A	?	-	THR	deletion	UNP P32639
A	?	-	LYS	deletion	UNP P32639
A	?	-	PHE	deletion	UNP P32639
A	?	-	SER	deletion	UNP P32639
A	?	-	VAL	deletion	UNP P32639
A	?	-	THR	deletion	UNP P32639
A	?	-	ALA	deletion	UNP P32639
A	?	-	GLU	deletion	UNP P32639
A	?	-	VAL	deletion	UNP P32639
A	?	-	ASN	deletion	UNP P32639
A	?	-	GLY	deletion	UNP P32639
A	?	-	GLY	deletion	UNP P32639
A	?	-	ASP	deletion	UNP P32639
A	?	-	ASP	deletion	UNP P32639
A	?	-	GLU	deletion	UNP P32639
A	?	-	ALA	deletion	UNP P32639

- Molecule 2 is a protein called Pre-mRNA-splicing factor 8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	J	251	2012	1298	325	383	6	0	0	0

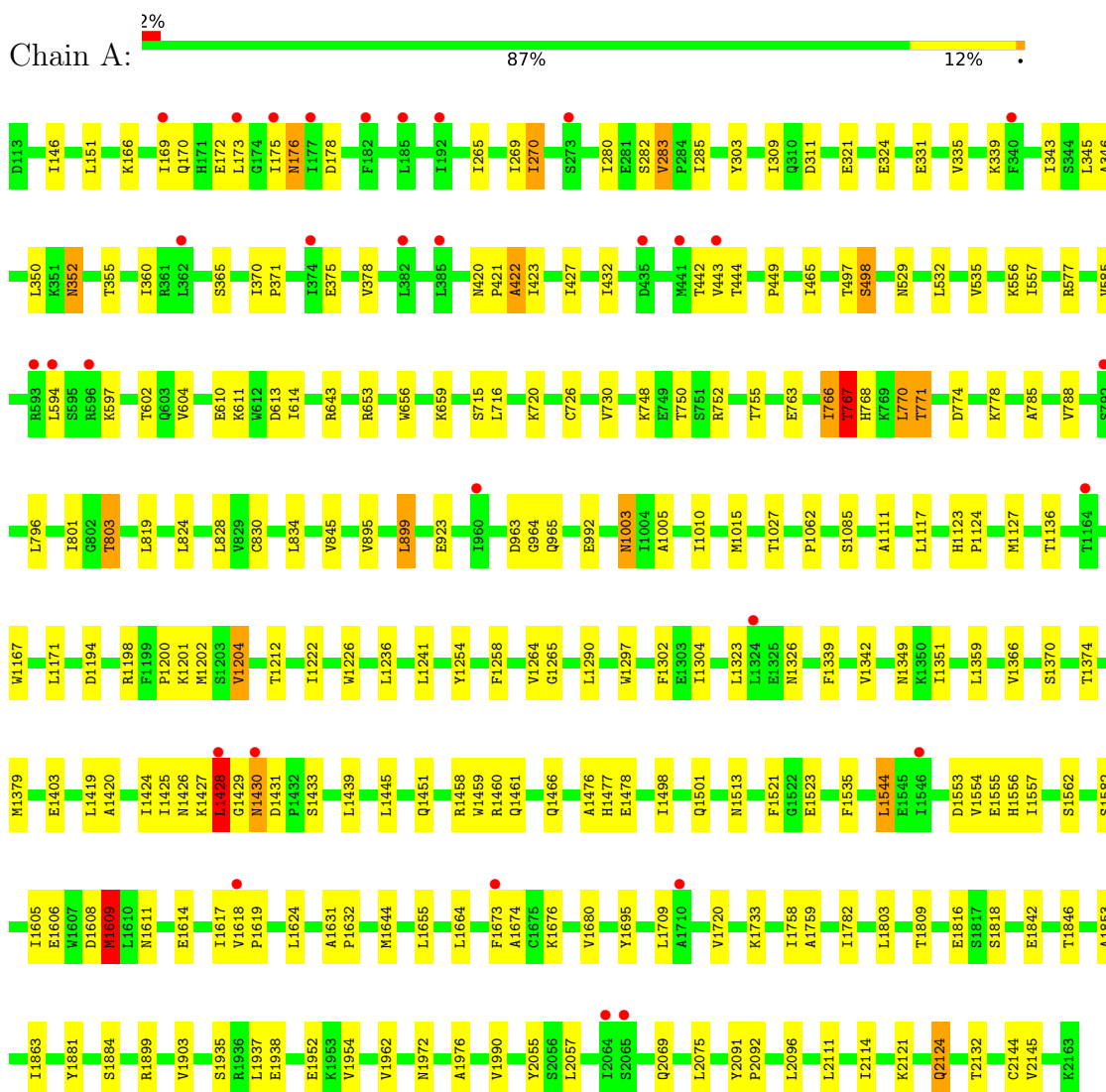
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	169	Total 169	O 169	0	0
3	J	22	Total 22	O 22	0	0

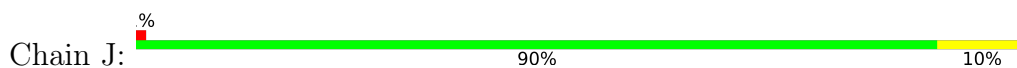
3 Residue-property plots

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: Pre-mRNA-splicing helicase BRR2



- Molecule 2: Pre-mRNA-splicing factor 8





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	107.85Å 178.85Å 181.11Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.80 50.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	98.5 (50.00-2.80) 98.4 (50.00-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.13 (at 2.73Å)	Xtrriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.202 , 0.255 0.205 , 0.253	Depositor DCC
R_{free} test set	4481 reflections (4.76%)	wwPDB-VP
Wilson B-factor (Å ²)	85.3	Xtrriage
Anisotropy	0.245	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 50.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	0.020 for -h,l,k	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	17842	wwPDB-VP
Average B, all atoms (Å ²)	102.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.21% 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](#)

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	0.45	0/15960	0.74	2/21620 (0.0%)
2	J	0.44	0/2060	0.70	0/2792
All	All	0.45	0/18020	0.74	2/24412 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1428	LEU	N-CA-C	-6.69	100.26	110.30
1	A	1304	ILE	N-CA-C	5.00	113.29	109.19

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	15639	0	15665	129	0
2	J	2012	0	1972	19	0
3	A	169	0	0	3	0
3	J	22	0	0	0	0
All	All	17842	0	17637	144	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 4.

All (144) 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)
2:J:2387:HIS:C	2:J:2388:ARG:N	2.05	1.15
1:A:1439:LEU:HA	1:A:1445:LEU:HD11	1.64	0.80
1:A:1555:GLU:C	1:A:1556:HIS:N	2.41	0.79
1:A:1015:MET:HE1	1:A:1111:ALA:HB1	1.73	0.70
1:A:767:THR:O	1:A:771:THR:N	2.25	0.70
1:A:2121:LYS:O	1:A:2124:GLN:NE2	2.24	0.69
1:A:1027:THR:HG21	2:J:2160:THR:HG23	1.74	0.69
1:A:557:ILE:HD11	1:A:604:VAL:HG22	1.76	0.68
1:A:1554:VAL:HG23	1:A:1557:ILE:HD11	1.77	0.66
1:A:303:TYR:HB2	1:A:309:ILE:HD11	1.79	0.64
1:A:1609:MET:O	3:A:2201:HOH:O	2.15	0.64
1:A:1556:HIS:C	1:A:1557:ILE:N	2.56	0.63
1:A:1339:PHE:O	1:A:1342:VAL:HG22	1.99	0.63
1:A:766:ILE:O	1:A:768:HIS:N	2.32	0.62
2:J:2296:THR:O	2:J:2297:PRO:C	2.43	0.61
1:A:375:GLU:HA	1:A:378:VAL:HG12	1.83	0.61
1:A:420:ASN:N	1:A:421:PRO:CD	2.65	0.59
1:A:343:ILE:O	1:A:343:ILE:HG22	2.01	0.59
1:A:1556:HIS:N	1:A:1557:ILE:N	2.53	0.57
1:A:175:ILE:HG23	1:A:178:ASP:HB3	1.86	0.56
1:A:1614:GLU:O	1:A:1618:VAL:HG23	2.06	0.56
2:J:2383:TYR:O	2:J:2388:ARG:NH1	2.40	0.55
1:A:1124:PRO:HA	1:A:1127:MET:HE3	1.89	0.55
1:A:283:VAL:HG11	1:A:355:THR:OG1	2.07	0.54
1:A:442:THR:O	1:A:444:THR:N	2.40	0.54
1:A:1617:ILE:HD11	1:A:1655:LEU:HD22	1.89	0.54
1:A:427:ILE:HD12	1:A:432:ILE:HD11	1.88	0.54
1:A:1990:VAL:HG12	1:A:1990:VAL:O	2.07	0.54
1:A:1680:VAL:CG1	1:A:1720:VAL:HG22	2.38	0.54
1:A:166:LYS:O	1:A:170:GLN:N	2.37	0.53
1:A:1618:VAL:N	1:A:1619:PRO:HD2	2.25	0.52
2:J:2225:VAL:HG11	2:J:2242:PRO:HG3	1.92	0.52
1:A:423:ILE:HD11	1:A:992:GLU:HA	1.92	0.52
1:A:1005:ALA:HB2	1:A:1015:MET:HG3	1.92	0.52
1:A:343:ILE:HG23	1:A:346:ALA:HB3	1.91	0.52
1:A:1419:LEU:O	1:A:1420:ALA:HB3	2.11	0.51
1:A:1370:SER:OG	1:A:1374:THR:OG1	2.21	0.51
1:A:613:ASP:OD1	1:A:653:ARG:NH2	2.45	0.50
1:A:529:ASN:HD21	1:A:577:ARG:HH22	1.60	0.50
1:A:766:ILE:HD12	1:A:766:ILE:N	2.27	0.50
1:A:1062:PRO:O	2:J:2388:ARG:NH2	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1202:MET:HE3	1:A:1222:ILE:HG21	1.93	0.50
1:A:755:THR:HG22	1:A:796:LEU:HD21	1.93	0.50
1:A:614:ILE:HG23	3:A:2301:HOH:O	2.12	0.49
1:A:1426:ASN:HD21	1:A:1428:LEU:CD2	2.25	0.49
1:A:1544:LEU:HD21	1:A:1720:VAL:HG23	1.94	0.49
1:A:557:ILE:CD1	1:A:604:VAL:HG22	2.42	0.49
2:J:2330:GLU:HB3	2:J:2332:THR:HG22	1.93	0.49
1:A:1123:HIS:HB3	1:A:1124:PRO:HD3	1.95	0.49
1:A:1226:TRP:O	1:A:1264:VAL:HG11	2.13	0.49
1:A:1351:ILE:HG23	1:A:1535:PHE:CE2	2.48	0.48
1:A:1236:LEU:HD11	1:A:1258:PHE:HB3	1.96	0.48
1:A:360:ILE:HD11	1:A:365:SER:OG	2.14	0.48
1:A:1758:ILE:HG22	1:A:1846:THR:HG23	1.95	0.48
1:A:1359:LEU:HD21	1:A:1379:MET:HB3	1.94	0.48
1:A:1962:VAL:HG22	1:A:1976:ALA:HB3	1.96	0.48
1:A:151:LEU:C	1:A:151:LEU:HD12	2.39	0.48
1:A:610:GLU:OE2	1:A:643:ARG:HD2	2.14	0.47
1:A:750:THR:HG21	1:A:803:THR:HG23	1.95	0.47
1:A:828:LEU:HG	1:A:830:CYS:SG	2.53	0.47
1:A:1204:VAL:HG13	1:A:1222:ILE:HG12	1.96	0.47
1:A:169:ILE:HG23	1:A:716:LEU:HD13	1.96	0.47
1:A:556:LYS:NZ	1:A:602:THR:O	2.45	0.47
1:A:421:PRO:O	1:A:422:ALA:HB3	2.14	0.47
1:A:1476:ALA:HB1	1:A:1521:PHE:CZ	2.50	0.47
1:A:1194:ASP:O	1:A:1198:ARG:HG2	2.15	0.47
1:A:963:ASP:O	1:A:965:GLN:N	2.48	0.47
1:A:1370:SER:O	1:A:1513:ASN:HA	2.14	0.47
1:A:1429:GLY:O	1:A:1431:ASP:N	2.47	0.47
1:A:285:ILE:HD11	1:A:355:THR:HG22	1.97	0.47
2:J:2388:ARG:O	2:J:2389:PRO:C	2.57	0.46
1:A:774:ASP:HA	1:A:778:LYS:HB2	1.97	0.46
1:A:1003:ASN:HD22	1:A:1003:ASN:C	2.23	0.46
1:A:1608:ASP:O	1:A:1609:MET:HG2	2.16	0.46
1:A:1631:ALA:HB3	1:A:1632:PRO:HD3	1.97	0.46
1:A:1674:ALA:HB1	1:A:1709:LEU:HD13	1.97	0.46
1:A:283:VAL:HG11	1:A:355:THR:CB	2.45	0.46
1:A:285:ILE:HD12	1:A:285:ILE:N	2.31	0.46
1:A:1782:ILE:HG21	1:A:1803:LEU:HD21	1.97	0.46
1:A:1200:PRO:HG2	1:A:1297:TRP:CD1	2.51	0.46
1:A:1241:LEU:HD11	1:A:1290:LEU:HD11	1.98	0.45
1:A:1582:SER:HA	1:A:1664:LEU:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2111:LEU:HD21	1:A:2114:ILE:HB	1.98	0.45
1:A:1419:LEU:O	1:A:1420:ALA:CB	2.65	0.45
2:J:2152:TRP:CE2	2:J:2391:HIS:CE1	3.05	0.45
1:A:283:VAL:HG22	1:A:352:ASN:ND2	2.31	0.45
1:A:270:ILE:HD11	1:A:1733:LYS:HG3	1.99	0.44
1:A:1062:PRO:HD3	2:J:2395:PHE:CG	2.52	0.44
1:A:1853:ALA:HB2	1:A:1863:ILE:HD12	1.99	0.44
1:A:497:THR:O	1:A:498:SER:CB	2.65	0.44
1:A:1349:ASN:HB2	3:A:2213:HOH:O	2.16	0.44
1:A:1759:ALA:HB2	1:A:1846:THR:HG21	1.98	0.44
2:J:2205:ALA:HB2	2:J:2226:LEU:HD23	2.00	0.44
1:A:449:PRO:HG2	1:A:465:ILE:HG23	2.00	0.44
1:A:653:ARG:NH1	1:A:923:GLU:OE2	2.51	0.44
1:A:1459:TRP:CG	1:A:1498:ILE:HD11	2.52	0.44
1:A:280:ILE:HG22	1:A:280:ILE:O	2.18	0.44
1:A:1426:ASN:OD1	1:A:1426:ASN:O	2.36	0.44
2:J:2290:ASP:OD1	2:J:2290:ASP:C	2.61	0.43
2:J:2387:HIS:C	2:J:2388:ARG:CA	2.88	0.43
1:A:345:LEU:HD13	1:A:345:LEU:O	2.18	0.43
2:J:2226:LEU:O	2:J:2352:PRO:HD3	2.19	0.43
1:A:1476:ALA:HB1	1:A:1521:PHE:HZ	1.82	0.43
1:A:370:ILE:N	1:A:371:PRO:HD2	2.34	0.43
1:A:1899:ARG:O	1:A:1903:VAL:HG23	2.19	0.43
1:A:1085:SER:HB3	2:J:2396:SER:HA	2.01	0.43
1:A:1881:TYR:O	1:A:1884:SER:OG	2.34	0.43
1:A:2055:TYR:O	1:A:2055:TYR:CG	2.71	0.43
1:A:1010:ILE:HG21	1:A:1015:MET:HE2	2.01	0.43
1:A:1477:HIS:CG	1:A:1513:ASN:OD1	2.71	0.43
1:A:1556:HIS:C	1:A:1695:TYR:CD1	2.97	0.43
2:J:2388:ARG:N	2:J:2389:PRO:HD3	2.33	0.43
1:A:1264:VAL:HG12	1:A:1265:GLY:N	2.34	0.42
1:A:1425:ILE:HG22	1:A:1426:ASN:O	2.19	0.42
1:A:1631:ALA:HB3	1:A:1632:PRO:CD	2.50	0.42
2:J:2189:LEU:HD13	2:J:2224:VAL:HG23	2.01	0.42
1:A:2075:LEU:HD21	1:A:2144:CYS:SG	2.59	0.42
1:A:282:SER:C	1:A:283:VAL:HG23	2.44	0.42
1:A:420:ASN:N	1:A:421:PRO:HD2	2.34	0.42
1:A:656:TRP:CD1	1:A:656:TRP:C	2.98	0.42
1:A:1370:SER:HG	1:A:1374:THR:HG1	1.45	0.42
1:A:1605:ILE:HG22	1:A:1606:GLU:N	2.34	0.42
1:A:269:ILE:O	1:A:270:ILE:C	2.62	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:331:GLU:O	1:A:335:VAL:HG23	2.19	0.42
1:A:1403:GLU:HG2	1:A:1673:PHE:HZ	1.84	0.42
1:A:176:ASN:HD22	1:A:176:ASN:N	2.18	0.42
1:A:1424:ILE:O	1:A:1425:ILE:HD13	2.19	0.42
1:A:1935:SER:HB2	1:A:1937:LEU:HD13	2.01	0.42
1:A:1429:GLY:HA3	1:A:1451:GLN:HG2	2.01	0.41
1:A:895:VAL:O	1:A:899:LEU:HB2	2.21	0.41
2:J:2204:ALA:CB	2:J:2238:ILE:HD11	2.50	0.41
2:J:2238:ILE:HG22	2:J:2239:SER:O	2.21	0.41
1:A:535:VAL:HG22	1:A:557:ILE:HD12	2.02	0.41
1:A:819:LEU:HD23	1:A:824:LEU:HD12	2.03	0.41
1:A:1201:LYS:HA	1:A:1302:PHE:CZ	2.55	0.41
1:A:1117:LEU:HD11	1:A:1254:TYR:CG	2.56	0.41
1:A:1427:LYS:NZ	1:A:1445:LEU:HD13	2.36	0.40
1:A:1430:ASN:ND2	1:A:1952:GLU:O	2.55	0.40
1:A:1167:TRP:CZ3	1:A:1171:LEU:HD21	2.57	0.40
1:A:1339:PHE:CE1	1:A:1419:LEU:HD23	2.57	0.40
1:A:726:CYS:O	1:A:730:VAL:HG23	2.22	0.40
1:A:770:LEU:HD21	1:A:801:ILE:HG13	2.02	0.40
1:A:785:ALA:O	1:A:788:VAL:HG22	2.22	0.40
1:A:2091:TYR:HA	1:A:2092:PRO:HD3	1.83	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [\(i\)](#)

5.3.1 Protein backbone [\(i\)](#)

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	1937/1948 (99%)	1823 (94%)	97 (5%)	17 (1%)	14	41
2	J	247/251 (98%)	231 (94%)	16 (6%)	0	100	100
All	All	2184/2199 (99%)	2054 (94%)	113 (5%)	17 (1%)	16	44

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	270	ILE
1	A	498	SER
1	A	767	THR
1	A	172	GLU
1	A	321	GLU
1	A	422	ALA
1	A	443	VAL
1	A	1430	ASN
1	A	339	LYS
1	A	964	GLY
1	A	1644	MET
1	A	283	VAL
1	A	1972	ASN
1	A	1609	MET
1	A	1611	ASN
1	A	265	ILE
1	A	1676	LYS

5.3.2 Protein sidechains [i](#)

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	1762/1762 (100%)	1703 (97%)	59 (3%)	33	69
2	J	223/223 (100%)	221 (99%)	2 (1%)	70	89
All	All	1985/1985 (100%)	1924 (97%)	61 (3%)	35	70

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	146	ILE
1	A	173	LEU
1	A	176	ASN
1	A	311	ASP
1	A	324	GLU
1	A	350	LEU

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Mol	Chain	Res	Type
1	A	352	ASN
1	A	532	LEU
1	A	585	VAL
1	A	594	LEU
1	A	597	LYS
1	A	611	LYS
1	A	659	LYS
1	A	715	SER
1	A	720	LYS
1	A	748	LYS
1	A	752	ARG
1	A	763	GLU
1	A	766	ILE
1	A	767	THR
1	A	770	LEU
1	A	771	THR
1	A	803	THR
1	A	834	LEU
1	A	845	VAL
1	A	899	LEU
1	A	1003	ASN
1	A	1136	THR
1	A	1204	VAL
1	A	1212	THR
1	A	1323	LEU
1	A	1326	ASN
1	A	1366	VAL
1	A	1428	LEU
1	A	1433	SER
1	A	1458	ARG
1	A	1460	ARG
1	A	1461	GLN
1	A	1466	GLN
1	A	1478	GLU
1	A	1501	GLN
1	A	1523	GLU
1	A	1544	LEU
1	A	1553	ASP
1	A	1562	SER
1	A	1609	MET
1	A	1624	LEU
1	A	1809	THR

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Mol	Chain	Res	Type
1	A	1816	GLU
1	A	1818	SER
1	A	1842	GLU
1	A	1938	GLU
1	A	1954	VAL
1	A	2057	LEU
1	A	2069	GLN
1	A	2096	LEU
1	A	2124	GLN
1	A	2132	THR
1	A	2145	VAL
2	J	2310	GLU
2	J	2340	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	157	ASN
1	A	176	ASN
1	A	264	ASN
1	A	503	GLN
1	A	529	ASN
1	A	542	HIS
1	A	551	ASN
1	A	570	GLN
1	A	621	ASN
1	A	676	ASN
1	A	705	GLN
1	A	714	ASN
1	A	739	GLN
1	A	805	HIS
1	A	892	GLN
1	A	919	ASN
1	A	933	ASN
1	A	1003	ASN
1	A	1086	GLN
1	A	1296	ASN
1	A	1426	ASN
1	A	1461	GLN
1	A	1517	ASN
1	A	1547	ASN
1	A	1549	GLN

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Mol	Chain	Res	Type
1	A	1797	HIS
1	A	1855	HIS
1	A	2050	ASN
1	A	2059	ASN
1	A	2120	ASN
1	A	2161	ASN
2	J	2202	GLN
2	J	2232	HIS
2	J	2237	GLN
2	J	2240	ASN
2	J	2260	HIS
2	J	2355	ASN

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	5
2	J	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	192:ILE	C	258:ASN	N	48.54
1	A	393:GLU	C	420:ASN	N	23.97
1	A	1828:GLU	C	1841:THR	N	9.71
1	A	1556:HIS	C	1557:ILE	N	2.56
1	A	1555:GLU	C	1556:HIS	N	2.41
1	J	2387:HIS	C	2388:ARG	N	2.05

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	1948/1948 (100%)	-0.22	31 (1%) 70 61	57, 90, 184, 237	0
2	J	251/251 (100%)	-0.23	2 (0%) 82 75	59, 88, 151, 194	0
All	All	2199/2199 (100%)	-0.22	33 (1%) 72 63	57, 89, 182, 237	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1673	PHE	4.8
1	A	192	ILE	3.9
1	A	177	ILE	3.5
1	A	1428	LEU	3.4
1	A	173	LEU	3.3
1	A	1430	ASN	3.3
1	A	362	LEU	3.2
1	A	593	ARG	3.0
2	J	2321	ILE	2.9
1	A	169	ILE	2.9
1	A	182	PHE	2.8
1	A	2064	ILE	2.8
1	A	792	SER	2.7
1	A	385	LEU	2.7
1	A	594	LEU	2.7
1	A	2065	SER	2.7
1	A	185	LEU	2.6
1	A	1324	LEU	2.6
1	A	175	ILE	2.6
1	A	1164	THR	2.5
1	A	1710	ALA	2.5
1	A	443	VAL	2.5
1	A	382	LEU	2.5
1	A	441	MET	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	273	SER	2.4
1	A	374	ILE	2.3
1	A	1546	ILE	2.3
1	A	1618	VAL	2.2
2	J	2398	LEU	2.2
1	A	596	ARG	2.2
1	A	435	ASP	2.1
1	A	340	PHE	2.1
1	A	960	ILE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.