



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 08:39 AM UTC

PDB ID : 3U84 / pdb_00003u84
Title : Crystal Structure of Human Menin
Authors : Huang, J.; Wan, B.; Lei, M.
Deposited on : 2011-10-15
Resolution : 2.50 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

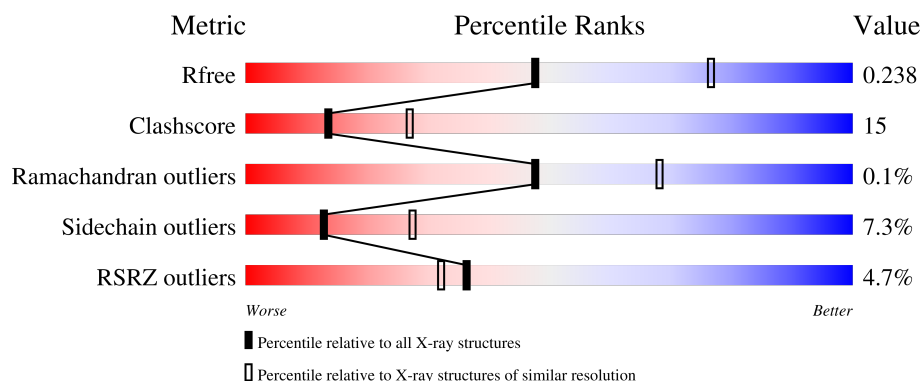
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	550	3% 68% 21% • 8%
1	B	550	6% 55% 27% • 14%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7753 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 Menin.

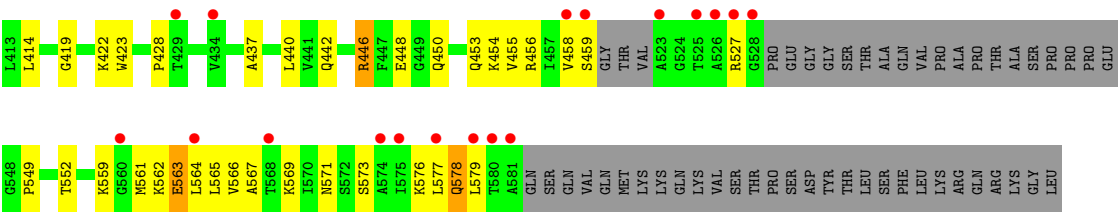
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	506	Total	C	N	O	S	0	0	0
			3981	2547	685	735	14			
1	B	472	Total	C	N	O	S	0	0	0
			3722	2390	633	685	14			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	SER	-	expression tag	UNP O00255
B	1	SER	-	expression tag	UNP O00255

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	27	Total	O	0	0
			27	27		
2	B	23	Total	O	0	0
			23	23		



4 Data and refinement statistics

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, α , β , γ	139.89Å 139.89Å 54.15Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.94 – 2.50 40.94 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.9 (40.94-2.50) 99.9 (40.94-2.50)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.98 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.7 _650	Depositor
R, R_{free}	0.198 , 0.235 0.199 , 0.238	Depositor DCC
R_{free} test set	3664 reflections (9.95%)	wwPDB-VP
Wilson B-factor (Å ²)	39.7	Xtriage
Anisotropy	0.064	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 65.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.022 for h,-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7753	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.08% 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	0.31	0/4070	0.72	2/5522 (0.0%)
1	B	0.29	0/3805	0.75	4/5165 (0.1%)
All	All	0.30	0/7875	0.74	6/10687 (0.1%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	68	ALA	CA-C-N	-7.83	111.83	120.14
1	A	68	ALA	C-N-CA	-7.83	111.83	120.14
1	B	208	GLY	N-CA-C	-6.45	107.40	115.08
1	B	56	THR	N-CA-C	-5.40	106.54	113.02
1	B	54	ILE	CA-C-N	5.25	126.06	119.98
1	B	54	ILE	C-N-CA	5.25	126.06	119.98

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	3981	0	3967	88	0
1	B	3722	0	3697	140	0
2	A	27	0	0	1	0
2	B	23	0	0	1	0
All	All	7753	0	7664	224	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 15.

All (224) 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:41:LEU:HD22	1:A:239:MET:HE2	1.45	0.98
1:B:300:THR:HG22	1:B:304:LYS:HE2	1.51	0.91
1:B:210:THR:HG23	1:B:212:ASN:H	1.36	0.90
1:B:134:PHE:CE2	1:B:151:LYS:HD3	2.06	0.90
1:A:210:THR:HG23	1:A:212:ASN:H	1.37	0.89
1:B:13:LEU:HB2	1:B:81:ALA:HB3	1.57	0.86
1:B:134:PHE:HE2	1:B:151:LYS:HD3	1.41	0.84
1:B:573:SER:O	1:B:577:LEU:HG	1.79	0.83
1:B:134:PHE:HD2	1:B:140:ILE:HD13	1.43	0.81
1:B:561:MET:HE2	1:B:578:GLN:HB3	1.68	0.75
1:B:349:GLN:HB2	1:B:422:LYS:HB3	1.72	0.72
1:A:527:ARG:HG2	1:A:528:GLY:N	2.06	0.70
1:B:134:PHE:CD2	1:B:140:ILE:HD13	2.25	0.69
1:A:41:LEU:CD2	1:A:239:MET:HE2	2.22	0.69
1:B:23:PHE:O	1:B:27:LEU:HB2	1.93	0.68
1:B:149:GLY:O	1:B:151:LYS:HG3	1.92	0.68
1:A:534:THR:HG22	1:A:535:ALA:N	2.09	0.68
1:B:177:LEU:HD21	1:B:238:PHE:CD2	2.28	0.68
1:A:177:LEU:HD21	1:A:238:PHE:CD2	2.29	0.67
1:B:193:THR:HG23	1:B:210:THR:OG1	1.95	0.67
1:A:38:SER:N	1:A:239:MET:HE1	2.10	0.67
1:B:211:VAL:HG12	1:B:215:VAL:HG23	1.76	0.66
1:B:159:PHE:CZ	1:B:239:MET:HE3	2.30	0.66
1:B:322:MET:HE3	1:B:344:THR:HG21	1.78	0.65
1:A:37:LEU:C	1:A:239:MET:HE1	2.21	0.65
1:B:561:MET:HG3	1:B:564:LEU:HD12	1.78	0.65
1:A:349:GLN:HB2	1:A:422:LYS:HB3	1.79	0.64
1:B:51:ASN:OD1	1:B:53:VAL:HG22	1.99	0.63
1:B:134:PHE:O	1:B:135:LYS:HD2	1.99	0.63
1:A:38:SER:HA	1:A:239:MET:HE1	1.81	0.63
1:B:134:PHE:HB3	1:B:137:ARG:HB3	1.82	0.62
1:B:453:GLN:HA	1:B:566:VAL:HG23	1.81	0.61
1:B:183:TRP:CE2	1:B:211:VAL:HG21	2.35	0.61
1:B:149:GLY:O	1:B:150:THR:HG22	2.02	0.60
1:B:377:LYS:HE2	1:B:442:GLN:OE1	2.02	0.60
1:B:233:LYS:HG2	1:B:272:HIS:CE1	2.36	0.60
1:B:437:ALA:HB1	1:B:576:LYS:HG2	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:134:PHE:HB3	1:B:137:ARG:CB	2.31	0.60
1:A:38:SER:CA	1:A:239:MET:HE1	2.32	0.60
1:B:103:LEU:HD21	1:B:168:LEU:HD22	1.84	0.59
1:A:31:GLU:OE2	1:A:232:ARG:HD2	2.02	0.59
1:A:415:ARG:HD2	2:A:616:HOH:O	2.03	0.59
1:A:38:SER:HA	1:A:239:MET:CE	2.34	0.58
1:A:521:THR:HG23	1:B:567:ALA:HB2	1.85	0.58
1:B:373:PRO:O	1:B:377:LYS:HG3	2.03	0.58
1:B:210:THR:HG23	1:B:212:ASN:N	2.13	0.58
1:B:355:ARG:HG2	1:B:356:GLU:N	2.17	0.58
1:A:437:ALA:HB1	1:A:576:LYS:HG2	1.86	0.58
1:B:559:LYS:O	1:B:562:LYS:HG3	2.04	0.58
1:B:177:LEU:HD21	1:B:238:PHE:HD2	1.69	0.57
1:A:316:GLU:HG3	1:A:351:TYR:OH	2.04	0.57
1:B:52:ARG:HD2	1:B:247:ILE:HG23	1.87	0.57
1:B:318:ILE:HG21	1:B:360:ILE:HD11	1.85	0.57
1:A:31:GLU:HG3	1:A:166:GLN:HE21	1.68	0.57
1:B:334:VAL:HG22	1:B:375:LEU:HD22	1.87	0.57
1:B:198:TRP:O	1:B:199:HIS:HB2	2.06	0.56
1:A:601:SER:HA	1:A:604:LYS:HG3	1.87	0.56
1:A:534:THR:CG2	1:A:535:ALA:N	2.69	0.55
1:B:409:CYS:HA	1:B:412:HIS:CD2	2.41	0.55
1:B:134:PHE:CD2	1:B:137:ARG:HD3	2.42	0.55
1:B:38:SER:HB2	1:B:239:MET:HE1	1.87	0.55
1:B:210:THR:HG23	1:B:211:VAL:N	2.22	0.55
1:B:300:THR:CG2	1:B:304:LYS:HE2	2.31	0.54
1:B:328:HIS:CG	1:B:336:GLU:HB2	2.42	0.54
1:B:440:LEU:HD22	1:B:579:LEU:CD1	2.38	0.54
1:B:180:ASP:HB2	1:B:220:TRP:CH2	2.43	0.53
1:B:453:GLN:C	1:B:455:VAL:H	2.16	0.53
1:B:206:ARG:O	1:B:209:GLN:HB2	2.08	0.53
1:B:288:GLU:OE2	1:B:330:ARG:HD2	2.07	0.53
1:A:267:LEU:HB3	1:A:273:LEU:HD13	1.91	0.53
1:B:134:PHE:CZ	1:B:151:LYS:HD3	2.43	0.53
1:B:440:LEU:HD22	1:B:579:LEU:HD12	1.91	0.53
1:B:35:VAL:HA	1:B:143:LEU:HD12	1.89	0.52
1:A:65:PRO:HB3	1:A:77:TYR:CE2	2.45	0.52
1:B:265:TRP:CE2	1:B:295:ARG:HD3	2.45	0.52
1:A:457:ILE:HG21	1:A:562:LYS:HB2	1.92	0.52
1:B:527:ARG:O	1:B:527:ARG:HG3	2.08	0.52
1:A:600:LEU:O	1:A:604:LYS:HG2	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:561:MET:HB3	1:A:578:GLN:OE1	2.10	0.52
1:B:211:VAL:HG13	1:B:222:TYR:CD2	2.45	0.51
1:A:369:ASN:O	1:A:373:PRO:HG2	2.10	0.51
1:A:404:LEU:HD21	1:A:446:ARG:HG3	1.91	0.51
1:B:181:HIS:HE1	1:B:195:GLU:OE2	1.94	0.51
1:B:456:ARG:NH1	1:B:549:PRO:HD2	2.25	0.51
1:A:596:SER:C	1:A:598:TYR:H	2.19	0.51
1:A:31:GLU:HG3	1:A:166:GLN:NE2	2.25	0.51
1:A:112:VAL:HG13	1:A:187:GLY:HA2	1.92	0.51
1:A:129:LEU:C	1:A:129:LEU:HD12	2.36	0.50
1:B:213:ALA:O	1:B:217:GLU:HG3	2.12	0.50
1:B:376:LEU:HB3	1:B:446:ARG:HG2	1.94	0.50
1:A:149:GLY:O	1:A:150:THR:OG1	2.29	0.50
1:B:384:GLU:O	1:B:385:ALA:HB3	2.11	0.50
1:B:233:LYS:HG2	1:B:272:HIS:NE2	2.27	0.50
1:B:219:SER:HB2	1:B:354:CYS:SG	2.51	0.50
1:A:555:SER:O	1:A:559:LYS:HG2	2.12	0.49
1:B:345:ALA:HB1	1:B:419:GLY:HA3	1.93	0.49
1:A:176:ALA:HB2	1:A:185:VAL:HG13	1.94	0.49
1:B:181:HIS:HB2	1:B:221:LEU:HD22	1.94	0.49
1:B:348:ILE:HD12	1:B:364:PHE:HE1	1.77	0.49
1:A:580:THR:O	1:A:581:ALA:HB2	2.13	0.49
1:B:108:ARG:HG2	1:B:108:ARG:HH11	1.77	0.49
1:B:357:ASP:O	1:B:360:ILE:HG22	2.13	0.49
1:A:47:PHE:O	1:A:52:ARG:HA	2.13	0.49
1:B:366:GLU:O	1:B:370:ASP:HB3	2.13	0.48
1:B:4:LYS:HD2	1:B:29:ARG:NH2	2.28	0.48
1:A:180:ASP:HB2	1:A:220:TRP:CH2	2.49	0.48
1:A:210:THR:HG23	1:A:211:VAL:N	2.27	0.48
1:B:211:VAL:HG12	1:B:215:VAL:CG2	2.42	0.48
1:B:377:LYS:HG2	1:B:446:ARG:NH1	2.28	0.48
1:B:458:VAL:HG12	1:B:459:SER:N	2.29	0.48
1:B:27:LEU:HD21	1:B:267:LEU:CD2	2.44	0.48
1:B:103:LEU:HD22	1:B:103:LEU:H	1.79	0.48
1:A:299:LEU:HD22	1:A:303:HIS:CD2	2.48	0.48
1:A:112:VAL:HG21	1:A:188:PRO:HG3	1.95	0.48
1:A:255:GLU:CD	1:A:255:GLU:H	2.22	0.48
1:B:377:LYS:HG2	1:B:446:ARG:NH2	2.29	0.48
1:B:371:VAL:O	1:B:375:LEU:HB2	2.13	0.47
1:A:175:LEU:HG	1:A:177:LEU:HD13	1.95	0.47
1:A:301:LEU:HD23	1:A:304:LYS:HD2	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:344:THR:HG22	1:B:364:PHE:CZ	2.49	0.47
1:B:569:LYS:HE2	1:B:571:ASN:HB2	1.96	0.47
1:A:421:CYS:SG	1:A:558:MET:CE	3.02	0.47
1:A:54:ILE:HD12	1:A:63:PHE:CG	2.50	0.47
1:B:165:CYS:HB3	1:B:170:LEU:HB2	1.97	0.47
1:A:527:ARG:HG2	1:A:528:GLY:H	1.77	0.47
1:B:214:GLY:HA3	1:B:222:TYR:CD1	2.50	0.47
1:B:59:PRO:O	1:B:60:GLU:HB2	2.16	0.46
1:B:134:PHE:O	1:B:137:ARG:HB2	2.16	0.46
1:B:342:ALA:O	1:B:346:THR:HG22	2.15	0.46
1:B:52:ARG:HD2	1:B:247:ILE:CG2	2.44	0.46
1:B:134:PHE:C	1:B:135:LYS:HD2	2.40	0.46
1:B:66:SER:O	1:B:76:THR:HG22	2.15	0.46
1:B:456:ARG:HH11	1:B:549:PRO:HD2	1.80	0.46
1:B:93:PHE:O	1:B:97:ILE:HG12	2.16	0.46
1:B:113:SER:OG	1:B:170:LEU:HD22	2.15	0.46
1:A:12:PRO:HG2	1:A:14:ARG:NH1	2.30	0.46
1:B:134:PHE:HA	1:B:135:LYS:HE3	1.97	0.46
1:A:70:ASP:C	1:A:72:PRO:HD2	2.41	0.45
1:A:521:THR:HG21	1:B:563:GLU:HB2	1.98	0.45
1:B:579:LEU:HD23	1:B:579:LEU:O	2.16	0.45
1:B:370:ASP:C	1:B:373:PRO:HD2	2.41	0.45
1:B:410:PHE:CE2	1:B:414:LEU:HD11	2.52	0.45
1:B:176:ALA:HB2	1:B:185:VAL:HG13	1.97	0.45
1:B:134:PHE:HB3	1:B:137:ARG:HB2	1.99	0.45
1:A:553:PHE:CZ	1:A:558:MET:HG3	2.52	0.45
1:B:92:ARG:HD2	2:B:621:HOH:O	2.17	0.45
1:B:216:ALA:O	1:B:218:ARG:HG3	2.17	0.45
1:B:448:GLU:HB3	1:B:450:GLN:HG2	1.99	0.45
1:B:377:LYS:HG2	1:B:446:ARG:HH12	1.82	0.45
1:B:27:LEU:HD21	1:B:267:LEU:HD23	1.99	0.44
1:B:300:THR:O	1:B:304:LYS:HG3	2.18	0.44
1:B:31:GLU:OE2	1:B:232:ARG:NH1	2.50	0.44
1:A:455:VAL:HG12	1:A:457:ILE:HD12	1.99	0.44
1:B:344:THR:HG22	1:B:364:PHE:HZ	1.82	0.44
1:B:377:LYS:HG2	1:B:446:ARG:HH22	1.82	0.44
1:A:353:TYR:O	1:A:428:PRO:HD2	2.18	0.44
1:A:539:ALA:O	1:B:563:GLU:HG3	2.18	0.44
1:B:563:GLU:CD	1:B:563:GLU:H	2.25	0.44
1:A:106:TYR:HA	1:A:107:PRO:HD3	1.78	0.44
1:B:333:ASN:HB3	1:B:336:GLU:CG	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:364:PHE:O	1:B:367:VAL:HG22	2.17	0.44
1:A:70:ASP:HA	1:A:71:PRO:C	2.42	0.44
1:B:183:TRP:HB2	1:B:194:ALA:O	2.18	0.44
1:B:150:THR:HG23	1:B:150:THR:O	2.18	0.44
1:A:101:VAL:HG23	1:A:103:LEU:HD13	2.00	0.43
1:A:358:GLU:HG2	1:A:362:LYS:HE3	1.99	0.43
1:A:332:ARG:HE	1:A:378:GLU:CD	2.26	0.43
1:B:31:GLU:HG3	1:B:166:GLN:HE21	1.84	0.43
1:B:103:LEU:HD22	1:B:103:LEU:N	2.34	0.43
1:B:295:ARG:HB3	1:B:296:PRO:HD2	2.01	0.43
1:B:4:LYS:CD	1:B:29:ARG:NH2	2.82	0.43
1:B:319:TYR:N	1:B:320:PRO:CD	2.82	0.43
1:A:603:LEU:HD12	1:A:603:LEU:HA	1.85	0.43
1:B:333:ASN:HB3	1:B:336:GLU:HG3	2.00	0.43
1:A:299:LEU:HG	1:A:327:TYR:CE2	2.53	0.43
1:A:328:HIS:CD2	1:A:336:GLU:HB3	2.54	0.43
1:B:41:LEU:HD12	1:B:41:LEU:HA	1.87	0.43
1:A:62:THR:HG22	1:A:63:PHE:N	2.34	0.42
1:A:355:ARG:HE	1:A:355:ARG:HB3	1.68	0.42
1:B:372:ILE:HB	1:B:373:PRO:HD3	2.01	0.42
1:B:561:MET:O	1:B:565:LEU:HG	2.19	0.42
1:A:228:MET:HG2	1:A:313:TYR:OH	2.18	0.42
1:B:326:GLY:O	1:B:330:ARG:HB2	2.19	0.42
1:A:152:LEU:HD12	1:A:152:LEU:HA	1.89	0.42
1:B:58:VAL:HA	1:B:59:PRO:HD3	1.84	0.42
1:A:451:VAL:HA	1:A:454:LYS:HD3	2.02	0.42
1:A:12:PRO:CG	1:A:14:ARG:NH1	2.82	0.42
1:A:338:LEU:CD1	1:A:409:CYS:HB3	2.49	0.42
1:A:580:THR:HG22	1:A:581:ALA:N	2.35	0.42
1:A:48:LEU:HD22	1:A:255:GLU:HG3	2.02	0.42
1:B:211:VAL:O	1:B:215:VAL:HG23	2.20	0.42
1:A:263:LEU:HD12	1:A:263:LEU:HA	1.83	0.42
1:B:353:TYR:HB2	1:B:423:TRP:CE2	2.55	0.42
1:B:328:HIS:CD2	1:B:336:GLU:HB2	2.54	0.42
1:A:185:VAL:HG12	1:A:193:THR:HG22	2.02	0.41
1:B:108:ARG:HG2	1:B:108:ARG:NH1	2.34	0.41
1:A:360:ILE:HD12	1:A:360:ILE:HA	1.92	0.41
1:A:559:LYS:HB3	1:A:559:LYS:HE2	1.84	0.41
1:B:29:ARG:H	1:B:29:ARG:HG2	1.61	0.41
1:B:334:VAL:HG22	1:B:375:LEU:CD2	2.49	0.41
1:A:416:PHE:CZ	1:A:420:ILE:HD11	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:146:PHE:O	1:A:150:THR:HA	2.19	0.41
1:A:310:LYS:HE3	1:A:321:TYR:OH	2.20	0.41
1:A:458:VAL:HG22	1:A:459:SER:O	2.20	0.41
1:B:133:TYR:O	1:B:134:PHE:HB2	2.19	0.41
1:B:446:ARG:N	1:B:446:ARG:HD2	2.35	0.41
1:A:318:ILE:HG23	1:A:344:THR:HG23	2.01	0.41
1:A:338:LEU:HD13	1:A:409:CYS:HB3	2.01	0.41
1:A:527:ARG:HG3	1:A:534:THR:O	2.21	0.41
1:B:134:PHE:O	1:B:137:ARG:N	2.53	0.41
1:B:318:ILE:HG23	1:B:344:THR:HG23	2.02	0.41
1:A:177:LEU:HB3	1:A:228:MET:HE3	2.03	0.41
1:B:284:ALA:HB2	1:B:301:LEU:HB2	2.03	0.41
1:A:239:MET:HE3	1:A:239:MET:HB2	1.95	0.41
1:A:103:LEU:HD12	1:A:103:LEU:HA	1.83	0.40
1:A:383:LEU:HD23	1:A:383:LEU:HA	1.90	0.40
1:B:102:ASP:OD2	1:B:104:SER:HB2	2.22	0.40
1:B:198:TRP:O	1:B:199:HIS:CB	2.69	0.40
1:A:363:GLU:O	1:A:367:VAL:HG23	2.21	0.40
1:B:285:ASP:O	1:B:288:GLU:HB3	2.22	0.40
1:A:42:GLY:HA3	1:A:144:PHE:HB3	2.04	0.40
1:B:353:TYR:O	1:B:428:PRO:HD2	2.22	0.40
1:A:521:THR:CG2	1:B:567:ALA:HB2	2.49	0.40
1:B:453:GLN:C	1:B:455:VAL:N	2.79	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	496/550 (90%)	467 (94%)	29 (6%)	0	100	100
1	B	460/550 (84%)	430 (94%)	29 (6%)	1 (0%)	43	63

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	956/1100 (87%)	897 (94%)	58 (6%)	1 (0%)	48 68

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	454	LYS

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	424/461 (92%)	393 (93%)	31 (7%)	13 27
1	B	396/461 (86%)	367 (93%)	29 (7%)	13 27
All	All	820/922 (89%)	760 (93%)	60 (7%)	13 27

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	LEU
1	A	41	LEU
1	A	70	ASP
1	A	101	VAL
1	A	103	LEU
1	A	117	LEU
1	A	177	LEU
1	A	210	THR
1	A	211	VAL
1	A	221	LEU
1	A	232	ARG
1	A	254	LEU
1	A	255	GLU
1	A	263	LEU
1	A	280	LEU
1	A	299	LEU
1	A	322	MET

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Mol	Chain	Res	Type
1	A	363	GLU
1	A	375	LEU
1	A	382	LEU
1	A	405	GLN
1	A	429	THR
1	A	432	LEU
1	A	556	GLU
1	A	566	VAL
1	A	568	THR
1	A	579	LEU
1	A	597	ASP
1	A	600	LEU
1	A	603	LEU
1	A	604	LYS
1	B	3	LEU
1	B	13	LEU
1	B	27	LEU
1	B	29	ARG
1	B	41	LEU
1	B	105	LEU
1	B	117	LEU
1	B	131	ARG
1	B	135	LYS
1	B	177	LEU
1	B	195	GLU
1	B	198	TRP
1	B	199	HIS
1	B	210	THR
1	B	229	ARG
1	B	239	MET
1	B	251	THR
1	B	254	LEU
1	B	280	LEU
1	B	292	THR
1	B	332	ARG
1	B	336	GLU
1	B	346	THR
1	B	375	LEU
1	B	383	LEU
1	B	446	ARG
1	B	552	THR
1	B	563	GLU

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Mol	Chain	Res	Type
1	B	578	GLN

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	64	GLN
1	A	250	HIS
1	A	258	GLN
1	A	261	GLN
1	A	303	HIS
1	A	328	HIS
1	A	333	ASN
1	A	339	GLN
1	A	349	GLN
1	B	96	GLN
1	B	328	HIS
1	B	412	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 ⓘ

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	506/550 (92%)	0.03	14 (2%) 55 50	20, 41, 82, 129	0
1	B	472/550 (85%)	0.36	32 (6%) 23 20	20, 48, 93, 133	0
All	All	978/1100 (88%)	0.19	46 (4%) 36 32	20, 45, 90, 133	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	132	SER	6.7
1	A	539	ALA	5.3
1	B	134	PHE	4.8
1	B	133	TYR	4.4
1	A	71	PRO	4.3
1	B	206	ARG	4.1
1	B	527	ARG	4.0
1	B	581	ALA	3.8
1	B	525	THR	3.7
1	B	69	PRO	3.6
1	B	528	GLY	3.6
1	A	528	GLY	3.5
1	B	523	ALA	3.5
1	B	131	ARG	3.4
1	A	534	THR	3.3
1	B	434	VAL	3.2
1	B	199	HIS	3.1
1	A	548	GLY	3.1
1	B	198	TRP	3.0
1	B	210	THR	2.8
1	A	535	ALA	2.8
1	B	459	SER	2.6
1	A	72	PRO	2.6
1	B	207	ARG	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	197	THR	2.6
1	B	568	THR	2.6
1	A	56	THR	2.5
1	B	575	ILE	2.4
1	A	386	GLY	2.4
1	B	136	ASP	2.3
1	B	560	GLY	2.3
1	B	458	VAL	2.3
1	B	429	THR	2.2
1	A	1	SER	2.2
1	B	526	ALA	2.2
1	A	429	THR	2.2
1	B	188	PRO	2.2
1	B	580	THR	2.2
1	B	579	LEU	2.2
1	A	70	ASP	2.2
1	B	574	ALA	2.1
1	A	73	GLY	2.1
1	B	333	ASN	2.0
1	B	564	LEU	2.0
1	A	538	PRO	2.0
1	B	577	LEU	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.