



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:36 PM GMT

PDB ID : 3U84  
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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

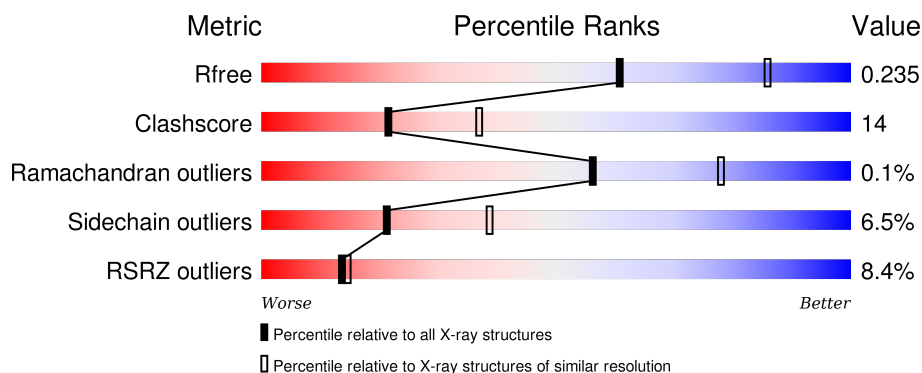
# 1 Overall quality at a glance

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))
$R_{free}$	91344	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	<div> <div>4%</div> <div>69%</div> <div>21%</div> <div>•</div> <div>8%</div> </div>
1	B	550	<div> <div>11%</div> <div>56%</div> <div>27%</div> <div>•</div> <div>14%</div> </div>

## 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 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	SER	-	EXPRESSION TAG	UNP O00255
A	?	-	GLY	SEE REMARK 999	UNP O00255
A	?	-	TRP	SEE REMARK 999	UNP O00255
A	?	-	SER	SEE REMARK 999	UNP O00255
A	?	-	PRO	SEE REMARK 999	UNP O00255
A	?	-	VAL	SEE REMARK 999	UNP O00255
B	1	SER	-	EXPRESSION TAG	UNP O00255
B	?	-	GLY	SEE REMARK 999	UNP O00255
B	?	-	TRP	SEE REMARK 999	UNP O00255
B	?	-	SER	SEE REMARK 999	UNP O00255
B	?	-	PRO	SEE REMARK 999	UNP O00255
B	?	-	VAL	SEE REMARK 999	UNP O00255

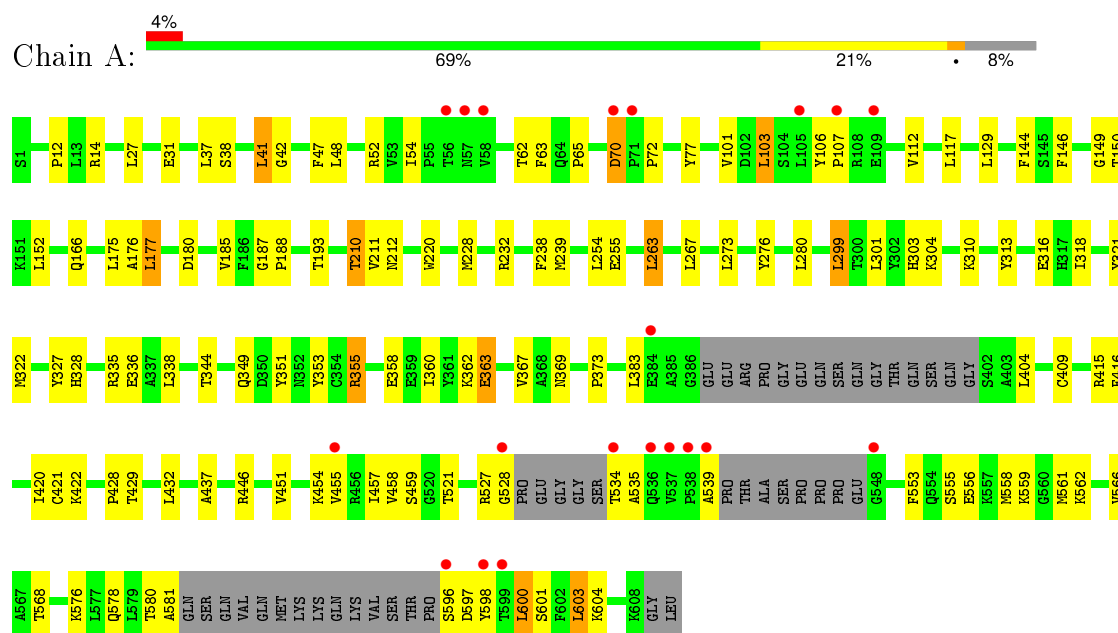
- Molecule 2 is water.

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

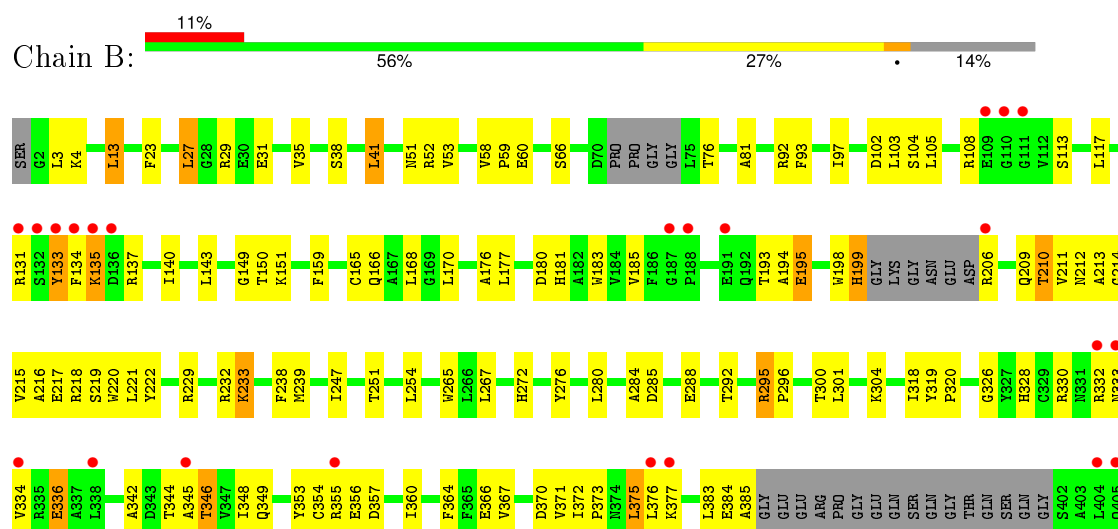
### 3 Residue-property plots

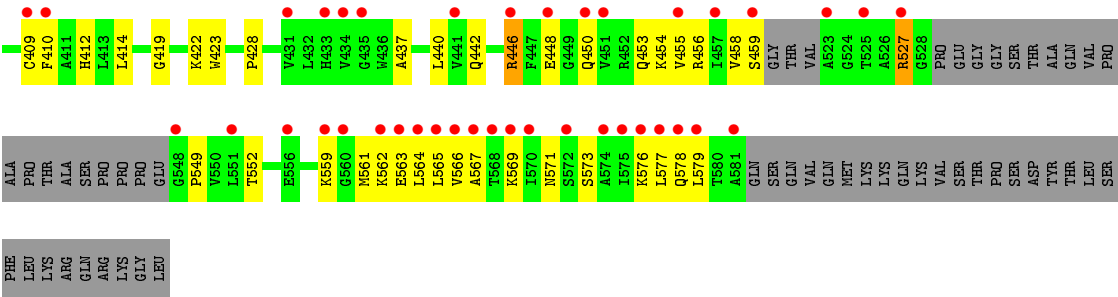
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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 ( $\text{RSRZ} > 2$ ). 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: Menin



#### • Molecule 1: Menin





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	139.89Å 139.89Å 54.15Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.94 – 2.50 49.46 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.9 (40.94-2.50) 99.9 (49.46-2.50)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.98 (at 2.51Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7_650)	Depositor
R, $R_{free}$	0.198 , 0.235 0.193 , 0.235	Depositor DCC
$R_{free}$ test set	3662 reflections (9.99%)	DCC
Wilson B-factor (Å <sup>2</sup> )	39.7	Xtriage
Anisotropy	0.064	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 65.9	EDS
Estimated twinning fraction	0.022 for h,-k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 36806 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	7753	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	0.24	0/4070	0.41	0/5522
1	B	0.23	0/3805	0.41	0/5165
All	All	0.23	0/7875	0.41	0/10687

There are no bond length outliers.

There are no bond angle outliers.

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	3981	0	3967	85	0
1	B	3722	0	3697	136	0
2	A	27	0	0	1	0
2	B	23	0	0	1	0
All	All	7753	0	7664	217	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 14.

All (217) 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:300:THR:HG22	1:B:304:LYS:HE2	1.51	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:38:SER:HA	1:A:239:MET:HE3	1.65	0.78
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: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:B:211:VAL:HG12	1:B:215:VAL:HG23	1.76	0.66
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:B:134:PHE:HB3	1:B:137:ARG:HB3	1.82	0.62
1:B:159:PHE:CZ	1:B:239:MET:HE3	2.34	0.62
1:A:38:SER:CA	1:A:239:MET:HE3	2.30	0.61
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
1:B:134:PHE:HB3	1:B:137:ARG:CB	2.31	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:B:373:PRO:O	1:B:377:LYS:HG3	2.03	0.58
1:A:521:THR:HG23	1:B:567:ALA:HB2	1.85	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:38:SER:HA	1:A:239:MET:CE	2.34	0.56
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: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: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:38:SER:HB2	1:B:239:MET:HE1	1.89	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:B:527:ARG:O	1:B:527:ARG:HG3	2.08	0.52
1:A:457:ILE:HG21	1:A:562:LYS:HB2	1.92	0.52
1:A:41:LEU:HD22	1:A:239:MET:HE2	1.92	0.52
1:A:600:LEU:O	1:A:604:LYS:HG2	2.09	0.52
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:41:LEU:HD22	1:A:239:MET:CE	2.40	0.51
1:A:404:LEU:HD21	1:A:446:ARG:HG3	1.91	0.51
1:A:369:ASN:O	1:A:373:PRO:HG2	2.10	0.51
1:B:456:ARG:NH1	1:B:549:PRO:HD2	2.25	0.51
1:B:181:HIS:HE1	1:B:195:GLU:OE2	1.94	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:B:376:LEU:HB3	1:B:446:ARG:HG2	1.94	0.50
1:B:213:ALA:O	1:B:217:GLU:HG3	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:345:ALA:HB1	1:B:419:GLY:HA3	1.93	0.49
1:A:555:SER:O	1:A:559:LYS:HG2	2.12	0.49
1:A:176:ALA:HB2	1:A:185:VAL:HG13	1.94	0.49
1:B:348:ILE:HD12	1:B:364:PHE:HE1	1.77	0.49
1:B:181:HIS:HB2	1:B:221:LEU:HD22	1.94	0.49
1:B:108:ARG:HG2	1:B:108:ARG:HH11	1.77	0.49
1:A:580:THR:O	1:A:581:ALA:HB2	2.13	0.49
1:B:357:ASP:O	1:B:360:ILE:HG22	2.13	0.49
1:B:453:GLN:C	1:B:455:VAL:H	2.16	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:B:211:VAL:HG12	1:B:215:VAL:CG2	2.42	0.48
1:A:210:THR:HG23	1:A:211:VAL:N	2.27	0.48
1:B:377:LYS:HG2	1:B:446:ARG:NH1	2.28	0.48
1:A:180:ASP:HB2	1:A:220:TRP:CH2	2.49	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:B:377:LYS:HG2	1:B:446:ARG:NH2	2.29	0.48
1:A:112:VAL:HG21	1:A:188:PRO:HG3	1.95	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
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:B:214:GLY:HA3	1:B:222:TYR:CD1	2.50	0.47
1:A:41:LEU:CD2	1:A:239:MET:HE2	2.45	0.47
1:A:527:ARG:HG2	1:A:528:GLY:H	1.77	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:596:SER:C	1:A:598:TYR:H	2.19	0.46
1:B:456:ARG:HH11	1:B:549:PRO:HD2	1.80	0.46
1:B:66:SER:O	1:B:76:THR:HG22	2.15	0.46
1:B:113:SER:OG	1:B:170:LEU:HD22	2.15	0.46
1:B:93:PHE:O	1:B:97:ILE:HG12	2.16	0.46
1:B:134:PHE:HA	1:B:135:LYS:HE3	1.97	0.46
1:A:129:LEU:C	1:A:129:LEU:HD12	2.36	0.46
1:A:12:PRO:HG2	1:A:14:ARG:NH1	2.30	0.46
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: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:216:ALA:O	1:B:218:ARG:HG3	2.17	0.45
1:B:92:ARG:HD2	2:B:621:HOH:O	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:B:377:LYS:HG2	1:B:446:ARG:HH22	1.82	0.44
1:B:344:THR:HG22	1:B:364:PHE:HZ	1.82	0.44
1:A:455:VAL:HG12	1:A:457:ILE:HD12	1.99	0.44
1:A:539:ALA:O	1:B:563:GLU:HG3	2.18	0.44
1:A:353:TYR:O	1:A:428:PRO:HD2	2.18	0.44
1:B:364:PHE:O	1:B:367:VAL:HG22	2.17	0.44
1:B:333:ASN:HB3	1:B:336:GLU:CG	2.48	0.44
1:A:106:TYR:HA	1:A:107:PRO:HD3	1.78	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: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:B:333:ASN:HB3	1:B:336:GLU:HG3	2.00	0.43
1:A:603:LEU:HA	1:A:603:LEU:HD12	1.85	0.43
1:A:255:GLU:H	1:A:255:GLU:CD	2.22	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:299:LEU:HG	1:A:327:TYR:CE2	2.53	0.43
1:B:41:LEU:HD12	1:B:41:LEU:HA	1.87	0.43
1:A:328:HIS:CD2	1:A:336:GLU:HB3	2.54	0.43
1:B:561:MET:O	1:B:565:LEU:HG	2.19	0.42
1:B:372:ILE:HB	1:B:373:PRO:HD3	2.01	0.42
1:A:62:THR:HG22	1:A:63:PHE:N	2.34	0.42
1:A:355:ARG:HB3	1:A:355:ARG:HE	1.68	0.42
1:B:326:GLY:O	1:B:330:ARG:HB2	2.19	0.42
1:A:228:MET:HG2	1:A:313:TYR:OH	2.18	0.42
1:B:58:VAL:HA	1:B:59:PRO:HD3	1.84	0.42
1:A:152:LEU:HD12	1:A:152:LEU:HA	1.89	0.42
1:A:37:LEU:C	1:A:239:MET:HE1	2.39	0.42
1:A:451:VAL:HA	1:A:454:LYS:HD3	2.02	0.42
1:A:580:THR:HG22	1:A:581:ALA:N	2.35	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:B:211:VAL:O	1:B:215:VAL:HG23	2.20	0.42
1:A:48:LEU:HD22	1:A:255:GLU:HG3	2.02	0.42
1:A:421:CYS:SG	1:A:558:MET:HE2	2.60	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:NH1	1:B:108:ARG:HG2	2.34	0.41
1:B:134:PHE:C	1:B:135:LYS:HD2	2.40	0.41
1:B:334:VAL:HG22	1:B:375:LEU:CD2	2.49	0.41
1:A:559:LYS:HE2	1:A:559:LYS:HB3	1.84	0.41
1:B:29:ARG:H	1:B:29:ARG:HG2	1.61	0.41
1:A:360:ILE:HA	1:A:360:ILE:HD12	1.92	0.41
1:A:416:PHE:CZ	1:A:420:ILE:HD11	2.55	0.41
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:HD2	1:B:446:ARG:N	2.35	0.41
1:A:338:LEU:HD13	1:A:409:CYS:HB3	2.01	0.41
1:A:318:ILE:HG23	1:A:344:THR:HG23	2.01	0.41
1:B:134:PHE:O	1:B:137:ARG:N	2.53	0.41
1:A:527:ARG:HG3	1:A:534:THR:O	2.21	0.41
1:B:318:ILE:HG23	1:B:344:THR:HG23	2.02	0.41
1:B:284:ALA:HB2	1:B:301:LEU:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:198:TRP:O	1:B:199:HIS:CB	2.69	0.40
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:A:363:GLU:O	1:A:367:VAL:HG23	2.21	0.40
1:B:370:ASP:C	1:B:373:PRO:HD2	2.41	0.40
1:B:285:ASP:O	1:B:288:GLU:HB3	2.22	0.40
1:A:70:ASP:C	1:A:72:PRO:HD2	2.41	0.40
1:B:353:TYR:O	1:B:428:PRO:HD2	2.22	0.40
1:A:42:GLY:HA3	1:A:144:PHE:HB3	2.04	0.40
1:A:521:THR:CG2	1:B:567:ALA:HB2	2.49	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%)	52	75
All	All	956/1100 (87%)	897 (94%)	58 (6%)	1 (0%)	56	78

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	454	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	424/461 (92%)	400 (94%)	24 (6%)	25	46
1	B	396/461 (86%)	367 (93%)	29 (7%)	17	32
All	All	820/922 (89%)	767 (94%)	53 (6%)	21	39

All (53) 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	103	LEU
1	A	117	LEU
1	A	177	LEU
1	A	210	THR
1	A	254	LEU
1	A	263	LEU
1	A	276	TYR
1	A	280	LEU
1	A	299	LEU
1	A	322	MET
1	A	335	ARG
1	A	355	ARG
1	A	363	GLU
1	A	429	THR
1	A	432	LEU
1	A	556	GLU
1	A	566	VAL
1	A	568	THR
1	A	597	ASP
1	A	600	LEU
1	A	603	LEU
1	B	3	LEU
1	B	13	LEU
1	B	27	LEU
1	B	41	LEU
1	B	105	LEU
1	B	117	LEU
1	B	131	ARG
1	B	133	TYR
1	B	135	LYS

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Mol	Chain	Res	Type
1	B	195	GLU
1	B	199	HIS
1	B	210	THR
1	B	229	ARG
1	B	233	LYS
1	B	251	THR
1	B	254	LEU
1	B	276	TYR
1	B	280	LEU
1	B	292	THR
1	B	295	ARG
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	527	ARG
1	B	552	THR
1	B	578	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	303	HIS
1	B	412	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

There are no ligands in this entry.

## 5.7 Other polymers

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	506/550 (92%)	0.17	20 (3%) 42 47	21, 41, 82, 129	0
1	B	472/550 (85%)	0.61	62 (13%) 5 4	20, 48, 93, 133	0
All	All	978/1100 (88%)	0.38	82 (8%) 14 14	20, 45, 90, 133	0

All (82) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	534	THR	10.4
1	B	134	PHE	7.3
1	A	71	PRO	5.9
1	A	56	THR	5.6
1	B	574	ALA	5.5
1	B	568	THR	5.2
1	B	434	VAL	5.1
1	B	132	SER	5.0
1	B	110	GLY	4.8
1	B	459	SER	4.7
1	B	133	TYR	4.6
1	B	578	GLN	4.5
1	A	538	PRO	4.2
1	B	569	LYS	4.1
1	B	109	GLU	4.1
1	B	188	PRO	4.1
1	B	567	ALA	4.1
1	B	560	GLY	4.0
1	A	109	GLU	4.0
1	B	564	LEU	4.0
1	B	332	ARG	4.0
1	B	410	PHE	3.9
1	B	111	GLY	3.8
1	A	58	VAL	3.8

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Mol	Chain	Res	Type	RSRZ
1	B	450	GLN	3.8
1	A	537	VAL	3.7
1	B	565	LEU	3.5
1	B	525	THR	3.5
1	B	579	LEU	3.5
1	B	523	ALA	3.4
1	B	377	LYS	3.4
1	B	575	ILE	3.2
1	B	576	LYS	3.2
1	B	334	VAL	3.2
1	A	57	ASN	3.1
1	B	527	ARG	3.1
1	B	187	GLY	3.0
1	B	455	VAL	3.0
1	B	338	LEU	3.0
1	B	566	VAL	2.9
1	B	577	LEU	2.8
1	A	107	PRO	2.8
1	A	528	GLY	2.7
1	A	70	ASP	2.7
1	B	435	GLY	2.7
1	B	572	SER	2.7
1	B	206	ARG	2.6
1	B	562	LYS	2.6
1	B	136	ASP	2.6
1	A	536	GLN	2.6
1	A	596	SER	2.5
1	B	405	GLN	2.5
1	B	559	LYS	2.5
1	A	598	TYR	2.5
1	A	105	LEU	2.5
1	B	581	ALA	2.5
1	B	570	ILE	2.5
1	B	448	GLU	2.4
1	A	539	ALA	2.4
1	B	409	CYS	2.4
1	B	135	LYS	2.4
1	A	599	THR	2.3
1	A	548	GLY	2.3
1	B	345	ALA	2.3
1	B	333	ASN	2.3
1	A	455	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	376	LEU	2.3
1	B	441	VAL	2.3
1	B	551	LEU	2.2
1	B	431	VAL	2.2
1	B	446	ARG	2.2
1	B	131	ARG	2.2
1	B	451	VAL	2.1
1	B	556	GLU	2.1
1	B	563	GLU	2.1
1	B	457	ILE	2.1
1	B	355	ARG	2.1
1	B	433	HIS	2.1
1	B	404	LEU	2.1
1	A	384	GLU	2.0
1	B	548	GLY	2.0
1	B	191	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](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.