Full wwPDB X-ray Structure Validation Report (i)

Jun 12, 2024 – 08:39 PM EDT

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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (1)) were used in the production of this report:

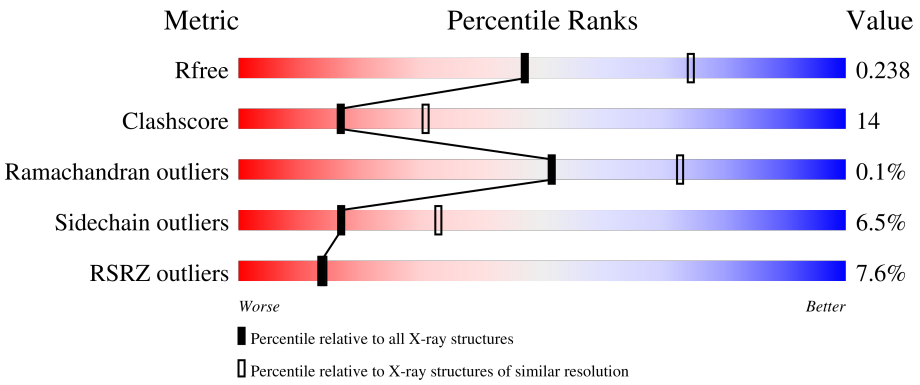
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.20.1
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

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}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (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 <=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% 69% 21% • 8%
1	B	550	10% 56% 27% • 14%

2 Entry composition (i)

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
			Total	C	N	O	S			
1	A	506	3981	2547	685	735	14	0	0	0
1	B	472	3722	2390	633	685	14	0	0	0

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.

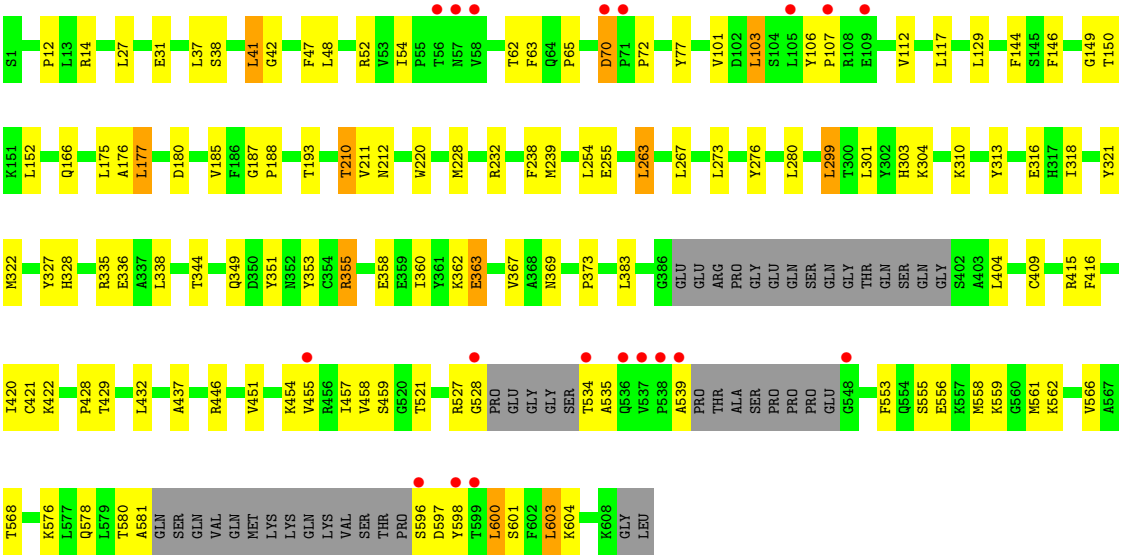
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	A	27	27	27	0	0
2	B	23	23	23	0	0

3 Residue-property plots (i)

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.

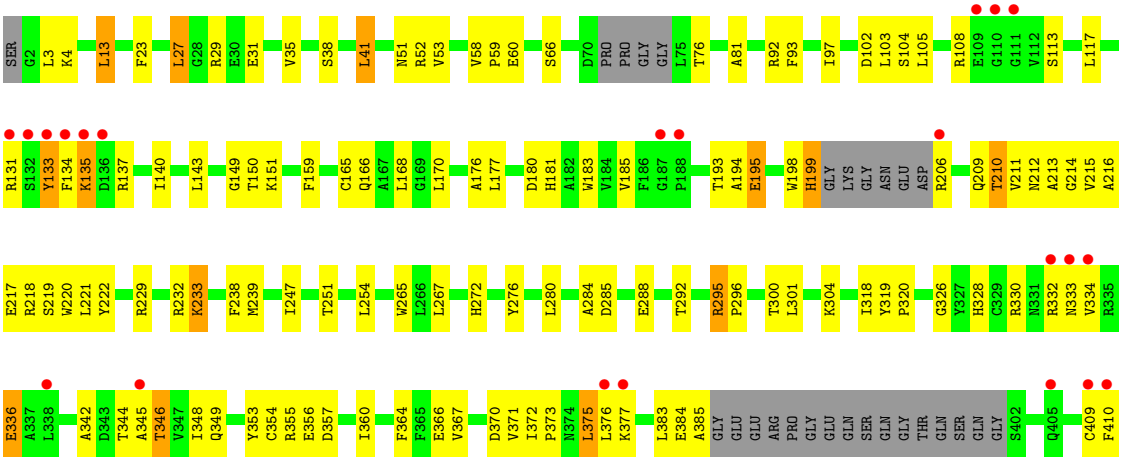
- Molecule 1: Menin

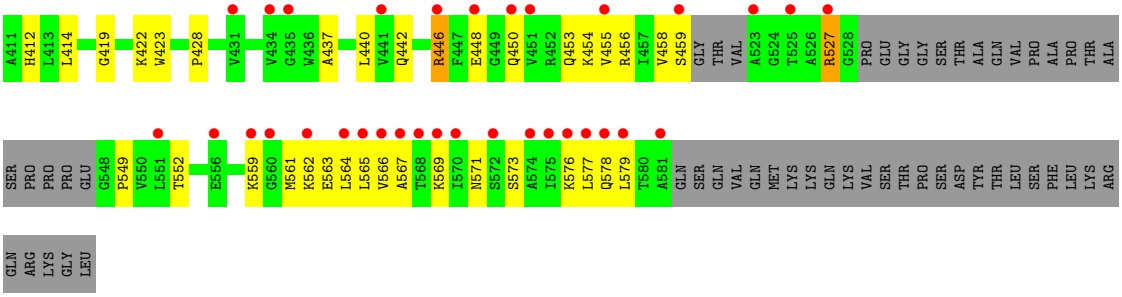
Chain A:



- Molecule 1: Menin

Chain B:




A411 H412 L413 L414 G419 K422 W423 P428 V431 V434 G435 W436 A437 L440 V441 Q442 R446 F447 E448 G449 Q450 V451 R452 Q453 K454 V455 R456 I457 V458 S459 GLY THR VAL A523 G524 T525 A526 R527 G528 PRO GLU GLY GLY SER THR ALA GLN VAL PRO ALA PRO THR ALA
SER PRO PRO PRO GLU G548 P549 V550 L551 T552 E556 K559 G560 M561 K562 E563 L564 L565 V566 A567 T568 K569 I570 N571 S572 S573 A574 I575 K576 L577 Q578 L579 T580 A581 GLN SER GLN VAL GLN MET LYS LYS GLN LYS VAL SER THR PRO SER ASP TYR THR LEU SER PHE LEU LYS ARG
GLN ARG LYS GLY LEU

4 Data and refinement statistics (i)

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 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
$< I/\sigma(I) >$ [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 , 65.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.022 for h,-k,-l	Xtriage
F_o,F_c correlation	0.94	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.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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	0.24	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 (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	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: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

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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: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: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: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: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: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

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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: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:453:GLN:C	1:B:455:VAL:H	2.16	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: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
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: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: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:A:596:SER:C	1:A:598:TYR:H	2.19	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:52:ARG:HD2	1:B:247:ILE:CG2	2.44	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:A:129:LEU:C	1:A:129:LEU:HD12	2.36	0.46
1:B:134:PHE:HA	1:B:135:LYS:HE3	1.97	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: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: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
1:B:364:PHE:O	1:B:367:VAL:HG22	2.17	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:A:255:GLU:CD	1:A:255:GLU:H	2.22	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

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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: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: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: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:A:421:CYS:SG	1:A:558:MET:HE2	2.60	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: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: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: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: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: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:A:70:ASP:C	1:A:72:PRO:HD2	2.41	0.40
1:B:285:ASP:O	1:B:288:GLU:HB3	2.22	0.40
1:B:370:ASP:C	1:B:373:PRO:HD2	2.41	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

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%)	47	68
All	All	956/1100 (87%)	897 (94%)	58 (6%)	1 (0%)	51	73

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%)	20	39
1	B	396/461 (86%)	367 (93%)	29 (7%)	14	27
All	All	820/922 (89%)	767 (94%)	53 (6%)	17	33

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

Sometimes 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 (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 monosaccharides 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	506/550 (92%)	0.12	19 (3%)	40	43	20, 41, 82, 129	0
1	B	472/550 (85%)	0.53	55 (11%)	4	4	20, 48, 93, 133	0
All	All	978/1100 (88%)	0.32	74 (7%)	13	14	20, 45, 90, 133	0

All (74) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	534	THR	10.2
1	B	134	PHE	7.1
1	A	71	PRO	5.7
1	A	56	THR	5.3
1	B	574	ALA	5.2
1	B	568	THR	5.0
1	B	132	SER	4.8
1	B	434	VAL	4.8
1	B	110	GLY	4.6
1	B	459	SER	4.5
1	B	133	TYR	4.4
1	B	578	GLN	4.3
1	B	569	LYS	4.0
1	A	538	PRO	4.0
1	B	109	GLU	3.9
1	B	567	ALA	3.9
1	A	109	GLU	3.9
1	B	560	GLY	3.8
1	B	188	PRO	3.8
1	B	332	ARG	3.8
1	B	564	LEU	3.8
1	B	410	PHE	3.7
1	B	450	GLN	3.6
1	A	58	VAL	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	111	GLY	3.6
1	A	537	VAL	3.6
1	B	565	LEU	3.4
1	B	525	THR	3.3
1	B	579	LEU	3.3
1	B	377	LYS	3.3
1	B	523	ALA	3.2
1	B	575	ILE	3.1
1	B	576	LYS	3.1
1	A	57	ASN	3.0
1	B	527	ARG	3.0
1	B	334	VAL	3.0
1	B	338	LEU	2.9
1	B	187	GLY	2.8
1	B	455	VAL	2.8
1	B	566	VAL	2.7
1	B	577	LEU	2.7
1	A	107	PRO	2.6
1	A	528	GLY	2.6
1	B	572	SER	2.6
1	A	70	ASP	2.5
1	B	562	LYS	2.5
1	B	435	GLY	2.5
1	B	206	ARG	2.5
1	B	136	ASP	2.4
1	A	536	GLN	2.4
1	B	405	GLN	2.4
1	B	559	LYS	2.4
1	A	596	SER	2.4
1	A	598	TYR	2.4
1	A	105	LEU	2.4
1	B	135	LYS	2.3
1	B	570	ILE	2.3
1	B	448	GLU	2.3
1	A	539	ALA	2.3
1	B	581	ALA	2.3
1	B	409	CYS	2.3
1	A	599	THR	2.2
1	B	345	ALA	2.2
1	B	376	LEU	2.2
1	B	333	ASN	2.1
1	A	548	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	446	ARG	2.1
1	B	551	LEU	2.1
1	A	455	VAL	2.1
1	B	441	VAL	2.1
1	B	431	VAL	2.1
1	B	131	ARG	2.0
1	B	451	VAL	2.0
1	B	556	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 monosaccharides 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.