



Full wwPDB/EMDataBank EM Map/Model Validation Report ⓘ

Nov 2, 2017 – 02:53 AM EDT

PDB ID : 5WJ5
EMDB ID: : EMD-8840
Title : Human TRPML1 channel structure in closed conformation
Authors : Schmiede, P.; Li, X.
Deposited on : unknown
Resolution : 3.70 Å(reported)

This is a Full wwPDB/EMDataBank EM Map/Model Validation Report
for a publicly released PDB/EMDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20030345

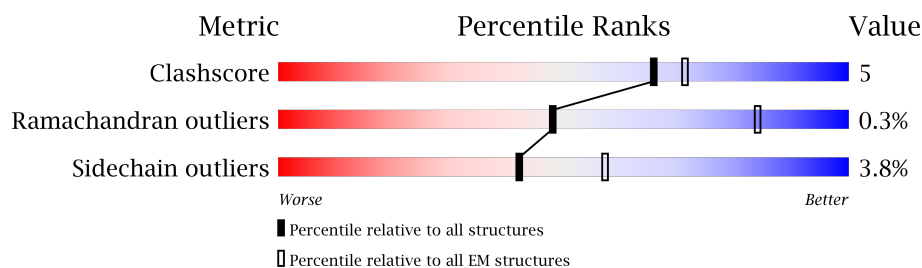
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.70 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)	EM structures (#Entries)
Clashscore	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	580	
1	B	580	
1	C	580	
1	D	580	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 14640 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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.

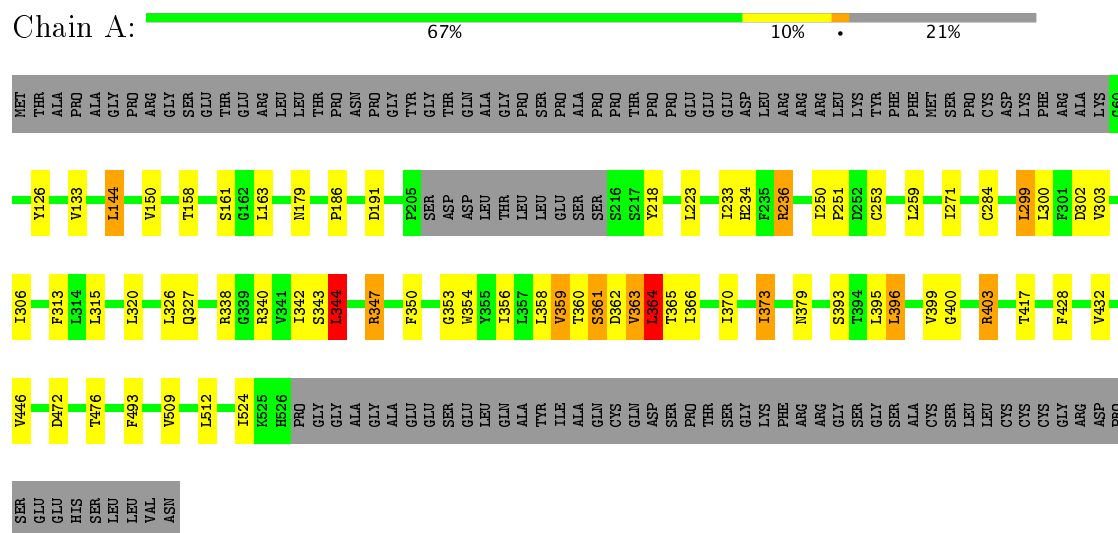
- Molecule 1 is a protein called Mucolipin-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	457	Total	C	N	O	S	0	0
			3660	2394	607	636	23		
1	B	457	Total	C	N	O	S	0	0
			3660	2394	607	636	23		
1	C	457	Total	C	N	O	S	0	0
			3660	2394	607	636	23		
1	D	457	Total	C	N	O	S	0	0
			3660	2394	607	636	23		

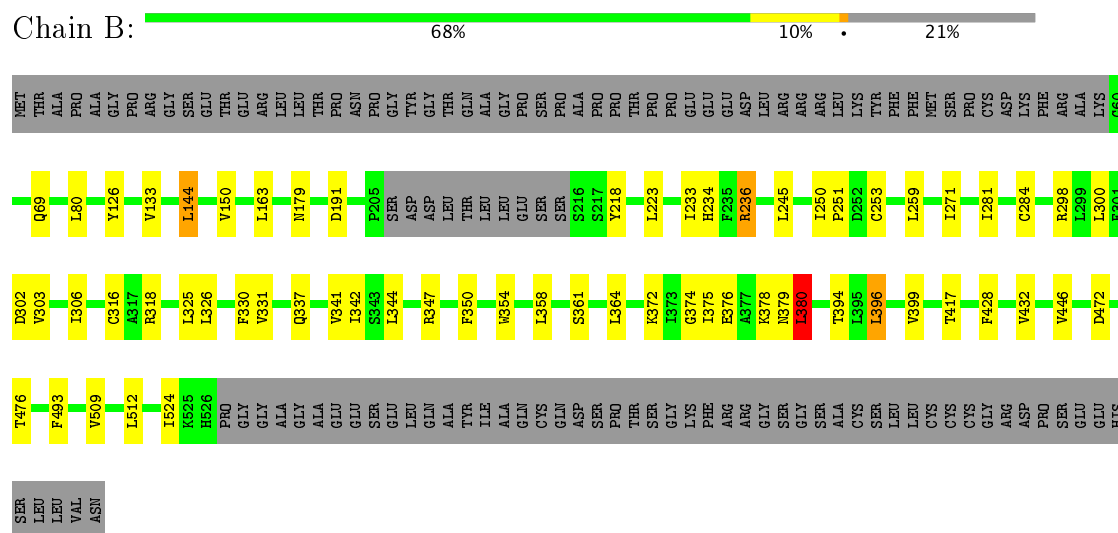
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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: Mucolin-1

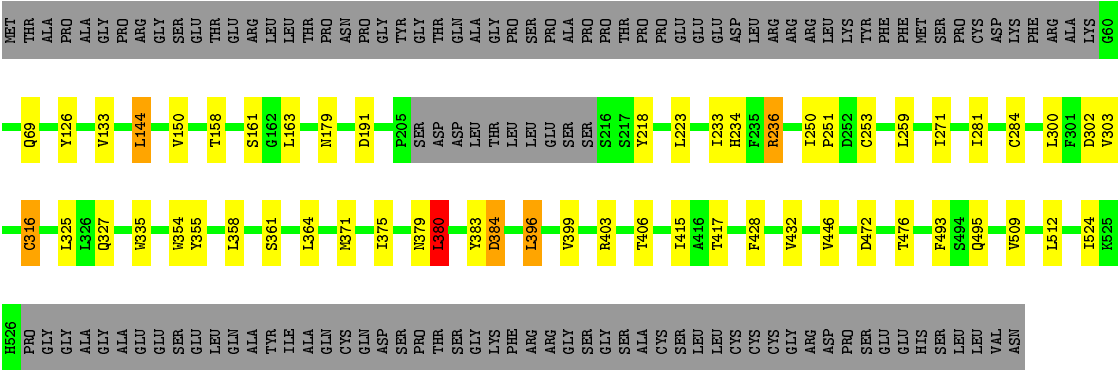


• Molecule 1: Mucolin-1

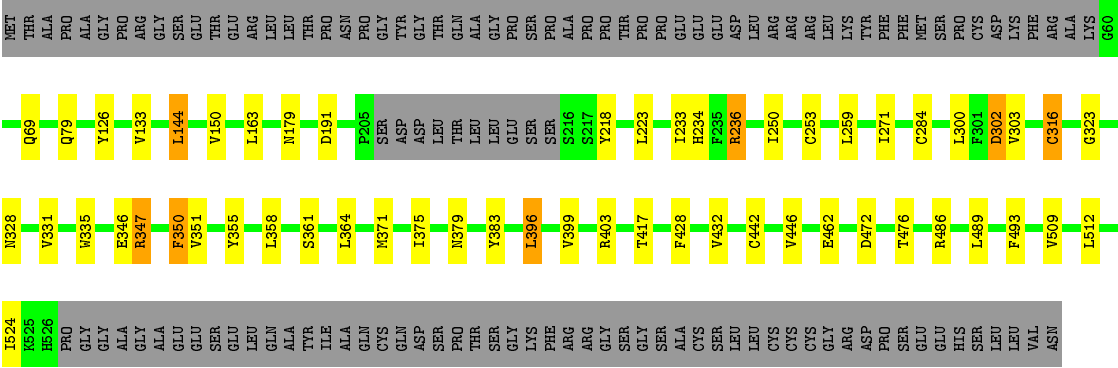


• Molecule 1: Mucolin-1





● Molecule 1: Mucolin-1



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	56105	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.6	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

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	$\# Z > 2$	RMSZ	$\# Z > 2$
1	A	0.46	1/3754 (0.0%)	0.64	2/5106 (0.0%)
1	B	0.43	0/3754	0.62	2/5106 (0.0%)
1	C	0.44	0/3754	0.63	3/5106 (0.1%)
1	D	0.44	0/3754	0.61	0/5106
All	All	0.44	1/15016 (0.0%)	0.63	7/20424 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	1
All	All	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	315	LEU	C-N	7.54	1.51	1.34

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	364	LEU	CA-CB-CG	8.75	135.42	115.30
1	C	380	LEU	N-CA-C	8.40	133.69	111.00
1	A	344	LEU	CA-CB-CG	7.29	132.06	115.30
1	C	354	TRP	CA-CB-CG	-5.97	102.36	113.70
1	B	380	LEU	CA-CB-CG	5.60	128.17	115.30
1	C	380	LEU	CA-CB-CG	5.54	128.05	115.30
1	B	354	TRP	CA-CB-CG	5.27	123.71	113.70

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	340	ARG	Peptide
1	B	341	VAL	Peptide
1	C	379	ASN	Peptide

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	3660	0	3684	51	0
1	B	3660	0	3684	34	0
1	C	3660	0	3684	28	0
1	D	3660	0	3684	31	0
All	All	14640	0	14736	137	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 5.

All (137) 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:359:VAL:O	1:A:362:ASP:HB3	1.57	1.04
1:A:347:ARG:O	1:A:350:PHE:HB2	1.61	0.99
1:A:344:LEU:HB2	1:A:347:ARG:HB3	1.67	0.76
1:A:299:LEU:HD23	1:A:373:ILE:HD11	1.71	0.71
1:B:372:LYS:HA	1:B:375:ILE:HG22	1.74	0.69
1:A:353:GLY:O	1:A:356:ILE:HG22	1.93	0.69
1:A:347:ARG:O	1:A:350:PHE:CB	2.38	0.68
1:A:362:ASP:O	1:A:365:THR:OG1	2.13	0.65
1:A:365:THR:HG23	1:A:393:SER:HB2	1.78	0.65
1:A:361:SER:HB3	1:A:396:LEU:HD22	1.83	0.60
1:A:344:LEU:CB	1:A:347:ARG:HB3	2.32	0.59
1:A:359:VAL:O	1:A:362:ASP:CB	2.43	0.59
1:A:360:THR:O	1:A:363:VAL:HG12	2.03	0.58
1:A:446:VAL:HG11	1:A:493:PHE:CD2	2.39	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:446:VAL:HG11	1:C:493:PHE:CD2	2.39	0.58
1:B:446:VAL:HG11	1:B:493:PHE:CD2	2.39	0.57
1:D:446:VAL:HG11	1:D:493:PHE:CD2	2.39	0.57
1:A:354:TRP:CG	1:A:403:ARG:HD2	2.39	0.56
1:A:320:LEU:HD11	1:A:356:ILE:HD12	1.88	0.56
1:C:406:THR:HG22	1:C:415:ILE:HG12	1.89	0.55
1:B:330:PHE:HB3	1:B:347:ARG:NH2	2.21	0.55
1:D:347:ARG:HA	1:D:350:PHE:HB3	1.89	0.54
1:A:365:THR:CG2	1:A:393:SER:HB2	2.38	0.53
1:C:300:LEU:O	1:C:303:VAL:HG22	2.09	0.53
1:A:300:LEU:O	1:A:303:VAL:HG22	2.09	0.52
1:D:300:LEU:O	1:D:303:VAL:HG22	2.09	0.52
1:B:300:LEU:O	1:B:303:VAL:HG22	2.09	0.52
1:A:313:PHE:HA	1:A:359:VAL:CG2	2.41	0.51
1:B:337:GLN:HB3	1:B:342:ILE:CD1	2.42	0.49
1:B:374:GLY:O	1:B:378:LYS:HB3	2.13	0.49
1:A:354:TRP:HZ2	1:A:400:GLY:CA	2.25	0.49
1:C:375:ILE:HG13	1:C:380:LEU:HA	1.95	0.49
1:A:344:LEU:HD13	1:A:347:ARG:HD2	1.96	0.48
1:C:69:GLN:NE2	1:C:358:LEU:HD21	2.29	0.48
1:A:313:PHE:HA	1:A:359:VAL:HG21	1.96	0.47
1:A:361:SER:CB	1:A:396:LEU:HD22	2.44	0.47
1:D:79:GLN:NE2	1:D:302:ASP:OD1	2.45	0.47
1:A:364:LEU:HD12	1:A:393:SER:HB3	1.96	0.47
1:A:150:VAL:HG21	1:A:236:ARG:CZ	2.45	0.47
1:D:150:VAL:HG21	1:D:236:ARG:CZ	2.45	0.47
1:B:150:VAL:HG21	1:B:236:ARG:CZ	2.45	0.47
1:B:69:GLN:NE2	1:B:358:LEU:HD21	2.29	0.47
1:A:446:VAL:HG11	1:A:493:PHE:CE2	2.50	0.47
1:C:150:VAL:HG21	1:C:236:ARG:CZ	2.45	0.47
1:C:383:TYR:O	1:C:384:ASP:C	2.53	0.47
1:D:316:CYS:SG	1:D:355:TYR:HB3	2.55	0.47
1:B:446:VAL:HG11	1:B:493:PHE:CE2	2.50	0.47
1:C:428:PHE:CE1	1:C:512:LEU:HD23	2.50	0.47
1:D:446:VAL:HG11	1:D:493:PHE:CE2	2.50	0.47
1:D:347:ARG:O	1:D:350:PHE:HD1	1.98	0.46
1:A:396:LEU:HA	1:A:399:VAL:HG22	1.97	0.46
1:B:344:LEU:HD23	1:B:347:ARG:HG3	1.98	0.46
1:A:306:ILE:HG12	1:A:366:ILE:HD11	1.96	0.46
1:C:446:VAL:HG11	1:C:493:PHE:CE2	2.50	0.46
1:D:331:VAL:HG22	1:D:335:TRP:HA	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:126:TYR:CE1	1:D:223:LEU:HD13	2.51	0.46
1:B:428:PHE:CE1	1:B:512:LEU:HD23	2.50	0.46
1:C:126:TYR:CE1	1:C:223:LEU:HD13	2.51	0.46
1:D:323:GLY:O	1:D:350:PHE:CZ	2.69	0.46
1:B:303:VAL:HA	1:B:306:ILE:HG12	1.98	0.46
1:D:350:PHE:CE1	1:D:351:VAL:HG23	2.50	0.46
1:D:69:GLN:NE2	1:D:358:LEU:HD21	2.30	0.46
1:C:316:CYS:SG	1:C:355:TYR:HB3	2.56	0.45
1:A:428:PHE:CE1	1:A:512:LEU:HD23	2.50	0.45
1:D:428:PHE:CE1	1:D:512:LEU:HD23	2.50	0.45
1:B:126:TYR:CE1	1:B:223:LEU:HD13	2.51	0.45
1:B:380:LEU:HD13	1:B:380:LEU:O	2.17	0.45
1:D:234:HIS:CE1	1:D:259:LEU:HD13	2.52	0.45
1:C:472:ASP:O	1:C:476:THR:HG23	2.17	0.45
1:C:234:HIS:CE1	1:C:259:LEU:HD13	2.52	0.45
1:D:396:LEU:HA	1:D:399:VAL:HG22	1.98	0.45
1:D:150:VAL:HG11	1:D:236:ARG:NH2	2.32	0.45
1:A:126:TYR:CE1	1:A:223:LEU:HD13	2.51	0.45
1:B:150:VAL:HG11	1:B:236:ARG:NH2	2.32	0.45
1:C:150:VAL:HG11	1:C:236:ARG:NH2	2.32	0.45
1:C:396:LEU:HA	1:C:399:VAL:HG22	1.99	0.45
1:A:234:HIS:CE1	1:A:259:LEU:HD13	2.52	0.44
1:B:396:LEU:HA	1:B:399:VAL:HG22	1.98	0.44
1:B:472:ASP:O	1:B:476:THR:HG23	2.17	0.44
1:A:343:SER:O	1:A:344:LEU:C	2.55	0.44
1:A:472:ASP:O	1:A:476:THR:HG23	2.17	0.44
1:B:234:HIS:CE1	1:B:259:LEU:HD13	2.52	0.44
1:C:250:ILE:HG23	1:C:251:PRO:HD2	1.99	0.44
1:A:150:VAL:HG11	1:A:236:ARG:NH2	2.32	0.44
1:B:271:ILE:HD12	1:C:144:LEU:HD22	2.00	0.44
1:C:281:ILE:HB	1:C:380:LEU:HD21	2.00	0.44
1:D:163:LEU:HD11	1:D:233:ILE:HG22	2.00	0.44
1:B:250:ILE:HG23	1:B:251:PRO:HD2	1.99	0.44
1:B:298:ARG:NH2	1:B:376:GLU:OE2	2.51	0.43
1:C:253:CYS:SG	1:C:284:CYS:N	2.85	0.43
1:A:250:ILE:HG23	1:A:251:PRO:HD2	1.99	0.43
1:D:253:CYS:SG	1:D:284:CYS:N	2.85	0.43
1:D:346:GLU:O	1:D:350:PHE:HB3	2.18	0.43
1:D:347:ARG:HG2	1:D:350:PHE:CE1	2.53	0.43
1:A:354:TRP:CH2	1:A:358:LEU:HD22	2.54	0.43
1:A:395:LEU:HB2	1:D:442:CYS:HB2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:271:ILE:HD12	1:B:144:LEU:HD22	2.00	0.43
1:A:354:TRP:HZ2	1:A:400:GLY:HA2	1.83	0.43
1:C:271:ILE:HD12	1:D:144:LEU:HD22	2.01	0.43
1:D:472:ASP:O	1:D:476:THR:HG23	2.17	0.43
1:B:163:LEU:HD11	1:B:233:ILE:HG22	2.00	0.42
1:D:133:VAL:HG11	1:D:218:TYR:CE2	2.55	0.42
1:D:375:ILE:HG21	1:D:383:TYR:CE1	2.53	0.42
1:B:331:VAL:HG22	1:B:342:ILE:HD13	2.00	0.42
1:C:133:VAL:HG11	1:C:218:TYR:CE2	2.55	0.42
1:A:163:LEU:HD11	1:A:233:ILE:HG22	2.00	0.42
1:A:326:LEU:HD22	1:A:350:PHE:CE1	2.54	0.42
1:A:338:ARG:CG	1:A:342:ILE:HD11	2.49	0.42
1:D:417:THR:HG22	1:D:524:ILE:HG21	2.02	0.42
1:A:133:VAL:HG11	1:A:218:TYR:CE2	2.55	0.42
1:B:133:VAL:HG11	1:B:218:TYR:CE2	2.55	0.42
1:B:253:CYS:SG	1:B:284:CYS:N	2.85	0.42
1:C:163:LEU:HD11	1:C:233:ILE:HG22	2.00	0.42
1:A:354:TRP:CD1	1:A:403:ARG:HD2	2.55	0.42
1:A:144:LEU:HD22	1:D:271:ILE:HD12	2.01	0.42
1:D:432:VAL:HG21	1:D:509:VAL:HG13	2.02	0.41
1:A:417:THR:HG22	1:A:524:ILE:HG21	2.02	0.41
1:B:372:LYS:CA	1:B:375:ILE:HG22	2.47	0.41
1:C:417:THR:HG22	1:C:524:ILE:HG21	2.01	0.41
1:C:495:GLN:NE2	1:D:462:GLU:OE2	2.53	0.41
1:B:432:VAL:HG21	1:B:509:VAL:HG13	2.03	0.41
1:A:432:VAL:HG21	1:A:509:VAL:HG13	2.03	0.41
1:C:432:VAL:HG21	1:C:509:VAL:HG13	2.03	0.41
1:A:163:LEU:HD11	1:A:233:ILE:CG2	2.51	0.41
1:A:186:PRO:HG3	1:B:245:LEU:HD22	2.03	0.41
1:C:163:LEU:HD11	1:C:233:ILE:CG2	2.51	0.41
1:B:163:LEU:HD11	1:B:233:ILE:CG2	2.51	0.41
1:A:363:VAL:HA	1:A:366:ILE:HG22	2.02	0.41
1:C:158:THR:N	1:C:161:SER:OG	2.54	0.41
1:A:253:CYS:SG	1:A:284:CYS:N	2.85	0.40
1:B:417:THR:HG22	1:B:524:ILE:HG21	2.02	0.40
1:C:69:GLN:HE22	1:C:358:LEU:HD21	1.85	0.40
1:D:163:LEU:HD11	1:D:233:ILE:CG2	2.51	0.40
1:A:158:THR:N	1:A:161:SER:OG	2.54	0.40
1:B:326:LEU:HD22	1:B:350:PHE:CE2	2.56	0.40
1:B:80:LEU:HD13	1:B:394:THR:OG1	2.22	0.40
1:B:281:ILE:H	1:B:380:LEU:HD21	1.85	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 PDB entries followed by that with respect to all EM entries.

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	453/580 (78%)	410 (90%)	42 (9%)	1 (0%)	51	85
1	B	453/580 (78%)	411 (91%)	41 (9%)	1 (0%)	51	85
1	C	453/580 (78%)	411 (91%)	40 (9%)	2 (0%)	38	77
1	D	453/580 (78%)	413 (91%)	39 (9%)	1 (0%)	51	85
All	All	1812/2320 (78%)	1645 (91%)	162 (9%)	5 (0%)	48	80

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	384	ASP
1	B	379	ASN
1	A	379	ASN
1	D	379	ASN
1	C	380	LEU

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 PDB entries followed by that with respect to all EM entries.

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	406/507 (80%)	389 (96%)	17 (4%)	34	70
1	B	406/507 (80%)	394 (97%)	12 (3%)	46	78
1	C	406/507 (80%)	391 (96%)	15 (4%)	39	73

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	D	406/507 (80%)	389 (96%)	17 (4%)	34 70
All	All	1624/2028 (80%)	1563 (96%)	61 (4%)	42 73

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

Mol	Chain	Res	Type
1	A	144	LEU
1	A	179	ASN
1	A	191	ASP
1	A	236	ARG
1	A	299	LEU
1	A	302	ASP
1	A	327	GLN
1	A	344	LEU
1	A	347	ARG
1	A	359	VAL
1	A	361	SER
1	A	363	VAL
1	A	364	LEU
1	A	370	ILE
1	A	373	ILE
1	A	396	LEU
1	A	403	ARG
1	B	144	LEU
1	B	179	ASN
1	B	191	ASP
1	B	236	ARG
1	B	302	ASP
1	B	316	CYS
1	B	318	ARG
1	B	325	LEU
1	B	361	SER
1	B	364	LEU
1	B	380	LEU
1	B	396	LEU
1	C	144	LEU
1	C	179	ASN
1	C	191	ASP
1	C	236	ARG
1	C	302	ASP
1	C	316	CYS
1	C	325	LEU

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Mol	Chain	Res	Type
1	C	327	GLN
1	C	335	TRP
1	C	361	SER
1	C	364	LEU
1	C	371	MET
1	C	380	LEU
1	C	396	LEU
1	C	403	ARG
1	D	144	LEU
1	D	179	ASN
1	D	191	ASP
1	D	236	ARG
1	D	250	ILE
1	D	302	ASP
1	D	316	CYS
1	D	328	ASN
1	D	347	ARG
1	D	350	PHE
1	D	361	SER
1	D	364	LEU
1	D	371	MET
1	D	396	LEU
1	D	403	ARG
1	D	486	ARG
1	D	489	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	97	ASN
1	A	124	GLN
1	A	179	ASN
1	A	410	ASN
1	B	69	GLN
1	B	97	ASN
1	B	124	GLN
1	B	179	ASN
1	B	379	ASN
1	B	469	ASN
1	B	483	GLN
1	C	69	GLN
1	C	97	ASN

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Mol	Chain	Res	Type
1	C	124	GLN
1	C	179	ASN
1	C	379	ASN
1	C	410	ASN
1	C	469	ASN
1	D	69	GLN
1	D	97	ASN
1	D	124	GLN
1	D	179	ASN
1	D	327	GLN
1	D	328	ASN
1	D	379	ASN
1	D	469	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 carbohydrates 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.