Full wwPDB/EMDataBank EM Map/Model Validation Report (i)

May 5, 2019 – 06:31 AM EDT

PDB ID	:	6QVD
EMDB ID:	:	EMD-4649
Title	:	CryoEM structure of the human ClC-1 chloride channel, CBS state 2
Authors	:	Wang, K.T.; Gourdon, P.E.; Zhou, Z.H.
Deposited on	:	2019-03-01
Resolution	:	4.34 Å(reported)
Based on PDB ID	:	5TQQ

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
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) symbol.

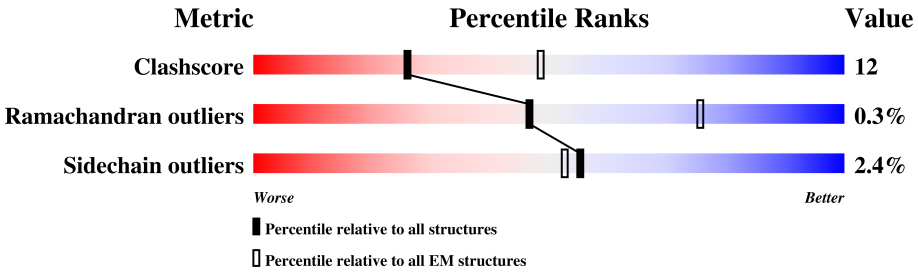
MolProbity	:	4.02b-467
Percentile statistics	:	20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20031633

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 4.34 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	136327	1886
Ramachandran outliers	132723	1663
Sidechain outliers	132532	1531

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 <=5%

Mol	Chain	Length	Quality of chain
1	A	988	41% 18% · 40%
1	B	988	40% 18% · 40%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 9212 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 Chloride channel protein 1.

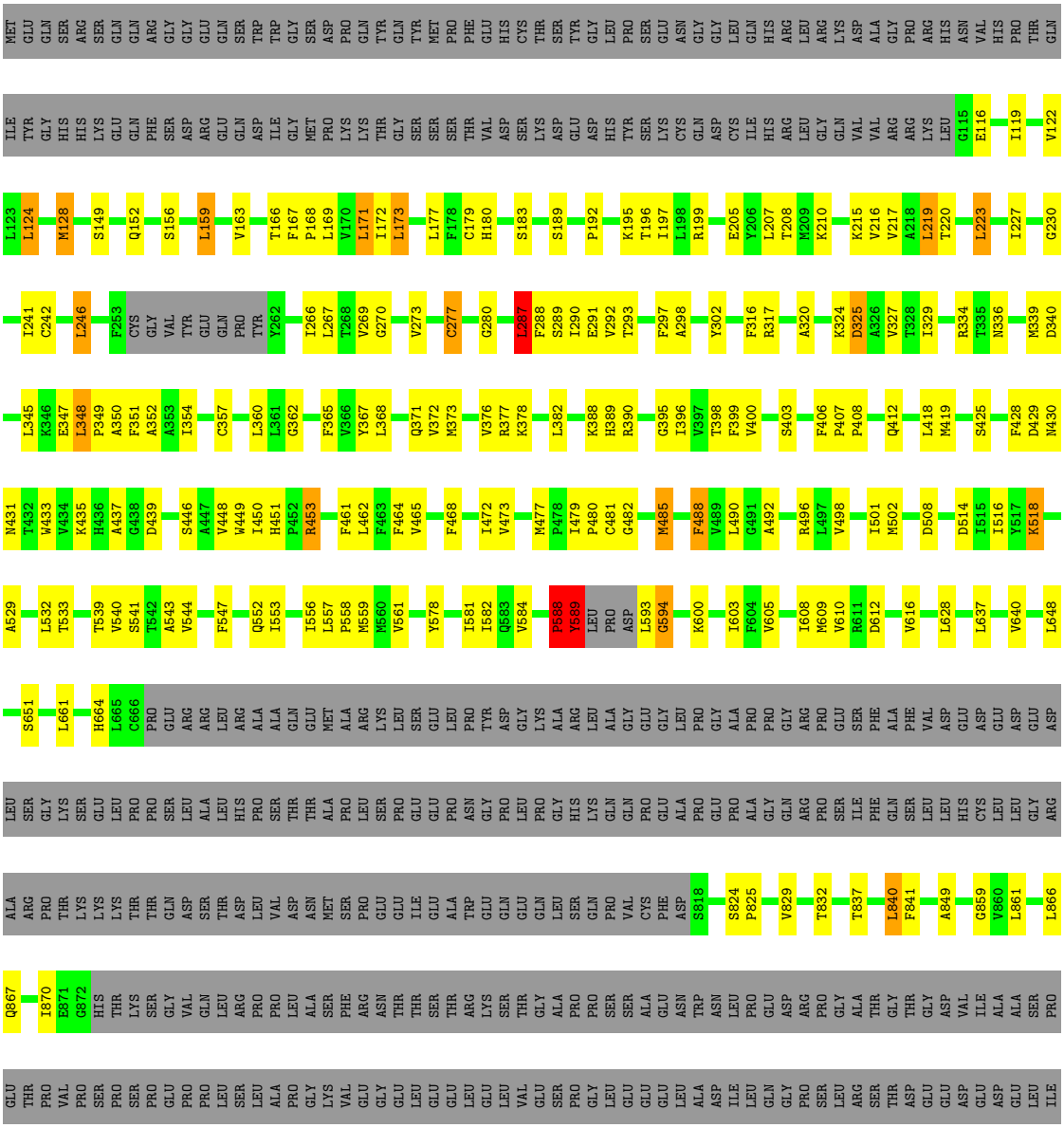
Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	596	Total	C	N	O	S	0	0
			4606	3047	736	788	35		
1	A	596	Total	C	N	O	S	0	0
			4606	3047	736	788	35		

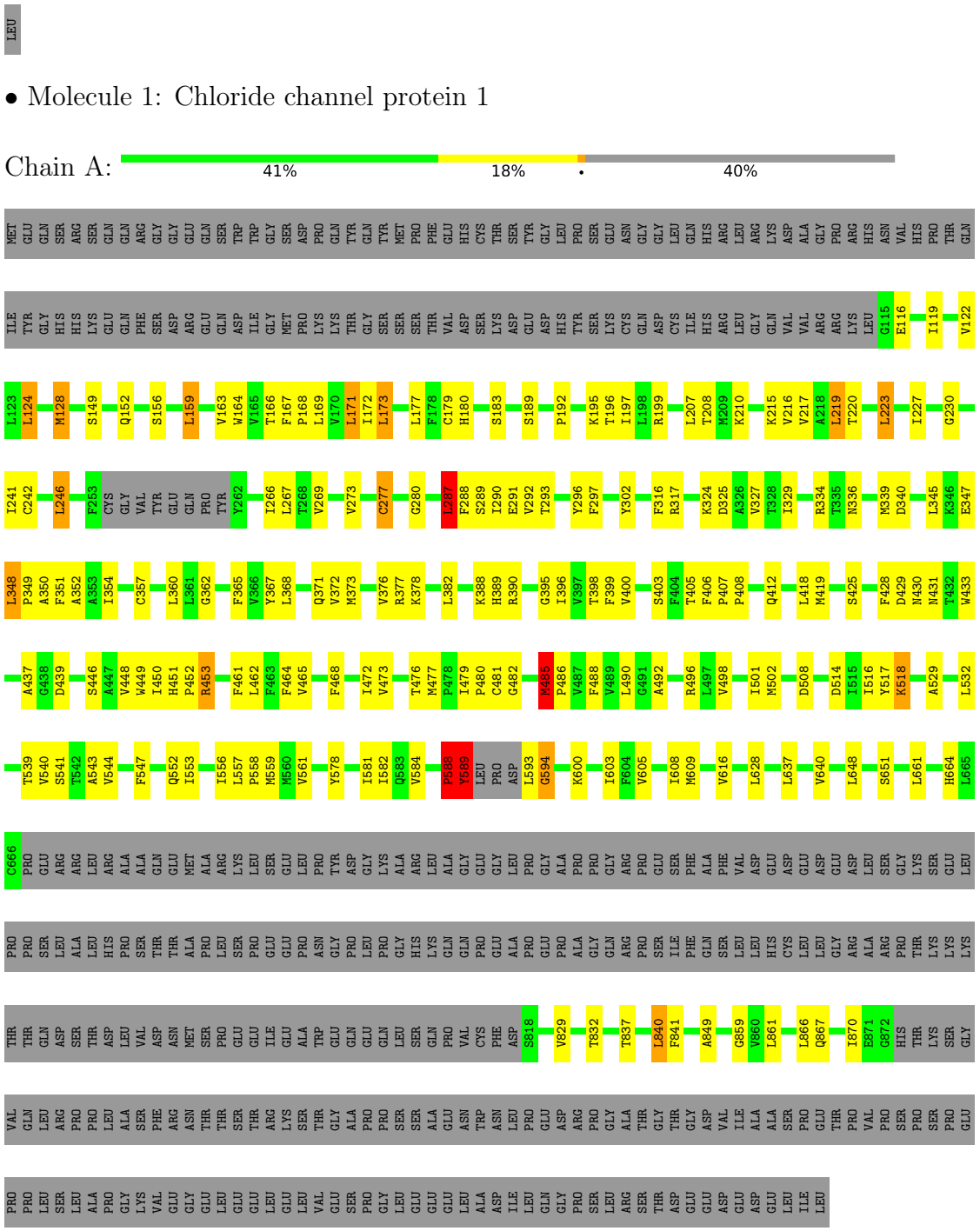
3 Residue-property plots (i)

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: Chloride channel protein 1

Chain B:





• Molecule 1: Chloride channel protein 1

Chain A: 41% 18% 40%

4 Experimental information (i)

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	74048	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	45	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	0.48	0/4721	0.94	22/6415 (0.3%)
1	B	0.48	0/4721	0.94	22/6415 (0.3%)
All	All	0.48	0/9442	0.94	44/12830 (0.3%)

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	8
1	B	0	8
All	All	0	16

There are no bond length outliers.

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	514	ASP	CB-CG-OD1	10.51	127.76	118.30
1	B	514	ASP	CB-CG-OD1	10.48	127.73	118.30
1	A	223	LEU	CA-CB-CG	8.92	135.82	115.30
1	B	223	LEU	CA-CB-CG	8.91	135.79	115.30
1	A	840	LEU	CA-CB-CG	8.39	134.61	115.30
1	B	840	LEU	CA-CB-CG	8.38	134.57	115.30
1	B	329	ILE	CG1-CB-CG2	-7.90	94.02	111.40
1	A	329	ILE	CG1-CB-CG2	-7.89	94.05	111.40
1	A	173	LEU	CA-CB-CG	7.51	132.57	115.30
1	B	173	LEU	CA-CB-CG	7.50	132.56	115.30
1	B	287	LEU	CA-CB-CG	7.44	132.42	115.30
1	B	177	LEU	CA-CB-CG	7.42	132.37	115.30
1	A	287	LEU	CA-CB-CG	7.42	132.37	115.30
1	A	177	LEU	CA-CB-CG	7.40	132.31	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	588	PRO	C-N-CA	7.37	140.12	121.70
1	A	588	PRO	C-N-CA	7.37	140.12	121.70
1	B	518	LYS	CD-CE-NZ	7.28	128.45	111.70
1	A	518	LYS	CD-CE-NZ	7.25	128.38	111.70
1	B	246	LEU	CA-CB-CG	6.85	131.06	115.30
1	A	246	LEU	CA-CB-CG	6.84	131.04	115.30
1	B	128	MET	CG-SD-CE	6.70	110.92	100.20
1	A	128	MET	CG-SD-CE	6.68	110.89	100.20
1	B	348	LEU	CA-CB-CG	6.47	130.19	115.30
1	A	348	LEU	CA-CB-CG	6.47	130.19	115.30
1	B	439	ASP	CB-CG-OD1	6.28	123.95	118.30
1	A	439	ASP	CB-CG-OD1	6.25	123.93	118.30
1	B	477	MET	CA-CB-CG	5.65	122.91	113.30
1	A	477	MET	CA-CB-CG	5.63	122.88	113.30
1	B	514	ASP	CB-CG-OD2	-5.52	113.33	118.30
1	A	514	ASP	CB-CG-OD2	-5.51	113.34	118.30
1	A	485	MET	CA-CB-CG	5.40	122.48	113.30
1	B	485	MET	CA-CB-CG	5.39	122.46	113.30
1	B	159	LEU	CA-CB-CG	5.38	127.68	115.30
1	A	159	LEU	CA-CB-CG	5.37	127.65	115.30
1	B	277	CYS	CA-CB-SG	5.37	123.66	114.00
1	A	277	CYS	CA-CB-SG	5.36	123.65	114.00
1	A	171	LEU	CA-CB-CG	5.34	127.58	115.30
1	B	171	LEU	CA-CB-CG	5.33	127.57	115.30
1	A	124	LEU	CA-CB-CG	5.29	127.47	115.30
1	B	124	LEU	CA-CB-CG	5.29	127.45	115.30
1	B	589	TYR	N-CA-C	5.22	125.10	111.00
1	A	589	TYR	N-CA-C	5.21	125.06	111.00
1	B	488	PHE	CB-CG-CD2	-5.17	117.18	120.80
1	A	488	PHE	CB-CG-CD2	-5.14	117.20	120.80

There are no chirality outliers.

All (16) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	290	ILE	Peptide
1	A	324	LYS	Peptide
1	A	325	ASP	Peptide
1	A	419	MET	Peptide
1	A	450	ILE	Peptide
1	A	508	ASP	Mainchain
1	A	588	PRO	Mainchain

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Mol	Chain	Res	Type	Group
1	A	594	GLY	Peptide
1	B	290	ILE	Peptide
1	B	324	LYS	Peptide
1	B	325	ASP	Peptide
1	B	419	MET	Peptide
1	B	450	ILE	Peptide
1	B	508	ASP	Mainchain
1	B	588	PRO	Mainchain
1	B	594	GLY	Peptide

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	4606	0	4751	116	0
1	B	4606	0	4751	118	0
All	All	9212	0	9502	228	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 12.

All (228) 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:637:LEU:O	1:A:651:SER:HA	1.80	0.82
1:B:637:LEU:O	1:B:651:SER:HA	1.80	0.82
1:A:396:ILE:O	1:A:399:PHE:HB3	1.85	0.77
1:B:396:ILE:O	1:B:399:PHE:HB3	1.85	0.76
1:B:280:GLY:HA3	1:B:317:ARG:HH12	1.51	0.75
1:A:280:GLY:HA3	1:A:317:ARG:HH12	1.51	0.73
1:B:395:GLY:O	1:B:398:THR:HB	1.89	0.72
1:A:395:GLY:O	1:A:398:THR:HB	1.89	0.71
1:A:376:VAL:HG12	1:A:377:ARG:HG2	1.75	0.69
1:B:376:VAL:HG12	1:B:377:ARG:HG2	1.75	0.69
1:B:156:SER:HB3	1:B:159:LEU:HG	1.76	0.68
1:B:163:VAL:HA	1:B:166:THR:HG22	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:340:ASP:OD1	1:A:334:ARG:NH2	2.27	0.67
1:A:163:VAL:HA	1:A:166:THR:HG22	1.77	0.66
1:A:156:SER:HB3	1:A:159:LEU:HG	1.76	0.65
1:B:373:MET:O	1:B:376:VAL:HB	1.98	0.63
1:B:431:ASN:O	1:B:496:ARG:NH2	2.31	0.63
1:A:373:MET:O	1:A:376:VAL:HB	1.98	0.63
1:A:357:CYS:O	1:A:360:LEU:HB3	1.99	0.62
1:A:431:ASN:O	1:A:496:ARG:NH2	2.31	0.62
1:B:357:CYS:O	1:B:360:LEU:HB3	1.99	0.61
1:B:189:SER:HB3	1:B:480:PRO:HB3	1.83	0.61
1:A:189:SER:HB3	1:A:480:PRO:HB3	1.83	0.60
1:A:287:LEU:HD21	1:A:544:VAL:HG11	1.84	0.60
1:A:418:LEU:HD21	1:A:448:VAL:HG21	1.83	0.60
1:A:273:VAL:O	1:A:277:CYS:CB	2.51	0.59
1:B:199:ARG:NH2	1:B:589:TYR:O	2.35	0.59
1:B:418:LEU:HD21	1:B:448:VAL:HG21	1.84	0.59
1:B:287:LEU:HD21	1:B:544:VAL:HG11	1.84	0.58
1:B:292:VAL:HG13	1:B:293:THR:HG23	1.86	0.58
1:B:297:PHE:HE2	1:B:302:TYR:HB2	1.67	0.58
1:A:199:ARG:NH2	1:A:589:TYR:O	2.35	0.58
1:B:273:VAL:O	1:B:277:CYS:CB	2.51	0.58
1:A:297:PHE:HE2	1:A:302:TYR:HB2	1.67	0.58
1:B:192:PRO:HB2	1:B:582:ILE:HG23	1.86	0.58
1:A:336:ASN:O	1:A:430:ASN:ND2	2.37	0.58
1:B:589:TYR:HD2	1:B:594:GLY:H	1.51	0.58
1:A:124:LEU:HD12	1:A:246:LEU:HD11	1.87	0.57
1:A:149:SER:HA	1:A:152:GLN:HG2	1.85	0.57
1:A:179:CYS:O	1:A:183:SER:OG	2.22	0.57
1:A:589:TYR:HD2	1:A:594:GLY:H	1.51	0.57
1:B:179:CYS:O	1:B:183:SER:OG	2.22	0.57
1:A:192:PRO:HA	1:A:195:LYS:HG2	1.86	0.57
1:A:192:PRO:HB2	1:A:582:ILE:HG23	1.86	0.57
1:B:149:SER:HA	1:B:152:GLN:HG2	1.85	0.57
1:B:192:PRO:HA	1:B:195:LYS:HG2	1.86	0.57
1:A:292:VAL:HG13	1:A:293:THR:HG23	1.86	0.57
1:B:351:PHE:HD1	1:B:354:ILE:HD12	1.69	0.57
1:B:336:ASN:O	1:B:430:ASN:ND2	2.37	0.57
1:A:498:VAL:HA	1:A:501:ILE:HG12	1.87	0.57
1:A:351:PHE:HD1	1:A:354:ILE:HD12	1.69	0.56
1:A:479:ILE:HD13	1:A:481:CYS:HB3	1.87	0.56
1:A:593:LEU:O	1:A:867:GLN:NE2	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:273:VAL:O	1:A:277:CYS:HB2	2.05	0.56
1:B:593:LEU:O	1:B:867:GLN:NE2	2.38	0.56
1:B:498:VAL:HA	1:B:501:ILE:HG12	1.87	0.56
1:A:199:ARG:HB3	1:A:593:LEU:HB2	1.88	0.56
1:B:124:LEU:HD12	1:B:246:LEU:HD11	1.87	0.56
1:A:289:SER:O	1:A:293:THR:OG1	2.24	0.55
1:B:289:SER:O	1:B:293:THR:OG1	2.24	0.55
1:B:588:PRO:O	1:B:593:LEU:HA	2.06	0.55
1:A:867:GLN:HA	1:A:870:ILE:HG22	1.88	0.55
1:B:273:VAL:O	1:B:277:CYS:HB2	2.05	0.55
1:A:588:PRO:O	1:A:593:LEU:HA	2.06	0.55
1:B:334:ARG:NH2	1:A:340:ASP:OD1	2.40	0.55
1:B:479:ILE:HD13	1:B:481:CYS:HB3	1.87	0.55
1:A:539:THR:OG1	1:A:540:VAL:N	2.40	0.55
1:B:199:ARG:HB3	1:B:593:LEU:HB2	1.88	0.55
1:B:348:LEU:O	1:B:351:PHE:HB2	2.06	0.55
1:B:867:GLN:HA	1:B:870:ILE:HG22	1.88	0.54
1:A:348:LEU:O	1:A:351:PHE:HB2	2.06	0.54
1:A:368:LEU:HA	1:A:371:GLN:HB2	1.90	0.54
1:A:372:VAL:O	1:A:376:VAL:N	2.41	0.54
1:B:609:MET:HB2	1:B:859:GLY:HA3	1.90	0.54
1:A:429:ASP:O	1:A:496:ARG:NH1	2.39	0.53
1:B:605:VAL:HA	1:B:608:ILE:HD13	1.89	0.53
1:B:368:LEU:HA	1:B:371:GLN:HB2	1.90	0.53
1:B:400:VAL:O	1:B:403:SER:HB3	2.09	0.53
1:A:400:VAL:O	1:A:403:SER:HB3	2.09	0.53
1:B:539:THR:OG1	1:B:540:VAL:N	2.40	0.53
1:A:605:VAL:HA	1:A:608:ILE:HD13	1.89	0.53
1:A:207:LEU:HD13	1:A:241:ILE:HG12	1.91	0.53
1:B:492:ALA:HB2	1:B:529:ALA:HB2	1.91	0.53
1:A:609:MET:HB2	1:A:859:GLY:HA3	1.90	0.53
1:B:196:THR:HG23	1:B:593:LEU:HD21	1.91	0.53
1:B:372:VAL:O	1:B:376:VAL:N	2.41	0.52
1:B:217:VAL:O	1:B:220:THR:HB	2.09	0.52
1:A:196:THR:HG23	1:A:593:LEU:HD21	1.91	0.52
1:B:207:LEU:HD13	1:B:241:ILE:HG12	1.91	0.52
1:B:429:ASP:O	1:B:496:ARG:NH1	2.39	0.52
1:B:547:PHE:HB3	1:B:553:ILE:HG22	1.91	0.52
1:A:167:PHE:CD1	1:A:168:PRO:HD3	2.44	0.52
1:A:217:VAL:O	1:A:220:THR:HB	2.09	0.52
1:B:208:THR:HG22	1:B:210:LYS:H	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:472:ILE:O	1:A:476:THR:OG1	2.19	0.51
1:A:373:MET:HB3	1:A:584:VAL:HG11	1.93	0.51
1:A:492:ALA:HB2	1:A:529:ALA:HB2	1.91	0.51
1:B:167:PHE:CD1	1:B:168:PRO:HD3	2.44	0.51
1:B:373:MET:HB3	1:B:584:VAL:HG11	1.93	0.51
1:B:349:PRO:O	1:B:352:ALA:HB3	2.11	0.51
1:A:616:VAL:HG22	1:A:628:LEU:HD13	1.93	0.51
1:A:208:THR:HG22	1:A:210:LYS:H	1.75	0.51
1:B:168:PRO:HA	1:B:171:LEU:HG	1.93	0.51
1:B:468:PHE:HE1	1:B:490:LEU:HD11	1.76	0.51
1:A:547:PHE:HB3	1:A:553:ILE:HG22	1.91	0.50
1:A:468:PHE:HE1	1:A:490:LEU:HD11	1.76	0.50
1:A:472:ILE:HD12	1:A:473:VAL:HG13	1.93	0.50
1:A:640:VAL:HG12	1:A:648:LEU:HA	1.93	0.50
1:B:287:LEU:O	1:B:291:GLU:HB3	2.11	0.50
1:A:349:PRO:O	1:A:352:ALA:HB3	2.11	0.50
1:A:287:LEU:O	1:A:291:GLU:HB3	2.11	0.50
1:B:616:VAL:HG22	1:B:628:LEU:HD13	1.93	0.50
1:B:640:VAL:HG12	1:B:648:LEU:HA	1.93	0.50
1:B:558:PRO:HA	1:B:561:VAL:HG22	1.94	0.50
1:A:388:LYS:HD3	1:A:389:HIS:HB2	1.95	0.49
1:B:446:SER:HA	1:B:449:TRP:HD1	1.78	0.49
1:A:168:PRO:HA	1:A:171:LEU:HG	1.93	0.49
1:B:388:LYS:HD3	1:B:389:HIS:HB2	1.94	0.49
1:B:362:GLY:HA2	1:B:365:PHE:CE1	2.48	0.49
1:B:433:TRP:O	1:B:437:ALA:N	2.46	0.49
1:B:472:ILE:HD12	1:B:473:VAL:HG13	1.93	0.49
1:B:172:ILE:HG13	1:B:398:THR:HG21	1.95	0.49
1:A:558:PRO:HA	1:A:561:VAL:HG22	1.94	0.48
1:B:220:THR:HA	1:B:223:LEU:HG	1.96	0.48
1:B:461:PHE:HA	1:B:464:PHE:CE1	2.49	0.48
1:A:433:TRP:O	1:A:437:ALA:N	2.46	0.48
1:A:451:HIS:CD2	1:A:453:ARG:H	2.32	0.48
1:B:116:GLU:HG2	1:B:119:ILE:HD12	1.96	0.48
1:B:451:HIS:CD2	1:B:453:ARG:H	2.32	0.48
1:A:446:SER:HA	1:A:449:TRP:HD1	1.78	0.48
1:A:347:GLU:O	1:A:350:ALA:HB3	2.14	0.48
1:A:172:ILE:HG13	1:A:398:THR:HG21	1.95	0.48
1:A:116:GLU:HG2	1:A:119:ILE:HD12	1.96	0.47
1:B:298:ALA:HB2	1:A:296:TYR:HE1	1.79	0.47
1:A:362:GLY:HA2	1:A:365:PHE:CE1	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:841:PHE:HZ	1:A:849:ALA:HB2	1.80	0.47
1:A:216:VAL:O	1:A:219:LEU:HB2	2.15	0.47
1:A:220:THR:HA	1:A:223:LEU:HG	1.96	0.47
1:B:205:GLU:O	1:B:208:THR:OG1	2.28	0.47
1:B:273:VAL:O	1:B:277:CYS:HB3	2.14	0.47
1:A:461:PHE:HA	1:A:464:PHE:CE1	2.49	0.47
1:B:841:PHE:HZ	1:B:849:ALA:HB2	1.79	0.47
1:B:347:GLU:O	1:B:350:ALA:HB3	2.14	0.47
1:B:367:TYR:HD2	1:B:368:LEU:HD22	1.80	0.47
1:A:516:ILE:HD11	1:A:518:LYS:NZ	2.30	0.47
1:A:273:VAL:O	1:A:277:CYS:HB3	2.14	0.46
1:B:516:ILE:HD11	1:B:518:LYS:NZ	2.30	0.46
1:B:216:VAL:O	1:B:219:LEU:HB2	2.14	0.46
1:A:192:PRO:HB3	1:A:578:TYR:HB3	1.98	0.46
1:A:461:PHE:HD2	1:A:462:LEU:HD22	1.81	0.46
1:A:408:PRO:O	1:A:412:GLN:NE2	2.49	0.46
1:A:661:LEU:HA	1:A:664:HIS:CE1	2.51	0.46
1:B:408:PRO:O	1:B:412:GLN:NE2	2.49	0.46
1:B:288:PHE:HD1	1:B:541:SER:HG	1.63	0.46
1:B:661:LEU:HA	1:B:664:HIS:CE1	2.51	0.46
1:A:288:PHE:HD1	1:A:541:SER:HG	1.63	0.45
1:B:180:HIS:ND1	1:B:390:ARG:HD3	2.32	0.45
1:A:230:GLY:HA3	1:A:482:GLY:O	2.17	0.45
1:B:339:MET:SD	1:A:552:GLN:NE2	2.86	0.45
1:B:461:PHE:HD2	1:B:462:LEU:HD22	1.81	0.45
1:A:219:LEU:O	1:A:223:LEU:N	2.41	0.45
1:A:266:ILE:HA	1:A:269:VAL:HG12	1.99	0.45
1:B:192:PRO:HB3	1:B:578:TYR:HB3	1.98	0.45
1:A:197:ILE:HG22	1:A:267:LEU:HD21	1.99	0.45
1:A:291:GLU:OE2	1:A:539:THR:OG1	2.27	0.45
1:A:367:TYR:HD2	1:A:368:LEU:HD22	1.80	0.45
1:B:197:ILE:HG22	1:B:267:LEU:HD21	1.99	0.45
1:A:532:LEU:HD13	1:A:532:LEU:HA	1.79	0.45
1:A:861:LEU:HD21	1:A:866:LEU:HB2	1.99	0.45
1:B:230:GLY:HA3	1:B:482:GLY:O	2.17	0.44
1:A:334:ARG:NH2	1:A:336:ASN:OD1	2.50	0.44
1:A:348:LEU:HD23	1:A:349:PRO:HD3	1.99	0.44
1:B:334:ARG:NH2	1:A:339:MET:O	2.50	0.44
1:B:556:ILE:O	1:B:559:MET:HG3	2.17	0.44
1:B:861:LEU:HD21	1:B:866:LEU:HB2	1.99	0.44
1:B:348:LEU:HD23	1:B:349:PRO:HD3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:266:ILE:HA	1:B:269:VAL:HG12	1.99	0.44
1:A:316:PHE:HD2	1:A:317:ARG:HH11	1.65	0.44
1:A:180:HIS:ND1	1:A:390:ARG:HD3	2.32	0.44
1:B:334:ARG:NH2	1:B:336:ASN:OD1	2.50	0.44
1:A:119:ILE:HA	1:A:122:VAL:HG12	2.00	0.44
1:B:552:GLN:NE2	1:A:339:MET:SD	2.86	0.44
1:B:316:PHE:HD2	1:B:317:ARG:HH11	1.65	0.43
1:A:406:PHE:HA	1:A:407:PRO:HD3	1.77	0.43
1:A:829:VAL:O	1:A:832:THR:OG1	2.28	0.43
1:B:171:LEU:HD12	1:B:172:ILE:HG12	2.00	0.43
1:B:219:LEU:O	1:B:223:LEU:N	2.41	0.43
1:B:297:PHE:CE2	1:B:302:TYR:HB2	2.52	0.43
1:A:556:ILE:O	1:A:559:MET:HG3	2.17	0.43
1:B:347:GLU:HG3	1:B:347:GLU:H	1.56	0.43
1:A:171:LEU:HD12	1:A:172:ILE:HG12	2.00	0.43
1:A:297:PHE:CE2	1:A:302:TYR:HB2	2.52	0.43
1:A:451:HIS:HA	1:A:452:PRO:HD3	1.89	0.43
1:B:578:TYR:HA	1:B:581:ILE:HD12	2.00	0.43
1:A:242:CYS:O	1:A:246:LEU:HG	2.19	0.42
1:B:215:LYS:HB2	1:B:215:LYS:HE2	1.79	0.42
1:B:242:CYS:O	1:B:246:LEU:HG	2.19	0.42
1:B:472:ILE:H	1:B:472:ILE:HG13	1.54	0.42
1:B:435:LYS:HG2	1:B:435:LYS:H	1.65	0.42
1:B:532:LEU:HA	1:B:532:LEU:HD13	1.79	0.42
1:A:465:VAL:HA	1:A:468:PHE:CD2	2.55	0.42
1:A:517:TYR:HA	1:A:517:TYR:HD1	1.74	0.42
1:A:578:TYR:HA	1:A:581:ILE:HD12	2.00	0.42
1:B:119:ILE:HA	1:B:122:VAL:HG12	2.00	0.42
1:B:829:VAL:O	1:B:832:THR:OG1	2.28	0.41
1:A:837:THR:HA	1:A:840:LEU:HG	2.01	0.41
1:B:837:THR:HA	1:B:840:LEU:HG	2.01	0.41
1:A:215:LYS:HE2	1:A:215:LYS:HB2	1.79	0.41
1:B:465:VAL:HA	1:B:468:PHE:CD2	2.55	0.41
1:B:425:SER:HA	1:B:428:PHE:CE1	2.55	0.41
1:B:556:ILE:HG23	1:B:557:LEU:HD22	2.03	0.41
1:B:543:ALA:HB1	1:B:559:MET:SD	2.61	0.41
1:B:824:SER:HA	1:B:825:PRO:HD3	1.87	0.41
1:A:164:TRP:NE1	1:A:405:THR:OG1	2.47	0.41
1:A:543:ALA:HB1	1:A:559:MET:SD	2.61	0.41
1:A:425:SER:HA	1:A:428:PHE:CE1	2.55	0.41
1:B:270:GLY:HA2	1:B:273:VAL:HG22	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:600:LYS:HD2	1:A:603:ILE:H	1.86	0.41
1:B:600:LYS:HD2	1:B:603:ILE:H	1.86	0.41
1:A:557:LEU:HD13	1:A:557:LEU:HA	1.92	0.40
1:B:488:PHE:CE1	1:B:533:THR:HG21	2.56	0.40
1:B:610:VAL:HG12	1:B:612:ASP:H	1.86	0.40
1:A:485:MET:HG2	1:A:486:PRO:HD3	2.03	0.40
1:B:320:ALA:O	1:B:325:ASP:HA	2.21	0.40
1:A:339:MET:HE2	1:A:339:MET:HB3	1.76	0.40
1:A:553:ILE:H	1:A:553:ILE:HG13	1.77	0.40
1:B:406:PHE:HA	1:B:407:PRO:HD3	1.77	0.40
1:B:589:TYR:HD2	1:B:594:GLY:N	2.19	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	590/988 (60%)	531 (90%)	57 (10%)	2 (0%)	43 80
1	B	590/988 (60%)	532 (90%)	56 (10%)	2 (0%)	43 80
All	All	1180/1976 (60%)	1063 (90%)	113 (10%)	4 (0%)	47 80

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	589	TYR
1	A	589	TYR
1	B	327	VAL
1	A	327	VAL

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	499/838 (60%)	487 (98%)	12 (2%)	52 75
1	B	499/838 (60%)	487 (98%)	12 (2%)	52 75
All	All	998/1676 (60%)	974 (98%)	24 (2%)	55 75

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	128	MET
1	B	169	LEU
1	B	173	LEU
1	B	219	LEU
1	B	227	ILE
1	B	287	LEU
1	B	345	LEU
1	B	378	LYS
1	B	382	LEU
1	B	453	ARG
1	B	485	MET
1	B	502	MET
1	A	128	MET
1	A	169	LEU
1	A	173	LEU
1	A	219	LEU
1	A	227	ILE
1	A	287	LEU
1	A	345	LEU
1	A	378	LYS
1	A	382	LEU
1	A	453	ARG
1	A	485	MET
1	A	502	MET

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

Mol	Chain	Res	Type
1	B	451	HIS
1	A	451	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.