



# Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Jan 3, 2018 – 10:54 AM EST

PDB ID : 5OYB  
EMDB ID: : EMD-3860  
Title : Structure of calcium-bound mTMEM16A chloride channel at 3.75 Å resolution  
Authors : Paulino, C.; Kalienkova, V.; Lam, K.M.; Neldner, Y.; Dutzler, R.  
Deposited on : 2017-09-08  
Resolution : 3.75 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](mailto: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.

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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-20030736

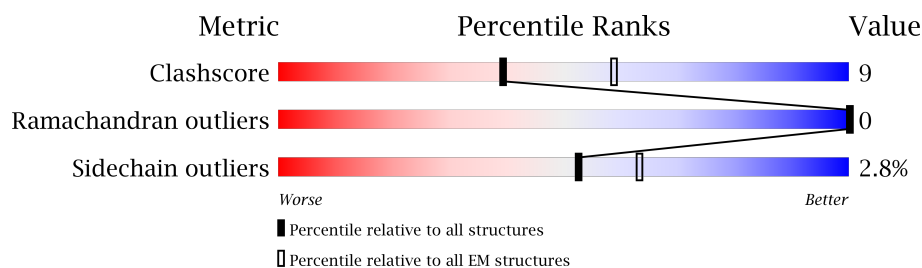
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*



The reported resolution of this entry is 3.75 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  $\geq 3$ , 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  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	A	960	
1	B	960	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 11770 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 Anoctamin-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	718	Total	C	N	O	S	0	0
			5883	3842	968	1036	37		
1	B	718	Total	C	N	O	S	0	0
			5883	3842	968	1036	37		

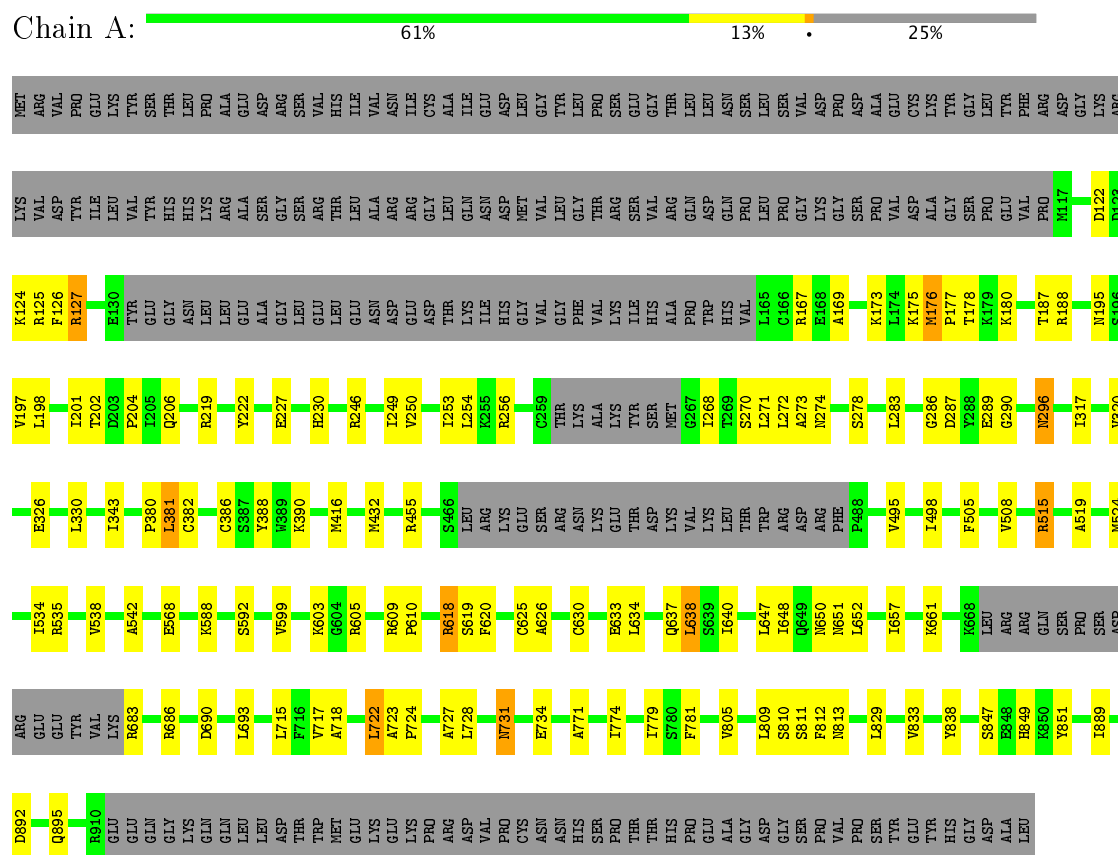
- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
2	B	2	Total	Ca	0
			2	2	
2	A	2	Total	Ca	0
			2	2	

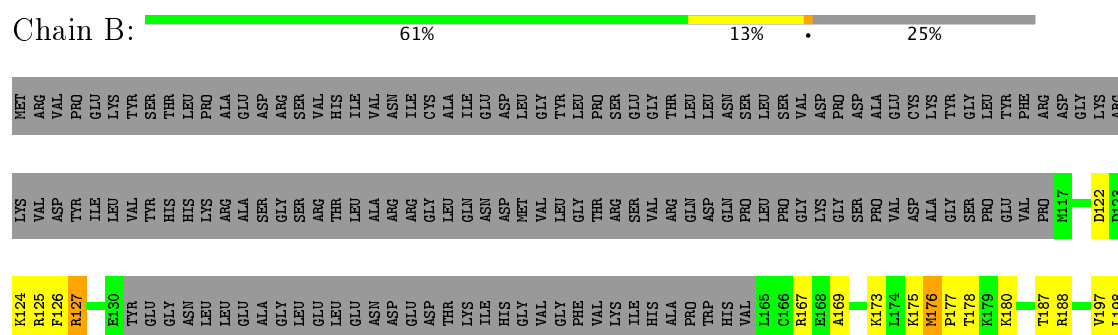
### 3 Residue-property plots

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: Anoctamin-1



#### • Molecule 1: Anoctamin-1



1889	GLU	1534	V320	1201
D892	GLU	R535	E326	T202
Q895	TYR	V538	L330	D203
Q896	VAL	A542	I343	P204
Q897	LYS	E568	P380	I205
Q898	R663	K588	S592	Q206
Q899	L693	S599	Y388	R219
Q900	L715	R603	K389	Y222
Q901	F716	G604	K390	E227
Q902	V717	R605	M416	H230
Q903	A718	R609	M432	L231
Q904	L722	P610	R455	R246
Q905	A723	R618	S466	I249
Q906	F724	S619	LEU	V250
Q907	A727	F620	ARG	I253
Q908	L728	C625	LYS	L254
Q909	N731	A626	GLU	K255
Q910	E734	C630	GLU	R256
Q911	A771	E633	ARG	C259
Q912	I774	L634	ASN	THR
Q913	I779	Q637	LYS	LYS
Q914	F780	L638	ASN	ALA
Q915	F781	S639	GLU	LYS
Q916	V805	I640	THR	TYR
Q917	L809	L647	ASP	LYS
Q918	S810	I648	LYS	MET
Q919	S811	Q649	VAL	G267
Q920	F812	N650	LYS	I268
Q921	N813	I651	LEU	F268
Q922	GLY	L652	THR	S270
Q923	SER	I657	TRP	L271
Q924	PRO	K661	ARG	L272
Q925	VAL	K668	ASP	A273
Q926	SER	LEU	ARG	N274
Q927	TYR	ARG	PHE	S276
Q928	GLU	GLN	F468	L283
Q929	TYR	SER	V495	G286
Q930	GLU	PRO	I498	D287
Q931	GLU	S847	F805	I286
Q932	HIS	E848	V508	E289
Q933	GLY	H849	R515	G290
Q934	ASP	K850	A519	N296
Q935	ALA	Y851	M524	W305
Q936	LEU	S854	P316	P316
Q937		K855	I317	I317

## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	147368	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; The contrast transfer function (CTF) parameters were estimated on the movie frames by ctffind4.1	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	80	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	46511	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA

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	0.40	0/6032	0.60	0/8160
1	B	0.40	0/6032	0.60	0/8160
All	All	0.40	0/12064	0.60	0/16320

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	5883	0	5898	105	0
1	B	5883	0	5898	104	0
2	A	2	0	0	1	0
2	B	2	0	0	1	0
All	All	11770	0	11796	209	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 9.

All (209) 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:812:PHE:CD1	1:B:813:ASN:N	2.33	0.97
1:A:812:PHE:CD1	1:A:813:ASN:N	2.33	0.97
1:B:812:PHE:HD1	1:B:813:ASN:H	1.09	0.91
1:B:176:MET:CE	1:B:180:LYS:HE3	2.03	0.89
1:A:380:PRO:O	1:A:381:LEU:HD12	1.74	0.88
1:B:176:MET:CE	1:B:180:LYS:CE	2.52	0.88
1:A:812:PHE:HD1	1:A:813:ASN:H	1.09	0.88
1:A:176:MET:CE	1:A:180:LYS:HE3	2.03	0.87
1:A:176:MET:CE	1:A:180:LYS:CE	2.52	0.87
1:B:380:PRO:O	1:B:381:LEU:HD12	1.74	0.86
1:A:176:MET:HE1	1:A:180:LYS:CE	2.07	0.85
1:B:176:MET:HE3	1:B:180:LYS:CE	2.08	0.84
1:B:515:ARG:HH21	1:B:519:ALA:HB2	1.44	0.83
1:B:187:THR:O	1:B:198:LEU:HB3	1.81	0.81
1:A:187:THR:O	1:A:198:LEU:HB3	1.81	0.81
1:B:610:PRO:HB2	1:B:812:PHE:CE2	2.17	0.80
1:A:610:PRO:HB2	1:A:812:PHE:CE2	2.17	0.80
1:A:515:ARG:HH21	1:A:519:ALA:HB2	1.44	0.80
1:B:176:MET:HE1	1:B:180:LYS:CE	2.16	0.75
1:A:176:MET:HE3	1:A:180:LYS:CE	2.17	0.75
1:B:619:SER:HG	1:B:620:PHE:HD1	1.37	0.73
1:B:176:MET:CE	1:B:180:LYS:HE2	2.17	0.73
1:B:812:PHE:CD1	1:B:851:TYR:OH	2.42	0.73
1:A:176:MET:CE	1:A:180:LYS:HE2	2.17	0.73
1:A:176:MET:HE3	1:A:180:LYS:HE3	1.71	0.72
1:B:812:PHE:HD1	1:B:851:TYR:HH	1.34	0.72
1:A:805:VAL:O	1:A:809:LEU:CD2	2.38	0.72
1:B:176:MET:HE3	1:B:180:LYS:HE3	1.67	0.71
1:A:812:PHE:CD1	1:A:851:TYR:OH	2.42	0.71
1:B:805:VAL:O	1:B:809:LEU:HD23	1.90	0.71
1:B:343:ILE:HD13	1:B:728:LEU:HD11	1.71	0.71
1:B:805:VAL:O	1:B:809:LEU:CD2	2.38	0.71
1:A:343:ILE:HD13	1:A:728:LEU:HD11	1.71	0.71
1:A:805:VAL:O	1:A:809:LEU:HD23	1.90	0.71
1:B:380:PRO:O	1:B:381:LEU:CD1	2.39	0.70
1:A:380:PRO:O	1:A:381:LEU:CD1	2.39	0.70
1:A:206:GLN:HE22	1:A:246:ARG:HG2	1.57	0.70
1:B:206:GLN:HE22	1:B:246:ARG:HG2	1.57	0.70
1:A:176:MET:HE1	1:A:180:LYS:HE2	1.72	0.69
1:B:812:PHE:HD1	1:B:851:TYR:OH	1.77	0.68
1:A:723:ALA:N	1:A:724:PRO:CD	2.57	0.68
1:B:270:SER:O	1:B:274:ASN:HB2	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:723:ALA:N	1:B:724:PRO:CD	2.57	0.67
1:A:812:PHE:HD1	1:A:851:TYR:HH	1.39	0.66
1:A:270:SER:O	1:A:274:ASN:HB2	1.95	0.65
1:A:812:PHE:HD1	1:A:851:TYR:OH	1.77	0.65
1:B:599:VAL:HG21	1:B:637:GLN:OE1	1.96	0.65
1:A:599:VAL:HG21	1:A:637:GLN:OE1	1.96	0.64
1:B:723:ALA:H	1:B:724:PRO:CD	2.11	0.64
1:A:810:SER:OG	1:A:838:TYR:CZ	2.51	0.63
1:B:810:SER:OG	1:B:838:TYR:CZ	2.51	0.63
1:B:289:GLU:HG2	1:B:290:GLY:H	1.64	0.63
1:A:289:GLU:HG2	1:A:290:GLY:H	1.64	0.63
1:A:610:PRO:HB2	1:A:812:PHE:CD2	2.34	0.63
1:B:610:PRO:HB2	1:B:812:PHE:CD2	2.34	0.63
1:B:268:ILE:HA	1:B:271:LEU:HB3	1.81	0.62
1:A:734:GLU:OE2	2:A:1001:CA:CA	1.77	0.62
1:A:723:ALA:H	1:A:724:PRO:CD	2.11	0.62
1:B:176:MET:HE3	1:B:180:LYS:HE2	1.76	0.62
1:A:268:ILE:HA	1:A:271:LEU:HB3	1.81	0.61
1:A:286:GLY:O	1:A:686:ARG:NH2	2.34	0.61
1:A:169:ALA:O	1:A:173:LYS:HB2	2.01	0.61
1:B:734:GLU:OE2	2:B:1001:CA:CA	1.77	0.60
1:B:286:GLY:O	1:B:686:ARG:NH2	2.34	0.60
1:A:812:PHE:HD1	1:A:813:ASN:N	1.84	0.60
1:B:169:ALA:O	1:B:173:LYS:HB2	2.01	0.60
1:A:125:ARG:HB3	1:A:197:VAL:HB	1.84	0.59
1:B:125:ARG:HB3	1:B:197:VAL:HB	1.84	0.58
1:A:605:ARG:NH2	1:A:781:PHE:O	2.36	0.58
1:B:810:SER:N	1:B:838:TYR:O	2.30	0.58
1:B:605:ARG:NH2	1:B:781:PHE:O	2.36	0.58
1:B:176:MET:HE1	1:B:180:LYS:HE2	1.84	0.58
1:B:289:GLU:HG2	1:B:290:GLY:N	2.19	0.58
1:A:289:GLU:HG2	1:A:290:GLY:N	2.19	0.58
1:B:538:VAL:O	1:B:542:ALA:HB2	2.04	0.57
1:A:715:LEU:HD23	1:A:771:ALA:HA	1.87	0.57
1:A:810:SER:N	1:A:838:TYR:O	2.30	0.57
1:B:326:GLU:O	1:B:330:LEU:HB2	2.05	0.57
1:B:715:LEU:HD23	1:B:771:ALA:HA	1.86	0.57
1:A:538:VAL:O	1:A:542:ALA:HB2	2.04	0.56
1:A:326:GLU:O	1:A:330:LEU:HB2	2.05	0.55
1:A:892:ASP:OD1	1:A:895:GLN:NE2	2.39	0.55
1:B:715:LEU:CD2	1:B:771:ALA:HA	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:805:VAL:O	1:B:809:LEU:HD22	2.07	0.55
1:A:812:PHE:CE1	1:A:813:ASN:O	2.60	0.55
1:A:715:LEU:CD2	1:A:771:ALA:HA	2.36	0.55
1:B:126:PHE:HD2	1:B:278:SER:HB3	1.70	0.55
1:A:126:PHE:HD2	1:A:278:SER:HB3	1.71	0.55
1:B:892:ASP:OD1	1:B:895:GLN:NE2	2.39	0.55
1:B:812:PHE:CE1	1:B:813:ASN:O	2.60	0.54
1:A:432:MET:HG2	1:A:889:ILE:HD12	1.90	0.54
1:B:390:LYS:HD3	1:B:829:LEU:HD13	1.90	0.54
1:A:805:VAL:O	1:A:809:LEU:HD22	2.07	0.54
1:B:432:MET:HG2	1:B:889:ILE:HD12	1.90	0.53
1:B:505:PHE:HA	1:B:508:VAL:HG12	1.90	0.53
1:A:690:ASP:HA	1:A:693:LEU:HD23	1.90	0.53
1:A:505:PHE:HA	1:A:508:VAL:HG12	1.90	0.53
1:A:390:LYS:HD3	1:A:829:LEU:HD13	1.90	0.53
1:A:588:LYS:O	1:A:592:SER:HB3	2.10	0.52
1:B:690:ASP:HA	1:B:693:LEU:HD23	1.90	0.52
1:B:588:LYS:O	1:B:592:SER:HB3	2.10	0.52
1:A:388:TYR:HE2	1:A:833:VAL:HG11	1.75	0.51
1:B:268:ILE:HG22	1:B:271:LEU:HD23	1.92	0.51
1:B:388:TYR:HE2	1:B:833:VAL:HG11	1.75	0.51
1:A:847:SER:OG	1:A:849:HIS:O	2.28	0.51
1:A:515:ARG:NE	1:A:515:ARG:HA	2.22	0.51
1:B:847:SER:OG	1:B:849:HIS:O	2.28	0.51
1:A:268:ILE:HG22	1:A:271:LEU:HD23	1.92	0.51
1:A:727:ALA:O	1:A:731:ASN:HB2	2.11	0.51
1:A:812:PHE:HE1	1:A:851:TYR:HH	1.52	0.50
1:B:727:ALA:O	1:B:731:ASN:HB2	2.11	0.50
1:B:253:ILE:HD12	1:B:256:ARG:HH21	1.77	0.50
1:A:202:THR:HG22	1:A:204:PRO:HD2	1.94	0.50
1:A:723:ALA:N	1:A:724:PRO:HD2	2.26	0.50
1:B:515:ARG:HA	1:B:515:ARG:NE	2.22	0.50
1:A:176:MET:SD	1:A:271:LEU:CD2	2.99	0.50
1:B:723:ALA:N	1:B:724:PRO:HD2	2.26	0.50
1:A:253:ILE:HD12	1:A:256:ARG:HH21	1.77	0.49
1:A:647:LEU:O	1:A:651:ASN:ND2	2.45	0.49
1:A:812:PHE:HB2	1:A:838:TYR:HE1	1.77	0.49
1:B:176:MET:SD	1:B:271:LEU:CD2	2.99	0.49
1:B:618:ARG:O	1:B:618:ARG:HG2	2.12	0.49
1:B:812:PHE:HB2	1:B:838:TYR:HE1	1.77	0.49
1:B:202:THR:HG22	1:B:204:PRO:HD2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:270:SER:HA	1:B:273:ALA:HB3	1.94	0.49
1:B:647:LEU:O	1:B:651:ASN:ND2	2.45	0.49
1:A:124:LYS:HE2	1:A:283:LEU:HD22	1.95	0.49
1:A:657:ILE:HG22	1:A:661:LYS:HE2	1.94	0.49
1:B:287:ASP:N	1:B:296:ASN:OD1	2.46	0.49
1:B:657:ILE:HG22	1:B:661:LYS:HE2	1.94	0.48
1:B:124:LYS:HE2	1:B:283:LEU:HD22	1.95	0.48
1:A:122:ASP:OD1	1:A:246:ARG:NH1	2.47	0.48
1:B:380:PRO:O	1:B:381:LEU:CG	2.62	0.48
1:A:603:LYS:NZ	1:A:633:GLU:OE1	2.46	0.48
1:A:618:ARG:O	1:A:618:ARG:HG2	2.13	0.48
1:A:270:SER:HA	1:A:273:ALA:HB3	1.94	0.48
1:A:287:ASP:N	1:A:296:ASN:OD1	2.46	0.48
1:A:380:PRO:O	1:A:381:LEU:CG	2.62	0.48
1:A:416:MET:HG3	1:A:717:VAL:HG21	1.95	0.48
1:B:122:ASP:OD1	1:B:246:ARG:NH1	2.47	0.48
1:B:715:LEU:HD22	1:B:774:ILE:HG21	1.96	0.48
1:B:416:MET:HG3	1:B:717:VAL:HG21	1.95	0.47
1:B:380:PRO:O	1:B:381:LEU:HG	2.14	0.47
1:B:625:CYS:SG	1:B:626:ALA:N	2.88	0.47
1:B:603:LYS:NZ	1:B:633:GLU:OE1	2.46	0.47
1:B:722:LEU:O	1:B:722:LEU:HD12	2.14	0.47
1:A:380:PRO:O	1:A:381:LEU:HG	2.14	0.47
1:A:812:PHE:HB2	1:A:838:TYR:CE1	2.49	0.47
1:B:125:ARG:NH2	1:B:254:LEU:HD11	2.30	0.47
1:A:722:LEU:O	1:A:722:LEU:HD12	2.14	0.47
1:A:715:LEU:HD22	1:A:774:ILE:HG21	1.96	0.47
1:A:201:ILE:HD13	1:A:250:VAL:HG22	1.96	0.47
1:B:201:ILE:HD13	1:B:250:VAL:HG22	1.96	0.47
1:A:268:ILE:O	1:A:272:LEU:CB	2.63	0.47
1:A:625:CYS:SG	1:A:626:ALA:N	2.88	0.47
1:B:723:ALA:H	1:B:724:PRO:HD2	1.80	0.47
1:A:125:ARG:NH2	1:A:254:LEU:HD11	2.30	0.46
1:B:268:ILE:O	1:B:272:LEU:CB	2.63	0.46
1:B:812:PHE:HD1	1:B:813:ASN:N	1.84	0.46
1:A:317:ILE:HA	1:A:320:VAL:HG12	1.98	0.46
1:B:317:ILE:HA	1:B:320:VAL:HG12	1.98	0.46
1:B:812:PHE:HB2	1:B:838:TYR:CE1	2.49	0.46
1:A:175:LYS:O	1:A:178:THR:OG1	2.32	0.46
1:A:718:ALA:HB1	1:A:779:ILE:HG13	1.99	0.45
1:A:625:CYS:SG	1:A:630:CYS:N	2.90	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:177:PRO:HA	1:B:180:LYS:HB2	1.99	0.45
1:B:625:CYS:SG	1:B:630:CYS:N	2.89	0.45
1:B:609:ARG:HD2	1:B:851:TYR:HB3	1.98	0.45
1:A:609:ARG:HD2	1:A:851:TYR:HB3	1.98	0.45
1:B:219:ARG:HD2	1:B:230:HIS:HB2	1.98	0.44
1:A:219:ARG:HD2	1:A:230:HIS:HB2	1.98	0.44
1:A:723:ALA:H	1:A:724:PRO:HD2	1.80	0.44
1:A:538:VAL:O	1:A:542:ALA:CB	2.66	0.44
1:B:515:ARG:NH2	1:B:519:ALA:HB2	2.24	0.44
1:B:718:ALA:HB1	1:B:779:ILE:HG13	1.99	0.44
1:B:495:VAL:HG21	1:B:568:GLU:HG2	2.00	0.44
1:A:177:PRO:HA	1:A:180:LYS:HB2	1.99	0.43
1:B:495:VAL:HG12	1:B:498:ILE:HD12	2.00	0.43
1:B:648:ILE:O	1:B:652:LEU:HB2	2.18	0.43
1:A:810:SER:OG	1:A:838:TYR:CE2	2.71	0.43
1:B:175:LYS:O	1:B:178:THR:OG1	2.32	0.43
1:B:538:VAL:O	1:B:542:ALA:CB	2.66	0.43
1:A:495:VAL:HG12	1:A:498:ILE:HD12	2.00	0.43
1:B:127:ARG:HH12	1:B:188:ARG:HH21	1.67	0.43
1:A:176:MET:HE3	1:A:180:LYS:HE2	1.88	0.42
1:B:222:TYR:HB3	1:B:227:GLU:HG2	2.01	0.42
1:A:495:VAL:HG21	1:A:568:GLU:HG2	2.00	0.42
1:A:127:ARG:HH12	1:A:188:ARG:HH21	1.67	0.42
1:A:648:ILE:O	1:A:652:LEU:HB2	2.18	0.42
1:B:634:LEU:O	1:B:638:LEU:HB2	2.20	0.42
1:A:534:ILE:HG13	1:A:534:ILE:H	1.59	0.42
1:A:619:SER:OG	1:A:620:PHE:HD1	2.03	0.42
1:A:805:VAL:HG12	1:A:809:LEU:CD2	2.50	0.41
1:A:222:TYR:HB3	1:A:227:GLU:HG2	2.01	0.41
1:A:515:ARG:HA	1:A:515:ARG:HD2	1.74	0.41
1:B:534:ILE:H	1:B:534:ILE:HG13	1.59	0.41
1:B:805:VAL:HG12	1:B:809:LEU:CD2	2.50	0.41
1:A:268:ILE:O	1:A:272:LEU:HB2	2.20	0.41
1:A:634:LEU:O	1:A:638:LEU:HB2	2.20	0.41
1:B:495:VAL:HA	1:B:498:ILE:HD12	2.02	0.41
1:A:495:VAL:HA	1:A:498:ILE:HD12	2.02	0.41
1:B:812:PHE:HE1	1:B:851:TYR:HH	1.54	0.41
1:B:854:SER:OG	1:B:855:LYS:N	2.55	0.40
1:B:268:ILE:O	1:B:272:LEU:HB2	2.20	0.40
1:A:127:ARG:HE	1:A:195:ASN:HB2	1.86	0.40
1:A:810:SER:OG	1:A:810:SER:O	2.39	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:231:LEU:HD13	1:B:231:LEU:HA	1.96	0.40
1:A:382:CYS:HB2	1:A:386:CYS:HB2	1.62	0.40
1:B:305:TRP:CD1	1:B:316:PRO:HD2	2.56	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	708/960 (74%)	654 (92%)	54 (8%)	0	100	100
1	B	708/960 (74%)	655 (92%)	53 (8%)	0	100	100
All	All	1416/1920 (74%)	1309 (92%)	107 (8%)	0	100	100

There are no Ramachandran outliers to report.

### 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	640/853 (75%)	622 (97%)	18 (3%)	49	76
1	B	640/853 (75%)	622 (97%)	18 (3%)	49	76
All	All	1280/1706 (75%)	1244 (97%)	36 (3%)	52	76

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	127	ARG
1	A	167	ARG
1	A	176	MET
1	A	249	ILE
1	A	296	ASN
1	A	381	LEU
1	A	455	ARG
1	A	515	ARG
1	A	524	MET
1	A	535	ARG
1	A	618	ARG
1	A	638	LEU
1	A	640	ILE
1	A	650	ASN
1	A	683	ARG
1	A	722	LEU
1	A	731	ASN
1	A	811	SER
1	B	127	ARG
1	B	167	ARG
1	B	176	MET
1	B	249	ILE
1	B	296	ASN
1	B	381	LEU
1	B	455	ARG
1	B	515	ARG
1	B	524	MET
1	B	535	ARG
1	B	618	ARG
1	B	638	LEU
1	B	640	ILE
1	B	650	ASN
1	B	683	ARG
1	B	722	LEU
1	B	731	ASN
1	B	811	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	183	HIS
1	A	206	GLN
1	A	650	ASN

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Mol	Chain	Res	Type
1	A	731	ASN
1	A	818	GLN
1	B	183	HIS
1	B	206	GLN
1	B	650	ASN
1	B	731	ASN

### 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 ⓘ

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

### 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.