



Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Feb 8, 2018 – 07:23 PM EST

PDB ID : 6BGJ
EMDB ID: : EMD-7096
Title : Cryo-EM structure of the TMEM16A calcium-activated chloride channel in LMNG
Authors : Dang, S.; Feng, S.; Tien, J.; Peters, C.J.; Bulkley, D.; Lolicato, M.; Zhao, J.; Zuberbuhler, K.; Ye, W.; Qi, L.; Chen, T.; Craik, C.S.; Jan, Y.N.; Minor, D.L.Jr.; Cheng, Y.; Jan, L.Y.
Deposited on : 2017-10-28
Resolution : 3.80 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-20030736

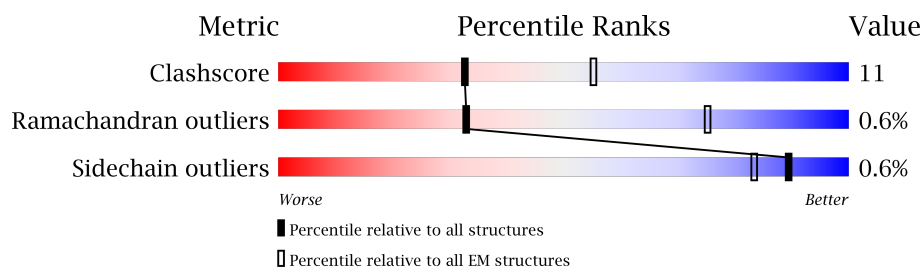
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.80 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	912	
1	B	912	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7418 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	490	Total	C	N	O	S	0	0
			3708	2446	597	641	24		
1	B	490	Total	C	N	O	S	0	0
			3708	2446	597	641	24		

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	904	SER	-	expression tag	UNP Q8BHY3
A	905	ASN	-	expression tag	UNP Q8BHY3
A	906	SER	-	expression tag	UNP Q8BHY3
A	907	LEU	-	expression tag	UNP Q8BHY3
A	908	GLU	-	expression tag	UNP Q8BHY3
A	909	VAL	-	expression tag	UNP Q8BHY3
A	910	LEU	-	expression tag	UNP Q8BHY3
A	911	PHE	-	expression tag	UNP Q8BHY3
A	912	GLN	-	expression tag	UNP Q8BHY3
B	904	SER	-	expression tag	UNP Q8BHY3
B	905	ASN	-	expression tag	UNP Q8BHY3
B	906	SER	-	expression tag	UNP Q8BHY3
B	907	LEU	-	expression tag	UNP Q8BHY3
B	908	GLU	-	expression tag	UNP Q8BHY3
B	909	VAL	-	expression tag	UNP Q8BHY3
B	910	LEU	-	expression tag	UNP Q8BHY3
B	911	PHE	-	expression tag	UNP Q8BHY3
B	912	GLN	-	expression tag	UNP Q8BHY3

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

Mol	Chain	Residues	Atoms		AltConf
2	B	1	Total	Ca	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
			Total	Ca	
2	A	1	1	1	0

- Molecule 1: Anoctamin-1

- Molecule 1: Anoctamin-1

Chain B: 41% 11% . 46%

Lys	S806	Tyr	V595	Tyr	V310	Phe	Val	Glut	Lys	Met
Asp		Val	A596	Glut	F311	Asp	Tyr	Asp	Val	Arg
Ile	N809	Lys		Ala	F311	Ser	His	Asp	Val	Val
Ser	S810	Arg	K599	Arg	Y312	Lys	Ile	Lys	Tyr	Pro
Gln	S811	Lys		Val		Thr	Ser	Arg	Ile	Glut
Ile	D812	Gln	D608	Leu	D318	Arg	Glut	Phe	Leu	Lys
			Y609	Glut	L319	Ser	Thr	Arg	Val	Tyr
His	A818		I612	Lys	V320	Thr	Arg	Arg	His	Ser
Lys	P819	V685	F613	Ser	R321	Ile	Leu	Glut	His	Leu
Glut	N820		R614	Arg	K322	Val	Leu	Tyr	Lys	Pro
Lys	D821	L689	R615	Arg	Y323	Tyr	Leu	Val	Lys	Ala
Val	L825		S615	Lys	F324	Glut	Lys	Glut	Arg	Ala
Leu		F716	F616	Glut	G325	Ile	Thr	Glut	Ala	Glut
Met	Glut		F616	Ser	E326	Lys	Ile	Asn	Glut	Asp
Val	Tyr	P720	E619	Arg	G329	Lys	Asn	Ser	Ser	Arg
Glut	Glut	L721		Asn		Arg	Val	Leu	Arg	Val
Leu	Val		A822	Glut	V352	Thr	Val	Ala	Thr	His
Ser	Gln	L724	P823	Thr		Cys	Gln	Leu	Leu	Ile
Asn	Ile	L725		Thr	V360	Thr	Lys	Leu	Ala	Val
Ser	Cys	N726	I632	Asp		Lys	Ile	Leu	Ala	Val
Leu	Arg	N727	Q633	Lys	I364	Ala	Thr	Leu	Arg	Asn
Glut	Tyr			Val	P365	Lys	Asp	Leu	Arg	Ile
Val	Lys	E730	I636	Lys	S366	Tyr	Pro	Asn	Gly	Cys
Leu	Asp			Leu	M367	Ser	Ile	Asp	Leu	Ala
Phe	Tyr	L742	L639	Thr	E368	Met	Ile	Glut	Gln	Ile
Leu	Arg	R743	G640	Trp	M369	Glut	Pro	Asp	Asn	Glut
Glut	Glut		K641	Arg		Lys	Val	Thr	Met	Leu
Pro	Pro	R749	Q642	Asp	M378	Ile	Val	Lys	Val	Gly
Pro				Arg		Thr	Ala	Ile	Val	Gly
Trp		G764	Q645	Phe	L381	Ser	Ala	His	Leu	Tyr
Ser	Glut	Y757	N646	Pro	C382	Leu	Gln	His	Gly	Leu
His			N647	Tyr	D383	Ala	Arg	Val	Thr	Pro
			Phe	Phe		Asn	Gln	Val	Arg	Ser
K346		L760	Leu	Thr	K390	Gly	Thr	Phe	Val	Gly
Y847		R761	Glut	Thr		Val	Ile	Val	Arg	Thr
D848		G782	Ile	Asn	F404	Tyr	Thr	Lys	Gln	Leu
I849		W783	Gly	Leu		Ser	Lys	Ile	Asp	Leu
S850		G784	Ile	Val	A408	Ala	Arg	His	Gln	Leu
K951		R765	Pro	Ser	T409	Ala	Leu	Ala	Pro	Asn
		L766	Lys		V410	Tyr	Ser	Pro	Leu	Ser
M854		A767	Met			Pro	Tyr	Trp	Pro	Leu
A855			Lys	I509	M416	Leu	Tyr	Trp	Pro	Ser
V856		A772	Lys			Leu	Pro	His	Gly	Val
L857			Phe	S513	W419	His	Phe	Val	Lys	Val
A858		W775	Ile			Asp	Ser	Leu	Gly	Pro
A859			Arg	A517	F423	Gly	Arg	Cys	Ser	Asp
R860		F781	Tyr		M424	Asp	Glut	Arg	Pro	Ala
L861			Leu	I546		Tyr	Lys	Glut	Val	Glut
A862		R784	Lys		F443	Glut	Gln	Ala	Asp	Cys
		L785	Leu	D650		Gly	His	Glut	Ala	Lys
I365			Arg			Asp	Leu	Phe	Gly	Tyr
		L788	Arg	Y553	Glut	N292	Phe	Leu	Ser	Gly
N869			Arg		Glut	M293	Asp	Lys	Pro	Leu
L870		Q793	Gln	I556	Glut		Leu	Leu	Glut	Tyr
			Ser		Asp	M296	Thr	Lys	Val	Phe
M874		F800	Ser	T568	Asp	D297	Arg	Met	Pro	Asp
			Asp	E569	Pro		Asp	Pro	Met	Asp
D884		N802	Arg	K570	Arg	L301	Arg	Thr	Asp	Gly
Ile			Glut		Ala		Ser	Lys	Tyr	Arg
Pro		L905	Glut	Y504	Glut	M206	Phe	Lys	His	Lys

4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	251851	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	80	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1900	Depositor
Magnification	29000	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	0/3801	0.63	1/5180 (0.0%)
1	B	0.40	0/3801	0.63	1/5180 (0.0%)
All	All	0.40	0/7602	0.63	2/10360 (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	11
1	B	0	11
All	All	0	22

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	810	VAL	CG1-CB-CG2	-6.26	100.88	110.90
1	A	810	VAL	CG1-CB-CG2	-6.25	100.91	110.90

There are no chirality outliers.

All (22) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	305	TRP	Peptide
1	A	404	PHE	Peptide
1	A	608	ASP	Peptide
1	A	622	ALA	Peptide

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Mol	Chain	Res	Type	Group
1	A	742	LEU	Peptide
1	A	785	LEU	Peptide
1	A	793	GLN	Peptide
1	A	802	ASN	Peptide
1	A	809	ASN	Peptide
1	A	810	VAL	Peptide
1	A	811	SER	Peptide
1	B	305	TRP	Peptide
1	B	404	PHE	Peptide
1	B	608	ASP	Peptide
1	B	622	ALA	Peptide
1	B	742	LEU	Peptide
1	B	785	LEU	Peptide
1	B	793	GLN	Peptide
1	B	802	ASN	Peptide
1	B	809	ASN	Peptide
1	B	810	VAL	Peptide
1	B	811	SER	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	3708	0	3540	80	0
1	B	3708	0	3540	75	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
All	All	7418	0	7080	154	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 11.

All (154) 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:383:ASP:OD2	1:B:614:ARG:NH2	2.14	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:383:ASP:OD2	1:A:614:ARG:NH2	2.14	0.80
1:B:424:MET:HE3	1:B:761:ARG:HA	1.64	0.79
1:B:321:ARG:NH2	1:B:326:GLU:OE2	2.19	0.76
1:A:321:ARG:NH2	1:A:326:GLU:OE2	2.19	0.75
1:A:821:ASP:OD2	1:A:846:LYS:N	2.22	0.72
1:B:821:ASP:OD2	1:B:846:LYS:N	2.22	0.72
1:A:424:MET:HE1	1:A:761:ARG:N	2.04	0.72
1:B:390:LYS:HZ2	1:B:623:PRO:HD2	1.57	0.69
1:A:685:VAL:O	1:A:743:ARG:NH1	2.27	0.68
1:B:685:VAL:O	1:B:743:ARG:NH1	2.27	0.67
1:A:424:MET:HE3	1:A:761:ARG:HA	1.75	0.66
1:A:390:LYS:HZ2	1:A:623:PRO:HD2	1.60	0.66
1:A:865:ILE:O	1:A:869:ASN:ND2	2.29	0.65
1:B:865:ILE:O	1:B:869:ASN:ND2	2.29	0.64
1:A:616:PHE:HB3	1:A:623:PRO:HG3	1.80	0.64
1:B:424:MET:HE1	1:B:761:ARG:N	2.13	0.64
1:A:640:GLY:O	1:A:726:ASN:ND2	2.32	0.63
1:B:640:GLY:O	1:B:726:ASN:ND2	2.32	0.62
1:A:851:LYS:HA	1:A:854:TRP:HD1	1.65	0.62
1:B:616:PHE:HB3	1:B:623:PRO:HG3	1.80	0.62
1:A:424:MET:SD	1:A:757:TYR:CE1	2.93	0.62
1:B:424:MET:SD	1:B:757:TYR:CE1	2.93	0.61
1:B:851:LYS:HA	1:B:854:TRP:HD1	1.64	0.61
1:A:727:ASN:HA	1:A:730:GLU:HB2	1.83	0.61
1:B:727:ASN:HA	1:B:730:GLU:HB2	1.83	0.60
1:B:297:ASP:O	1:B:301:LEU:N	2.35	0.60
1:A:821:ASP:CG	1:A:847:TYR:HD2	2.06	0.60
1:A:821:ASP:OD2	1:A:847:TYR:N	2.29	0.59
1:B:821:ASP:CG	1:B:847:TYR:HD2	2.06	0.59
1:A:410:VAL:HA	1:A:775:ILE:HD11	1.83	0.59
1:B:633:GLN:HG2	1:B:716:PHE:HB3	1.84	0.59
1:A:633:GLN:HG2	1:A:716:PHE:HB3	1.84	0.59
1:B:410:VAL:HA	1:B:775:ILE:HD11	1.83	0.59
1:A:297:ASP:O	1:A:301:LEU:N	2.35	0.57
1:A:761:ARG:O	1:A:765:LYS:N	2.37	0.57
1:A:820:ASN:HD22	1:A:849:ILE:HG12	1.70	0.56
1:B:820:ASN:HD22	1:B:849:ILE:HG12	1.70	0.56
1:A:642:GLN:HG2	1:A:645:GLN:HB2	1.88	0.56
1:A:424:MET:CE	1:A:761:ARG:HA	2.36	0.56
1:B:424:MET:CE	1:B:761:ARG:HA	2.36	0.55
1:B:642:GLN:HG2	1:B:645:GLN:HB2	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:369:MET:HG3	1:A:800:PHE:HB3	1.88	0.55
1:B:369:MET:HG3	1:B:800:PHE:HB3	1.88	0.54
1:B:546:ILE:O	1:B:550:ASP:N	2.41	0.54
1:B:806:SER:HA	1:B:809:ASN:HD22	1.73	0.54
1:A:390:LYS:HZ1	1:A:623:PRO:HB2	1.72	0.53
1:A:818:ALA:O	1:A:846:LYS:N	2.42	0.53
1:B:785:LEU:O	1:B:802:ASN:ND2	2.42	0.53
1:A:546:ILE:O	1:A:550:ASP:N	2.41	0.53
1:A:806:SER:HA	1:A:809:ASN:HD22	1.73	0.53
1:A:785:LEU:O	1:A:802:ASN:ND2	2.42	0.53
1:B:821:ASP:OD2	1:B:847:TYR:N	2.29	0.53
1:B:754:GLY:HA2	1:B:757:TYR:HB3	1.91	0.52
1:A:292:ASN:O	1:A:296:ASN:N	2.41	0.52
1:A:318:ASP:O	1:A:322:LYS:N	2.41	0.52
1:B:292:ASN:O	1:B:296:ASN:N	2.41	0.52
1:A:378:MET:HE2	1:A:381:LEU:HD22	1.91	0.52
1:B:818:ALA:O	1:B:846:LYS:N	2.42	0.52
1:A:754:GLY:HA2	1:A:757:TYR:HB3	1.91	0.52
1:B:761:ARG:O	1:B:765:LYS:N	2.37	0.51
1:B:378:MET:HE2	1:B:381:LEU:HD22	1.93	0.51
1:A:784:ARG:HH12	1:A:788:LEU:CD1	2.24	0.51
1:B:784:ARG:HH12	1:B:788:LEU:CD1	2.24	0.50
1:A:720:PRO:O	1:A:724:LEU:N	2.45	0.50
1:A:851:LYS:HB3	1:B:851:LYS:HB3	1.93	0.50
1:B:720:PRO:O	1:B:724:LEU:N	2.45	0.50
1:B:390:LYS:HZ1	1:B:623:PRO:HB2	1.75	0.50
1:B:416:MET:HA	1:B:419:TRP:HB3	1.94	0.50
1:A:416:MET:HA	1:A:419:TRP:HB3	1.94	0.50
1:B:820:ASN:HB2	1:B:849:ILE:HG21	1.94	0.49
1:B:609:TYR:OH	1:B:820:ASN:OD1	2.31	0.49
1:A:609:TYR:OH	1:A:820:ASN:OD1	2.31	0.49
1:B:820:ASN:HB2	1:B:849:ILE:HG12	1.95	0.49
1:B:318:ASP:O	1:B:322:LYS:N	2.41	0.49
1:A:784:ARG:HD2	1:A:856:VAL:HG22	1.95	0.49
1:B:858:ALA:O	1:B:862:ALA:N	2.44	0.48
1:B:326:GLU:H	1:B:749:ARG:HA	1.79	0.48
1:B:325:GLY:O	1:B:329:GLY:N	2.34	0.48
1:B:854:TRP:O	1:B:858:ALA:N	2.42	0.48
1:A:326:GLU:H	1:A:749:ARG:HA	1.79	0.48
1:B:553:TYR:HD1	1:B:556:ILE:HD12	1.78	0.48
1:A:360:VAL:HA	1:A:365:PRO:HD2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:360:VAL:HA	1:B:365:PRO:HD2	1.96	0.48
1:A:820:ASN:HB2	1:A:849:ILE:HG12	1.95	0.48
1:A:859:ALA:HA	1:A:862:ALA:HB3	1.96	0.48
1:B:859:ALA:HA	1:B:862:ALA:HB3	1.96	0.48
1:B:856:VAL:O	1:B:860:ARG:N	2.37	0.48
1:B:509:ILE:O	1:B:513:SER:N	2.43	0.48
1:A:553:TYR:HD1	1:A:556:ILE:HD12	1.78	0.47
1:A:820:ASN:HB2	1:A:849:ILE:HG21	1.94	0.47
1:A:364:ILE:HG12	1:A:368:GLU:HG3	1.97	0.47
1:B:364:ILE:HG12	1:B:368:GLU:HG3	1.96	0.47
1:B:636:ILE:HA	1:B:639:LEU:HB2	1.96	0.47
1:A:636:ILE:HA	1:A:639:LEU:HB2	1.96	0.47
1:B:784:ARG:HD2	1:B:856:VAL:HG22	1.95	0.47
1:B:310:VAL:HG12	1:B:312:TYR:H	1.80	0.47
1:A:310:VAL:HG12	1:A:312:TYR:H	1.80	0.47
1:A:325:GLY:O	1:A:329:GLY:N	2.34	0.47
1:B:360:VAL:HG12	1:B:367:MET:HG2	1.96	0.47
1:A:424:MET:HE1	1:A:760:LEU:C	2.35	0.46
1:B:424:MET:HE1	1:B:760:LEU:C	2.36	0.46
1:A:781:PHE:HE1	1:A:860:ARG:HH21	1.64	0.46
1:A:360:VAL:HG12	1:A:367:MET:HG2	1.96	0.46
1:A:513:SER:O	1:A:517:ALA:N	2.49	0.46
1:A:821:ASP:OD2	1:A:847:TYR:HD2	1.99	0.45
1:B:821:ASP:OD2	1:B:847:TYR:HD2	1.99	0.45
1:B:721:LEU:HA	1:B:724:LEU:HB3	1.98	0.45
1:A:721:LEU:HA	1:A:724:LEU:HB3	1.98	0.45
1:B:781:PHE:HE1	1:B:860:ARG:HH21	1.64	0.45
1:B:763:VAL:O	1:B:767:ALA:N	2.50	0.45
1:B:772:ALA:HA	1:B:775:ILE:HG22	1.99	0.44
1:B:513:SER:O	1:B:517:ALA:N	2.49	0.44
1:A:320:VAL:O	1:A:324:PHE:N	2.46	0.44
1:A:763:VAL:O	1:A:767:ALA:N	2.50	0.44
1:A:858:ALA:O	1:A:862:ALA:N	2.44	0.44
1:A:689:LEU:HD21	1:A:742:LEU:H	1.83	0.44
1:A:772:ALA:HA	1:A:775:ILE:HG22	1.99	0.44
1:B:293:VAL:HA	1:B:296:ASN:HD22	1.83	0.44
1:B:820:ASN:H	1:B:849:ILE:HG21	1.83	0.44
1:A:352:VAL:HG13	1:A:408:ALA:HB1	2.00	0.44
1:B:594:TYR:O	1:B:599:LYS:N	2.47	0.43
1:A:568:THR:HG22	1:A:570:LYS:H	1.84	0.43
1:B:689:LEU:HD21	1:B:742:LEU:H	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:293:VAL:HA	1:A:296:ASN:HD22	1.83	0.43
1:A:805:LEU:O	1:A:809:ASN:N	2.51	0.43
1:A:854:TRP:O	1:A:858:ALA:N	2.42	0.43
1:A:422:THR:O	1:A:426:HIS:N	2.41	0.43
1:B:596:ALA:HA	1:B:632:ILE:HD11	2.01	0.42
1:A:596:ALA:HA	1:A:632:ILE:HD11	2.01	0.42
1:B:352:VAL:HG13	1:B:408:ALA:HB1	2.01	0.42
1:B:805:LEU:O	1:B:809:ASN:N	2.51	0.42
1:A:820:ASN:H	1:A:849:ILE:HG21	1.83	0.42
1:A:851:LYS:HA	1:A:854:TRP:CD1	2.50	0.42
1:B:424:MET:CE	1:B:761:ARG:CA	2.98	0.42
1:A:350:VAL:O	1:A:354:LEU:N	2.47	0.42
1:A:729:ILE:O	1:A:733:LEU:N	2.37	0.42
1:B:870:LEU:O	1:B:874:MET:N	2.38	0.41
1:A:509:ILE:O	1:A:513:SER:N	2.43	0.41
1:B:419:TRP:O	1:B:423:PHE:N	2.38	0.41
1:A:414:VAL:HG22	1:A:867:PHE:HE1	1.86	0.41
1:A:594:TYR:O	1:A:599:LYS:N	2.47	0.41
1:A:614:ARG:HB3	1:A:619:GLU:OE2	2.21	0.41
1:B:856:VAL:HG12	1:B:860:ARG:HG3	2.02	0.41
1:B:568:THR:HG22	1:B:570:LYS:H	1.83	0.41
1:A:424:MET:CE	1:A:761:ARG:CA	2.98	0.41
1:A:784:ARG:HH12	1:A:788:LEU:HD12	1.86	0.41
1:A:870:LEU:O	1:A:874:MET:N	2.38	0.41
1:B:614:ARG:HB3	1:B:619:GLU:OE2	2.21	0.41
1:A:608:ASP:HA	1:A:612:ILE:HD12	2.03	0.40
1:A:811:SER:O	1:A:813:PHE:N	2.55	0.40
1:A:856:VAL:HG12	1:A:860:ARG:HG3	2.02	0.40
1:B:320:VAL:O	1:B:324:PHE:N	2.46	0.40
1:B:608:ASP:HA	1:B:612:ILE:HD12	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	482/912 (53%)	413 (86%)	66 (14%)	3 (1%)	28	70
1	B	482/912 (53%)	413 (86%)	66 (14%)	3 (1%)	28	70
All	All	964/1824 (53%)	826 (86%)	132 (14%)	6 (1%)	33	70

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	812	ASP
1	B	812	ASP
1	A	609	TYR
1	B	609	TYR
1	A	810	VAL
1	B	810	VAL

5.3.2 Protein sidechains ⓘ

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	363/812 (45%)	361 (99%)	2 (1%)	89	95
1	B	363/812 (45%)	361 (99%)	2 (1%)	89	95
All	All	726/1624 (45%)	722 (99%)	4 (1%)	89	95

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	321	ARG
1	A	784	ARG
1	B	321	ARG
1	B	784	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	296	ASN
1	A	794	ASN
1	A	809	ASN
1	B	296	ASN
1	B	794	ASN
1	B	809	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](#)

Of 2 ligands modelled in this entry, 2 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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.