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

May 7, 2019 – 01:55 AM EDT

PDB ID	:	6D73
EMDB ID:	:	EMD-7822
Title	:	Cryo-EM structure of the zebrafish TRPM2 channel in the presence of Ca2+M2
Authors	:	Yin, Y.; Wu, M.; Borschel, W.F.; Lander, G.C.; Lee, S.-Y.
Deposited on	:	2018-04-23
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
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) symbol.

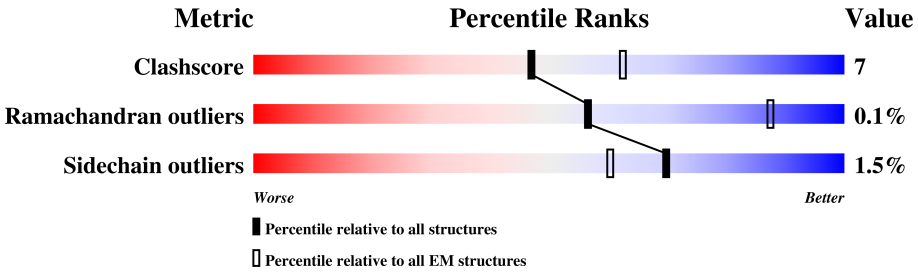
MolProbity	:	4.02b-467
Percentile statistics	:	20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20031633

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 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	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	1466	72% 11% 16%
1	B	1466	73% 13% 14%
1	C	1466	72% 11% 16%
1	D	1466	73% 13% 14%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 35340 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 Transient receptor potential cation channel, subfamily M.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	1256	Total	C	N	O	S	0	0
			8892	5756	1567	1534	35		
1	A	1227	Total	C	N	O	S	0	0
			8776	5690	1524	1523	39		
1	C	1227	Total	C	N	O	S	0	0
			8776	5690	1524	1523	39		
1	D	1256	Total	C	N	O	S	0	0
			8892	5756	1567	1534	35		

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

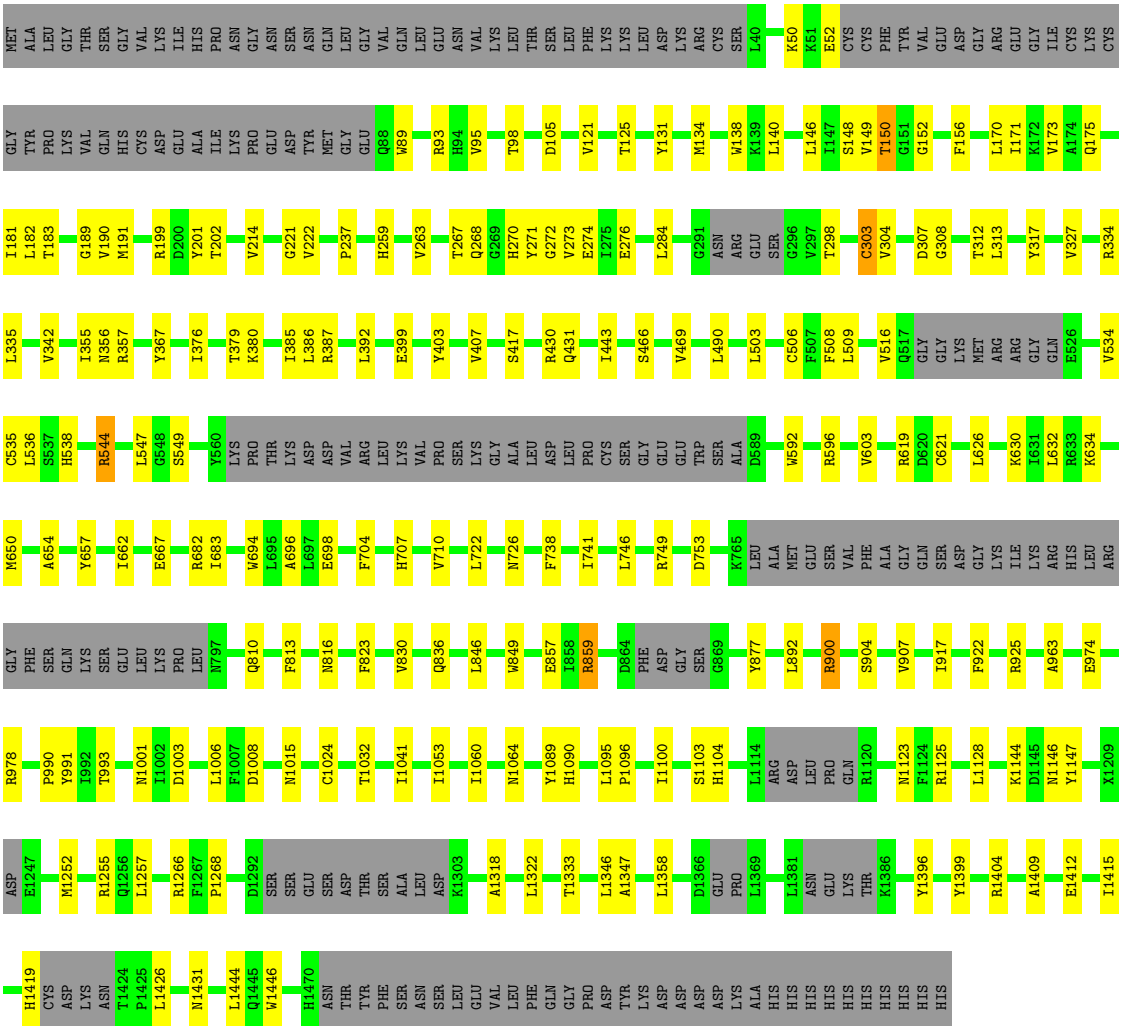
Mol	Chain	Residues	Atoms		AltConf
2	B	1	Total	Ca	0
			1	1	
2	A	1	Total	Ca	0
			1	1	
2	D	1	Total	Ca	0
			1	1	
2	C	1	Total	Ca	0
			1	1	

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.

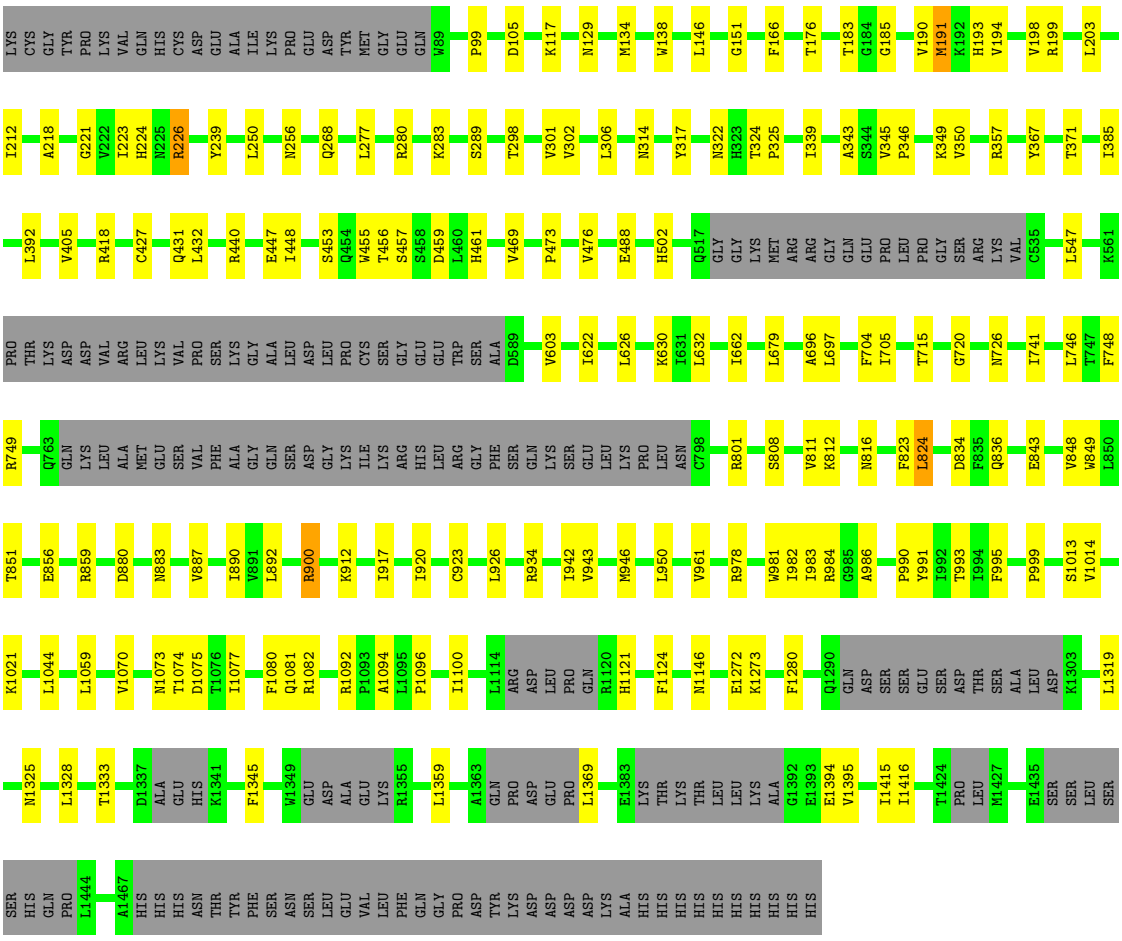
• Molecule 1: Transient receptor potential cation channel, subfamily M

Chain B:



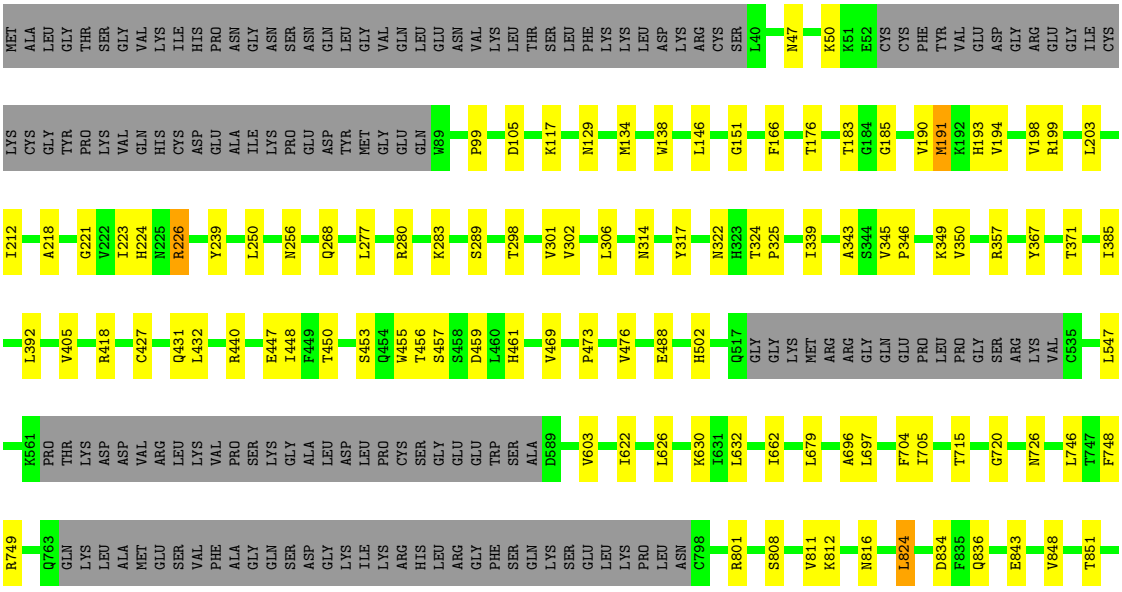
• Molecule 1: Transient receptor potential cation channel, subfamily M

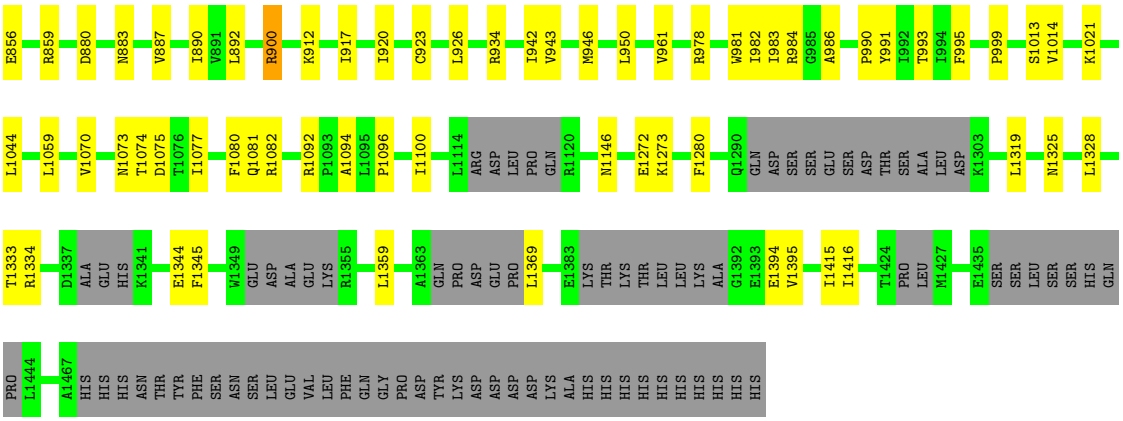
Chain A:



• Molecule 1: Transient receptor potential cation channel, subfamily M

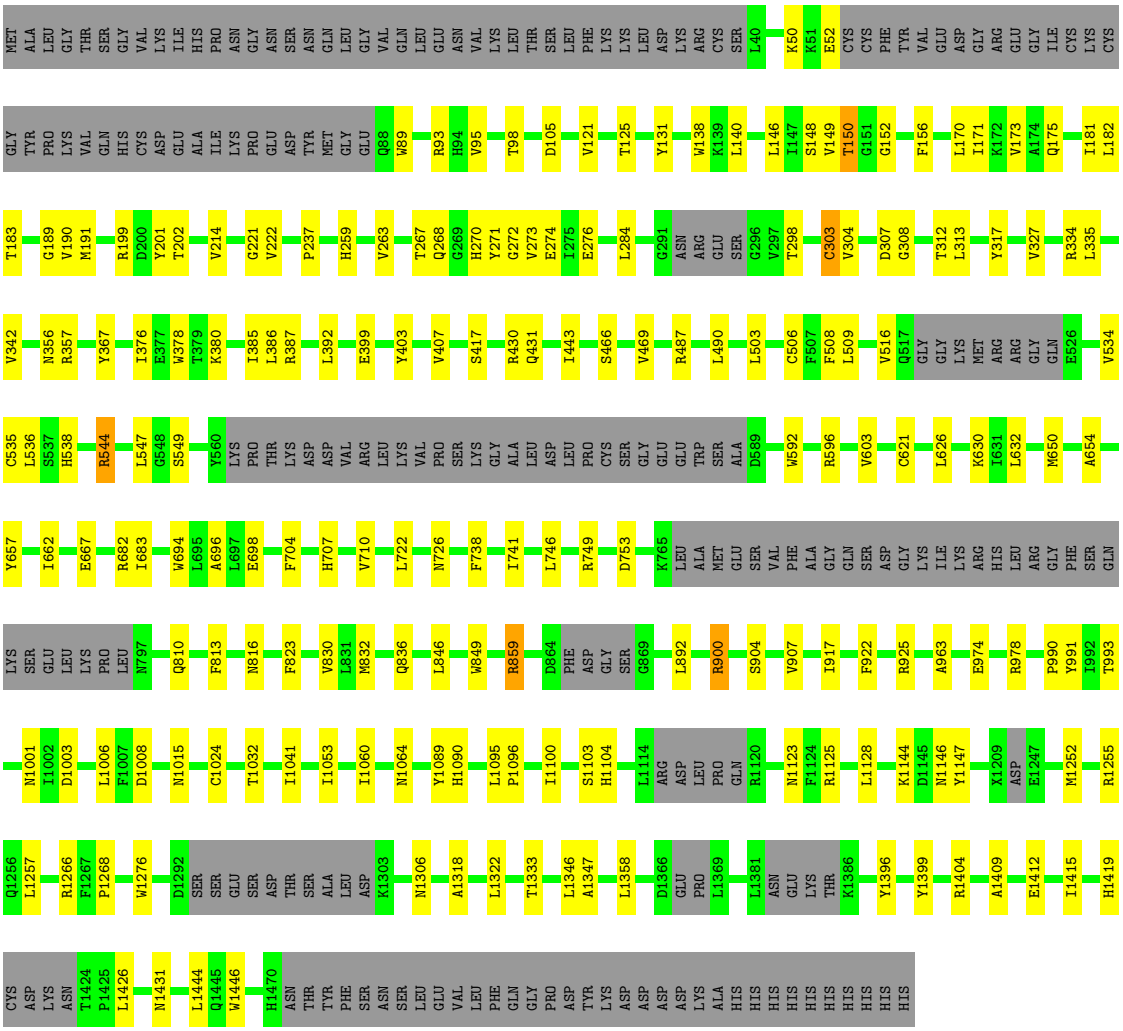
Chain C:





• Molecule 1: Transient receptor potential cation channel, subfamily M

Chain D:



4 Experimental information (i)

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	93573	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	63	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	36000	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	0.36	0/8871	0.59	5/12138 (0.0%)
1	B	0.35	0/8995	0.59	4/12326 (0.0%)
1	C	0.36	0/8871	0.59	5/12138 (0.0%)
1	D	0.36	0/8995	0.59	4/12326 (0.0%)
All	All	0.36	0/35732	0.59	18/48928 (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	2
1	C	0	2
All	All	0	4

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	203	LEU	CA-CB-CG	6.77	130.88	115.30
1	A	203	LEU	CA-CB-CG	6.76	130.84	115.30
1	D	272	GLY	N-CA-C	6.55	129.49	113.10
1	B	272	GLY	N-CA-C	6.53	129.42	113.10
1	C	1075	ASP	CB-CG-OD1	6.00	123.70	118.30
1	C	1359	LEU	CA-CB-CG	6.00	129.10	115.30
1	D	490	LEU	CA-CB-CG	6.00	129.09	115.30
1	B	490	LEU	CA-CB-CG	5.99	129.08	115.30
1	A	1359	LEU	CA-CB-CG	5.98	129.06	115.30
1	A	1075	ASP	CB-CG-OD1	5.97	123.68	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	650	MET	CA-CB-CG	5.91	123.35	113.30
1	D	650	MET	CA-CB-CG	5.90	123.33	113.30
1	C	697	LEU	CB-CG-CD2	-5.72	101.28	111.00
1	A	697	LEU	CB-CG-CD2	-5.71	101.30	111.00
1	C	824	LEU	CB-CG-CD1	-5.05	102.42	111.00
1	A	824	LEU	CB-CG-CD1	-5.04	102.44	111.00
1	D	1444	LEU	CA-CB-CG	5.02	126.84	115.30
1	B	1444	LEU	CA-CB-CG	5.01	126.83	115.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1013	SER	Peptide
1	A	1021	LYS	Peptide
1	C	1013	SER	Peptide
1	C	1021	LYS	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	8776	0	7824	109	0
1	B	8892	0	7798	136	0
1	C	8776	0	7824	105	0
1	D	8892	0	7798	133	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
All	All	35340	0	31244	468	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 7.

All (468) 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:C:346:PRO:HB2	1:C:349:LYS:CB	1.43	1.44
1:A:346:PRO:HB2	1:A:349:LYS:CB	1.43	1.44
1:C:367:TYR:O	1:C:371:THR:HG23	1.40	1.20
1:D:156:PHE:HE1	1:D:189:GLY:C	1.46	1.19
1:B:156:PHE:HE1	1:B:189:GLY:CA	1.57	1.18
1:B:156:PHE:HE1	1:B:189:GLY:C	1.46	1.16
1:D:156:PHE:HE1	1:D:189:GLY:CA	1.57	1.16
1:A:367:TYR:O	1:A:371:THR:HG23	1.40	1.14
1:C:346:PRO:CB	1:C:349:LYS:CB	2.27	1.12
1:A:346:PRO:CB	1:A:349:LYS:CB	2.27	1.12
1:D:149:VAL:HG22	1:D:304:VAL:CG2	1.80	1.11
1:B:149:VAL:HG22	1:B:304:VAL:CG2	1.80	1.10
1:D:156:PHE:CE1	1:D:189:GLY:C	2.27	1.08
1:D:149:VAL:HG22	1:D:304:VAL:HG22	1.34	1.08
1:B:156:PHE:CE1	1:B:189:GLY:C	2.27	1.07
1:B:222:VAL:HG11	1:B:271:TYR:CE1	1.91	1.06
1:D:222:VAL:HG11	1:D:271:TYR:CE1	1.91	1.05
1:B:149:VAL:HG22	1:B:304:VAL:HG22	1.34	1.02
1:B:156:PHE:CE1	1:B:189:GLY:HA2	1.97	1.00
1:D:156:PHE:CE1	1:D:189:GLY:HA2	1.97	0.99
1:C:367:TYR:CD1	1:C:371:THR:HG22	1.98	0.99
1:B:156:PHE:CE1	1:B:189:GLY:CA	2.45	0.98
1:D:50:LYS:HB3	1:D:98:THR:O	1.64	0.98
1:B:156:PHE:CE1	1:B:190:VAL:N	2.32	0.98
1:A:367:TYR:CD1	1:A:371:THR:HG22	1.97	0.97
1:D:156:PHE:CE1	1:D:189:GLY:CA	2.45	0.97
1:D:156:PHE:CE1	1:D:190:VAL:N	2.32	0.97
1:B:50:LYS:HB3	1:B:98:THR:O	1.64	0.95
1:B:156:PHE:HE1	1:B:189:GLY:HA2	1.31	0.92
1:A:367:TYR:O	1:A:371:THR:CG2	2.18	0.92
1:C:367:TYR:O	1:C:371:THR:CG2	2.18	0.90
1:D:156:PHE:HE1	1:D:189:GLY:HA2	1.31	0.90
1:D:222:VAL:CG1	1:D:271:TYR:CE1	2.57	0.88
1:B:222:VAL:CG1	1:B:271:TYR:CE1	2.56	0.88
1:D:105:ASP:O	1:D:237:PRO:HA	1.74	0.87
1:B:105:ASP:O	1:B:237:PRO:HA	1.74	0.86
1:B:152:GLY:H	1:B:308:GLY:HA2	1.40	0.86
1:D:152:GLY:H	1:D:308:GLY:HA2	1.40	0.85
1:A:991:TYR:HD1	1:A:995:PHE:CZ	1.96	0.84
1:C:991:TYR:HD1	1:C:995:PHE:CZ	1.96	0.82
1:C:367:TYR:CD1	1:C:371:THR:CG2	2.65	0.80
1:A:367:TYR:CD1	1:A:371:THR:CG2	2.65	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:149:VAL:HG13	1:B:304:VAL:HG23	1.65	0.77
1:D:149:VAL:HG13	1:D:304:VAL:HG23	1.65	0.76
1:C:350:VAL:HG12	1:C:350:VAL:O	1.86	0.76
1:A:367:TYR:CE1	1:A:371:THR:HG22	2.21	0.75
1:D:148:SER:O	1:D:303:CYS:HA	1.86	0.75
1:C:367:TYR:CE1	1:C:371:THR:HG22	2.21	0.75
1:B:148:SER:O	1:B:303:CYS:HA	1.86	0.74
1:A:350:VAL:O	1:A:350:VAL:HG12	1.86	0.74
1:A:367:TYR:CE1	1:A:371:THR:CG2	2.74	0.70
1:D:267:THR:HG22	1:D:270:HIS:CE1	2.27	0.70
1:C:367:TYR:CE1	1:C:371:THR:CG2	2.74	0.69
1:B:267:THR:HG22	1:B:270:HIS:CE1	2.27	0.69
1:D:506:CYS:SG	1:D:508:PHE:HB3	2.34	0.68
1:D:1006:LEU:HD12	1:D:1008:ASP:H	1.59	0.68
1:A:345:VAL:N	1:A:346:PRO:HD2	2.09	0.68
1:C:345:VAL:N	1:C:346:PRO:HD2	2.09	0.68
1:B:152:GLY:N	1:B:308:GLY:HA2	2.08	0.67
1:B:506:CYS:SG	1:B:508:PHE:HB3	2.34	0.67
1:D:317:TYR:HA	1:D:385:ILE:HD11	1.76	0.67
1:D:152:GLY:N	1:D:308:GLY:HA2	2.08	0.67
1:B:1006:LEU:HD12	1:B:1008:ASP:H	1.59	0.66
1:B:317:TYR:HA	1:B:385:ILE:HD11	1.77	0.66
1:C:961:VAL:HG11	1:C:991:TYR:CE2	2.32	0.65
1:C:47:ASN:HB3	1:C:129:ASN:HD21	1.61	0.65
1:D:222:VAL:HG11	1:D:271:TYR:HE1	1.59	0.65
1:A:47:ASN:HB3	1:A:129:ASN:HD21	1.61	0.65
1:A:961:VAL:HG11	1:A:991:TYR:CE2	2.32	0.64
1:B:222:VAL:HG11	1:B:271:TYR:HE1	1.59	0.64
1:C:1077:ILE:HG22	1:C:1081:GLN:HE22	1.61	0.64
1:A:1077:ILE:HG22	1:A:1081:GLN:HE22	1.61	0.64
1:A:339:ILE:O	1:A:343:ALA:HB2	1.98	0.64
1:C:339:ILE:O	1:C:343:ALA:HB2	1.98	0.63
1:B:52:GLU:O	1:B:95:VAL:HA	1.98	0.63
1:D:52:GLU:O	1:D:95:VAL:HA	1.98	0.62
1:D:267:THR:HG22	1:D:270:HIS:HE1	1.64	0.62
1:D:156:PHE:CZ	1:D:190:VAL:HA	2.35	0.62
1:C:289:SER:HA	1:C:298:THR:HA	1.81	0.62
1:D:1426:LEU:O	1:D:1431:ASN:ND2	2.33	0.62
1:B:1333:THR:HG23	1:B:1419:HIS:HB2	1.82	0.62
1:B:267:THR:CG2	1:B:270:HIS:CE1	2.83	0.62
1:D:149:VAL:CG2	1:D:304:VAL:CG2	2.69	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:978:ARG:HD2	1:A:981:TRP:HB2	1.81	0.61
1:C:978:ARG:HD2	1:C:981:TRP:HB2	1.81	0.61
1:B:1095:LEU:HD23	1:B:1103:SER:HB3	1.83	0.61
1:D:1095:LEU:HD23	1:D:1103:SER:HB3	1.82	0.61
1:B:156:PHE:CZ	1:B:190:VAL:HA	2.35	0.61
1:D:267:THR:CG2	1:D:270:HIS:CE1	2.83	0.61
1:D:156:PHE:HB2	1:D:307:ASP:CB	2.31	0.61
1:B:267:THR:HG22	1:B:270:HIS:HE1	1.64	0.61
1:A:961:VAL:HG22	1:A:990:PRO:HB2	1.83	0.61
1:B:1426:LEU:O	1:B:1431:ASN:ND2	2.33	0.61
1:B:156:PHE:HB2	1:B:307:ASP:CB	2.31	0.61
1:C:961:VAL:HG22	1:C:990:PRO:HB2	1.83	0.61
1:D:1333:THR:HG23	1:D:1419:HIS:HB2	1.82	0.60
1:A:289:SER:HA	1:A:298:THR:HA	1.81	0.60
1:B:974:GLU:O	1:A:912:LYS:NZ	2.35	0.59
1:C:843:GLU:OE2	1:C:900:ARG:NH1	2.35	0.59
1:A:991:TYR:CD1	1:A:995:PHE:CZ	2.86	0.59
1:C:912:LYS:NZ	1:D:974:GLU:O	2.34	0.59
1:D:694:TRP:O	1:D:698:GLU:HB2	2.02	0.59
1:C:357:ARG:NH1	1:C:367:TYR:OH	2.35	0.59
1:C:991:TYR:CD1	1:C:995:PHE:CZ	2.86	0.59
1:A:843:GLU:OE2	1:A:900:ARG:NH1	2.35	0.59
1:B:694:TRP:O	1:B:698:GLU:HB2	2.02	0.59
1:B:892:LEU:HD21	1:B:917:ILE:HG23	1.85	0.59
1:B:990:PRO:HA	1:B:993:THR:HG22	1.85	0.59
1:D:313:LEU:HD13	1:D:335:LEU:HD11	1.85	0.59
1:C:1059:LEU:HG	1:D:1060:ILE:HD11	1.85	0.59
1:C:190:VAL:HA	1:C:193:HIS:HD2	1.67	0.59
1:D:662:ILE:HG22	1:D:704:PHE:HD1	1.68	0.59
1:D:990:PRO:HA	1:D:993:THR:HG22	1.85	0.59
1:B:149:VAL:CG2	1:B:304:VAL:CG2	2.69	0.59
1:A:357:ARG:NH1	1:A:367:TYR:OH	2.35	0.58
1:C:715:THR:OG1	1:C:1082:ARG:NH2	2.36	0.58
1:B:662:ILE:HG22	1:B:704:PHE:HD1	1.68	0.58
1:A:715:THR:OG1	1:A:1082:ARG:NH2	2.36	0.58
1:D:978:ARG:NH1	1:D:1015:ASN:O	2.36	0.58
1:C:185:GLY:HA3	1:C:218:ALA:HB2	1.86	0.58
1:C:350:VAL:O	1:C:350:VAL:CG1	2.52	0.58
1:B:978:ARG:NH1	1:B:1015:ASN:O	2.36	0.58
1:B:313:LEU:HD13	1:B:335:LEU:HD11	1.85	0.58
1:D:171:ILE:O	1:D:175:GLN:HB2	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1060:ILE:HD11	1:A:1059:LEU:HG	1.86	0.57
1:A:190:VAL:HA	1:A:193:HIS:HD2	1.67	0.57
1:A:720:GLY:O	1:A:749:ARG:NH1	2.37	0.57
1:D:836:GLN:O	1:D:900:ARG:NH2	2.36	0.57
1:A:457:SER:O	1:A:461:HIS:ND1	2.37	0.57
1:C:720:GLY:O	1:C:749:ARG:NH1	2.37	0.57
1:A:418:ARG:NH1	1:A:447:GLU:OE2	2.38	0.57
1:A:982:ILE:O	1:A:986:ALA:HB2	2.04	0.57
1:B:171:ILE:O	1:B:175:GLN:HB2	2.04	0.57
1:D:892:LEU:HD21	1:D:917:ILE:HG23	1.85	0.57
1:C:982:ILE:O	1:C:986:ALA:HB2	2.04	0.57
1:D:1096:PRO:O	1:D:1100:ILE:N	2.38	0.57
1:A:221:GLY:HA3	1:A:268:GLN:HA	1.87	0.57
1:A:836:GLN:O	1:A:900:ARG:NH2	2.38	0.57
1:C:418:ARG:NH1	1:C:447:GLU:OE2	2.38	0.57
1:C:920:ILE:HG22	1:D:963:ALA:HB1	1.86	0.57
1:C:151:GLY:HA3	1:C:190:VAL:HG11	1.87	0.56
1:D:171:ILE:HD12	1:D:201:TYR:HB2	1.87	0.56
1:A:185:GLY:HA3	1:A:218:ALA:HB2	1.86	0.56
1:A:350:VAL:O	1:A:350:VAL:CG1	2.52	0.56
1:B:963:ALA:HB1	1:A:920:ILE:HG22	1.87	0.56
1:B:626:LEU:HD13	1:B:696:ALA:HB2	1.88	0.56
1:B:816:ASN:ND2	1:B:1089:TYR:OH	2.37	0.56
1:B:171:ILE:HD12	1:B:201:TYR:HB2	1.87	0.56
1:D:222:VAL:HG13	1:D:271:TYR:CZ	2.39	0.56
1:B:222:VAL:HG13	1:B:271:TYR:CZ	2.39	0.56
1:C:221:GLY:HA3	1:C:268:GLN:HA	1.87	0.56
1:D:816:ASN:ND2	1:D:1089:TYR:OH	2.37	0.56
1:A:301:VAL:O	1:A:324:THR:OG1	2.22	0.56
1:B:1096:PRO:O	1:B:1100:ILE:N	2.38	0.56
1:D:503:LEU:O	1:D:509:LEU:HD12	2.06	0.55
1:C:836:GLN:O	1:C:900:ARG:NH2	2.38	0.55
1:D:667:GLU:HG3	1:D:1147:TYR:HB2	1.87	0.55
1:A:151:GLY:HA3	1:A:190:VAL:HG11	1.87	0.55
1:B:503:LEU:O	1:B:509:LEU:HD12	2.06	0.55
1:D:626:LEU:HD13	1:D:696:ALA:HB2	1.88	0.55
1:B:667:GLU:HG3	1:B:1147:TYR:HB2	1.88	0.55
1:D:156:PHE:CZ	1:D:190:VAL:CA	2.90	0.55
1:B:619:ARG:NH2	1:C:239:TYR:OH	2.38	0.55
1:D:150:THR:OG1	1:D:312:THR:HA	2.07	0.55
1:B:836:GLN:O	1:B:900:ARG:NH2	2.36	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1252:MET:HA	1:D:1255:ARG:HD3	1.89	0.54
1:B:131:TYR:HB2	1:B:284:LEU:HD21	1.90	0.54
1:B:170:LEU:HA	1:B:173:VAL:HG22	1.90	0.54
1:D:222:VAL:HG13	1:D:271:TYR:CE1	2.43	0.54
1:B:156:PHE:CZ	1:B:190:VAL:CA	2.90	0.54
1:B:1041:ILE:HD11	1:A:983:ILE:HG23	1.89	0.54
1:C:983:ILE:HG23	1:D:1041:ILE:HD11	1.89	0.53
1:B:150:THR:OG1	1:B:312:THR:HA	2.07	0.53
1:A:432:LEU:HD13	1:A:448:ILE:HD11	1.91	0.53
1:C:1096:PRO:O	1:C:1100:ILE:N	2.41	0.53
1:C:301:VAL:O	1:C:324:THR:OG1	2.22	0.53
1:D:170:LEU:HA	1:D:173:VAL:HG22	1.90	0.53
1:D:1095:LEU:HD12	1:D:1096:PRO:HD2	1.91	0.53
1:B:1252:MET:HA	1:B:1255:ARG:HD3	1.89	0.53
1:B:1257:LEU:HA	1:B:1266:ARG:HG2	1.90	0.53
1:C:824:LEU:HD11	1:C:926:LEU:HD11	1.91	0.53
1:A:1096:PRO:O	1:A:1100:ILE:N	2.41	0.52
1:D:830:VAL:HG11	1:D:846:LEU:HD22	1.91	0.52
1:A:277:LEU:HA	1:A:280:ARG:HG2	1.91	0.52
1:C:432:LEU:HD13	1:C:448:ILE:HD11	1.91	0.52
1:D:131:TYR:HB2	1:D:284:LEU:HD21	1.90	0.52
1:B:830:VAL:HG11	1:B:846:LEU:HD22	1.91	0.52
1:C:457:SER:O	1:C:461:HIS:ND1	2.37	0.52
1:A:1070:VAL:O	1:A:1074:THR:HB	2.10	0.52
1:B:1095:LEU:HD12	1:B:1096:PRO:HD2	1.91	0.52
1:B:222:VAL:HG13	1:B:271:TYR:CE1	2.43	0.52
1:B:1006:LEU:HD21	1:B:1032:THR:CB	2.40	0.52
1:B:149:VAL:HG22	1:B:304:VAL:HG23	1.85	0.52
1:D:1006:LEU:HD21	1:D:1032:THR:CB	2.40	0.52
1:A:1319:LEU:HD23	1:A:1325:ASN:HD22	1.75	0.52
1:B:140:LEU:HD21	1:B:259:HIS:HE1	1.75	0.52
1:A:824:LEU:HD11	1:A:926:LEU:HD11	1.91	0.52
1:C:277:LEU:HA	1:C:280:ARG:HG2	1.92	0.52
1:B:813:PHE:HD1	1:B:1089:TYR:HE2	1.57	0.52
1:D:1257:LEU:HA	1:D:1266:ARG:HG2	1.90	0.52
1:D:503:LEU:O	1:D:509:LEU:CD1	2.58	0.52
1:D:547:LEU:HD12	1:D:630:LYS:HD3	1.92	0.52
1:C:1070:VAL:O	1:C:1074:THR:HB	2.10	0.51
1:C:456:THR:HG23	1:C:459:ASP:H	1.75	0.51
1:B:342:VAL:HG12	1:B:386:LEU:HD22	1.93	0.51
1:C:547:LEU:O	1:C:630:LYS:NZ	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:892:LEU:HD21	1:C:917:ILE:HG23	1.92	0.51
1:A:367:TYR:CE1	1:A:371:THR:HG21	2.45	0.51
1:B:503:LEU:O	1:B:509:LEU:CD1	2.58	0.51
1:D:148:SER:O	1:D:303:CYS:CA	2.58	0.51
1:A:812:LYS:HE2	1:A:1094:ALA:HB2	1.92	0.51
1:C:812:LYS:HE2	1:C:1094:ALA:HB2	1.92	0.51
1:A:456:THR:HG23	1:A:459:ASP:H	1.75	0.51
1:D:298:THR:OG1	1:D:430:ARG:NH1	2.44	0.51
1:D:738:PHE:HA	1:D:741:ILE:HD12	1.93	0.51
1:A:990:PRO:O	1:A:993:THR:HG22	2.11	0.51
1:D:121:VAL:HB	1:D:125:THR:HG21	1.93	0.51
1:C:880:ASP:OD2	1:C:883:ASN:ND2	2.44	0.51
1:C:990:PRO:O	1:C:993:THR:HG22	2.11	0.51
1:D:342:VAL:HG12	1:D:386:LEU:HD22	1.93	0.51
1:B:298:THR:OG1	1:B:430:ARG:NH1	2.44	0.51
1:C:622:ILE:HD12	1:C:679:LEU:HD23	1.93	0.51
1:D:140:LEU:HD21	1:D:259:HIS:HE1	1.75	0.51
1:B:1053:ILE:HD13	1:A:950:LEU:HD13	1.92	0.50
1:B:547:LEU:HD12	1:B:630:LYS:HD3	1.92	0.50
1:A:223:ILE:O	1:A:226:ARG:NH1	2.42	0.50
1:B:1396:TYR:HB2	1:B:1415:ILE:HG23	1.94	0.50
1:C:367:TYR:CE1	1:C:371:THR:HG21	2.45	0.50
1:C:950:LEU:HD13	1:D:1053:ILE:HD13	1.94	0.50
1:A:892:LEU:HD21	1:A:917:ILE:HG23	1.92	0.50
1:A:943:VAL:HA	1:A:946:MET:HG2	1.94	0.50
1:C:1319:LEU:HD23	1:C:1325:ASN:HD22	1.75	0.50
1:D:221:GLY:HA3	1:D:268:GLN:HA	1.93	0.50
1:A:1070:VAL:O	1:A:1074:THR:CB	2.60	0.50
1:B:221:GLY:HA3	1:B:268:GLN:HA	1.93	0.50
1:B:121:VAL:HB	1:B:125:THR:HG21	1.93	0.50
1:B:1318:ALA:HB3	1:B:1404:ARG:HD2	1.94	0.50
1:D:1318:ALA:HB3	1:D:1404:ARG:HD2	1.94	0.50
1:D:813:PHE:HD1	1:D:1089:TYR:HE2	1.57	0.50
1:A:622:ILE:HD12	1:A:679:LEU:HD23	1.93	0.50
1:A:880:ASP:OD2	1:A:883:ASN:ND2	2.44	0.50
1:B:385:ILE:HG22	1:B:392:LEU:HD11	1.94	0.50
1:C:345:VAL:N	1:C:346:PRO:CD	2.75	0.50
1:C:943:VAL:HA	1:C:946:MET:HG2	1.94	0.50
1:A:345:VAL:N	1:A:346:PRO:CD	2.75	0.49
1:B:148:SER:O	1:B:303:CYS:CA	2.58	0.49
1:C:473:PRO:HA	1:C:476:VAL:HG12	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1396:TYR:HB2	1:D:1415:ILE:HG23	1.94	0.49
1:D:149:VAL:CG1	1:D:304:VAL:HG23	2.40	0.49
1:D:385:ILE:HG22	1:D:392:LEU:HD11	1.95	0.49
1:A:1272:GLU:HG3	1:A:1273:LYS:HG2	1.94	0.49
1:A:183:THR:HG22	1:A:191:MET:HG3	1.94	0.49
1:B:738:PHE:HA	1:B:741:ILE:HD12	1.93	0.49
1:C:1070:VAL:O	1:C:1074:THR:CB	2.60	0.49
1:C:183:THR:HG22	1:C:191:MET:HG3	1.94	0.49
1:C:942:ILE:HG13	1:C:1074:THR:HG21	1.94	0.49
1:A:239:TYR:OH	1:D:487:ARG:NH2	2.46	0.49
1:A:547:LEU:O	1:A:630:LYS:NZ	2.43	0.49
1:A:942:ILE:HG13	1:A:1074:THR:HG21	1.94	0.49
1:C:166:PHE:HA	1:C:405:VAL:HG21	1.95	0.49
1:A:1273:LYS:HD2	1:A:1280:PHE:HB3	1.95	0.49
1:A:166:PHE:HA	1:A:405:VAL:HG21	1.95	0.49
1:C:1272:GLU:HG3	1:C:1273:LYS:HG2	1.94	0.49
1:C:224:HIS:HA	1:C:250:LEU:HD12	1.95	0.49
1:D:823:PHE:HB2	1:D:849:TRP:CZ2	2.48	0.49
1:A:473:PRO:HA	1:A:476:VAL:HG12	1.94	0.49
1:B:149:VAL:CG1	1:B:304:VAL:HG23	2.40	0.48
1:A:982:ILE:HD11	1:D:832:MET:HB3	1.95	0.48
1:D:149:VAL:HA	1:D:304:VAL:O	2.13	0.48
1:D:149:VAL:HG22	1:D:304:VAL:HG23	1.86	0.48
1:B:149:VAL:HA	1:B:304:VAL:O	2.13	0.48
1:C:226:ARG:HH22	1:C:268:GLN:HE21	1.62	0.48
1:A:151:GLY:HA2	1:A:306:LEU:H	1.79	0.48
1:B:823:PHE:HB2	1:B:849:TRP:CZ2	2.48	0.48
1:D:156:PHE:CD1	1:D:189:GLY:HA2	2.48	0.48
1:A:224:HIS:HA	1:A:250:LEU:HD12	1.95	0.47
1:A:226:ARG:HH22	1:A:268:GLN:HE21	1.62	0.47
1:B:138:TRP:HB3	1:B:140:LEU:HD23	1.95	0.47
1:C:961:VAL:HG22	1:C:990:PRO:CB	2.43	0.47
1:D:156:PHE:CZ	1:D:190:VAL:N	2.81	0.47
1:B:356:ASN:OD1	1:B:367:TYR:OH	2.30	0.47
1:C:1328:LEU:HD11	1:C:1369:LEU:HD12	1.97	0.47
1:A:961:VAL:HG22	1:A:990:PRO:CB	2.43	0.47
1:C:1273:LYS:HD2	1:C:1280:PHE:HB3	1.95	0.47
1:A:1395:VAL:N	1:A:1415:ILE:O	2.48	0.47
1:A:302:VAL:HG23	1:A:325:PRO:HG2	1.96	0.47
1:C:705:ILE:HD13	1:C:1080:PHE:HA	1.96	0.47
1:D:859:ARG:HG2	1:D:1104:HIS:HE1	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:547:LEU:O	1:B:630:LYS:NZ	2.39	0.47
1:B:191:MET:SD	1:B:191:MET:N	2.87	0.47
1:D:138:TRP:HB3	1:D:140:LEU:HD23	1.95	0.47
1:D:544:ARG:HE	1:D:549:SER:HA	1.80	0.47
1:A:887:VAL:HA	1:A:890:ILE:HG22	1.97	0.47
1:B:682:ARG:HG2	1:B:1128:LEU:HD23	1.97	0.47
1:C:469:VAL:HG23	1:C:502:HIS:HB3	1.97	0.47
1:A:283:LYS:HB3	1:A:322:ASN:HD21	1.80	0.47
1:A:705:ILE:HD13	1:A:1080:PHE:HA	1.96	0.47
1:A:923:CYS:HA	1:A:926:LEU:HD13	1.97	0.47
1:B:1090:HIS:HE1	1:B:1123:ASN:HD22	1.62	0.47
1:B:859:ARG:HG2	1:B:1104:HIS:HE1	1.80	0.47
1:A:856:GLU:OE2	1:A:1092:ARG:NE	2.49	0.46
1:A:1328:LEU:HD11	1:A:1369:LEU:HD12	1.97	0.46
1:B:183:THR:HG22	1:B:191:MET:HG3	1.98	0.46
1:B:417:SER:HB3	1:B:431:GLN:HE22	1.79	0.46
1:C:302:VAL:HG23	1:C:325:PRO:HG2	1.96	0.46
1:A:134:MET:O	1:A:138:TRP:HB2	2.15	0.46
1:A:986:ALA:O	1:A:990:PRO:HG2	2.16	0.46
1:C:283:LYS:HB3	1:C:322:ASN:HD21	1.80	0.46
1:D:417:SER:HB3	1:D:431:GLN:HE22	1.80	0.46
1:A:427:CYS:SG	1:A:431:GLN:NE2	2.89	0.46
1:C:198:VAL:HG23	1:C:212:ILE:HD11	1.97	0.46
1:C:223:ILE:O	1:C:226:ARG:NH1	2.42	0.46
1:C:427:CYS:SG	1:C:431:GLN:NE2	2.89	0.46
1:C:887:VAL:HA	1:C:890:ILE:HG22	1.97	0.46
1:B:387:ARG:NH1	1:B:1252:MET:SD	2.87	0.46
1:D:682:ARG:HG2	1:D:1128:LEU:HD23	1.97	0.46
1:C:450:THR:O	1:C:453:SER:OG	2.29	0.46
1:C:856:GLU:OE2	1:C:1092:ARG:NE	2.49	0.46
1:C:151:GLY:HA2	1:C:306:LEU:H	1.79	0.46
1:A:626:LEU:HD13	1:A:696:ALA:HB2	1.98	0.46
1:B:181:ILE:HB	1:B:214:VAL:HG12	1.98	0.46
1:C:134:MET:O	1:C:138:TRP:HB2	2.15	0.46
1:C:986:ALA:O	1:C:990:PRO:HG2	2.16	0.46
1:A:198:VAL:HG23	1:A:212:ILE:HD11	1.97	0.46
1:A:999:PRO:HB2	1:A:1044:LEU:HD21	1.98	0.46
1:B:544:ARG:HE	1:B:549:SER:HA	1.80	0.46
1:B:726:ASN:HD22	1:B:746:LEU:HD23	1.81	0.46
1:D:183:THR:HG22	1:D:191:MET:HG3	1.98	0.46
1:B:156:PHE:CZ	1:B:190:VAL:N	2.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1395:VAL:N	1:C:1415:ILE:O	2.48	0.46
1:D:506:CYS:SG	1:D:509:LEU:N	2.89	0.45
1:C:923:CYS:HA	1:C:926:LEU:HD13	1.97	0.45
1:C:999:PRO:HB2	1:C:1044:LEU:HD21	1.98	0.45
1:D:1090:HIS:HE1	1:D:1123:ASN:HD22	1.62	0.45
1:A:469:VAL:HG23	1:A:502:HIS:HB3	1.97	0.45
1:C:626:LEU:HD13	1:C:696:ALA:HB2	1.98	0.45
1:D:1322:LEU:HA	1:D:1409:ALA:HB2	1.98	0.45
1:D:726:ASN:HD22	1:D:746:LEU:HD23	1.81	0.45
1:B:592:TRP:O	1:B:596:ARG:NH1	2.50	0.45
1:B:506:CYS:SG	1:B:509:LEU:N	2.89	0.45
1:D:148:SER:O	1:D:304:VAL:N	2.48	0.45
1:D:181:ILE:HB	1:D:214:VAL:HG12	1.98	0.45
1:D:683:ILE:HD13	1:D:1125:ARG:HE	1.82	0.45
1:B:273:VAL:O	1:B:276:GLU:N	2.43	0.45
1:D:722:LEU:HD23	1:D:810:GLN:HE21	1.82	0.45
1:B:1347:ALA:HA	1:B:1358:LEU:HA	1.99	0.44
1:D:156:PHE:CZ	1:D:189:GLY:C	2.86	0.44
1:B:722:LEU:HD21	1:B:726:ASN:HD21	1.83	0.44
1:D:1347:ALA:HA	1:D:1358:LEU:HA	1.99	0.44
1:D:407:VAL:HG22	1:D:443:ILE:HD11	1.99	0.44
1:D:1346:LEU:HA	1:D:1446:TRP:HA	2.00	0.44
1:B:1322:LEU:HA	1:B:1409:ALA:HB2	1.99	0.44
1:B:263:VAL:HG21	1:B:274:GLU:HA	1.99	0.44
1:C:1334:ARG:NE	1:C:1344:GLU:OE1	2.41	0.44
1:D:263:VAL:HG21	1:D:274:GLU:HA	1.99	0.44
1:B:1346:LEU:HA	1:B:1446:TRP:HA	2.00	0.44
1:B:407:VAL:HG22	1:B:443:ILE:HD11	1.99	0.44
1:B:722:LEU:HD23	1:B:810:GLN:HE21	1.82	0.44
1:C:385:ILE:HG22	1:C:392:LEU:HD11	2.00	0.44
1:B:1090:HIS:CE1	1:B:1123:ASN:HD22	2.36	0.43
1:D:621:CYS:SG	1:D:1144:LYS:HD2	2.58	0.43
1:B:621:CYS:SG	1:B:1144:LYS:HD2	2.58	0.43
1:B:632:LEU:HB3	1:B:654:ALA:HB2	2.00	0.43
1:D:722:LEU:HD21	1:D:726:ASN:HD21	1.83	0.43
1:D:191:MET:SD	1:D:191:MET:N	2.87	0.43
1:D:592:TRP:O	1:D:596:ARG:NH1	2.50	0.43
1:A:183:THR:HG21	1:A:194:VAL:HG11	2.01	0.43
1:C:1394:GLU:HA	1:C:1416:ILE:HA	2.01	0.43
1:A:199:ARG:CZ	1:A:256:ASN:HD21	2.32	0.43
1:B:857:GLU:OE1	1:B:877:TYR:OH	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1090:HIS:CE1	1:D:1123:ASN:HD22	2.37	0.43
1:D:632:LEU:HB3	1:D:654:ALA:HB2	2.00	0.43
1:D:657:TYR:HA	1:D:657:TYR:HD1	1.68	0.43
1:B:694:TRP:O	1:B:698:GLU:CB	2.67	0.43
1:B:89:TRP:O	1:B:93:ARG:CB	2.67	0.43
1:C:199:ARG:CZ	1:C:256:ASN:HD21	2.31	0.43
1:A:453:SER:HB3	1:A:455:TRP:CD1	2.54	0.43
1:B:148:SER:O	1:B:304:VAL:N	2.48	0.43
1:B:535:CYS:H	1:B:538:HIS:HD2	1.66	0.43
1:B:904:SER:HB2	1:B:907:VAL:HG22	2.01	0.43
1:D:466:SER:HA	1:D:469:VAL:HG12	2.01	0.43
1:D:707:HIS:HB3	1:D:710:VAL:HG12	2.00	0.43
1:D:904:SER:HB2	1:D:907:VAL:HG22	2.01	0.43
1:B:683:ILE:HD13	1:B:1125:ARG:HE	1.82	0.43
1:D:146:LEU:HD11	1:D:182:LEU:HB2	2.01	0.43
1:C:461:HIS:NE2	1:C:488:GLU:O	2.52	0.43
1:C:808:SER:HB2	1:C:811:VAL:HG12	2.00	0.43
1:A:848:VAL:HA	1:A:851:THR:HG22	2.01	0.42
1:B:376:ILE:HG23	1:B:1268:PRO:HG2	2.01	0.42
1:A:1333:THR:HG22	1:A:1345:PHE:HB3	2.01	0.42
1:C:183:THR:HG21	1:C:194:VAL:HG11	2.01	0.42
1:C:848:VAL:HA	1:C:851:THR:HG22	2.01	0.42
1:C:984:ARG:NE	1:D:1003:ASP:O	2.52	0.42
1:D:273:VAL:O	1:D:276:GLU:N	2.43	0.42
1:A:808:SER:HB2	1:A:811:VAL:HG12	2.00	0.42
1:D:199:ARG:HA	1:D:202:THR:HG22	2.01	0.42
1:B:105:ASP:OD1	1:B:105:ASP:N	2.52	0.42
1:B:156:PHE:CD1	1:B:189:GLY:HA2	2.48	0.42
1:B:466:SER:HA	1:B:469:VAL:HG12	2.01	0.42
1:B:707:HIS:HB3	1:B:710:VAL:HG12	2.00	0.42
1:C:1333:THR:HG22	1:C:1345:PHE:HB3	2.01	0.42
1:D:694:TRP:O	1:D:698:GLU:CB	2.67	0.42
1:A:385:ILE:HG22	1:A:392:LEU:HD11	2.00	0.42
1:B:380:LYS:HD2	1:B:1257:LEU:HD11	2.01	0.42
1:D:387:ARG:NH1	1:D:1252:MET:SD	2.87	0.42
1:D:89:TRP:O	1:D:93:ARG:CB	2.67	0.42
1:B:603:VAL:HG22	1:B:632:LEU:HD21	2.01	0.42
1:C:726:ASN:HD22	1:C:746:LEU:HD22	1.85	0.42
1:D:356:ASN:OD1	1:D:367:TYR:OH	2.30	0.42
1:D:376:ILE:HG23	1:D:1268:PRO:HG2	2.01	0.42
1:D:859:ARG:HG2	1:D:1104:HIS:CE1	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1003:ASP:O	1:A:984:ARG:NE	2.52	0.42
1:A:461:HIS:NE2	1:A:488:GLU:O	2.52	0.42
1:B:199:ARG:HA	1:B:202:THR:HG22	2.02	0.42
1:B:657:TYR:HD1	1:B:657:TYR:HA	1.68	0.42
1:C:176:THR:HG21	1:C:440:ARG:HH11	1.85	0.42
1:A:346:PRO:HB3	1:A:349:LYS:CB	2.40	0.42
1:A:1394:GLU:HA	1:A:1416:ILE:HA	2.01	0.42
1:C:453:SER:HB3	1:C:455:TRP:CD1	2.54	0.42
1:D:399:GLU:H	1:D:403:TYR:HB2	1.85	0.42
1:D:535:CYS:SG	1:D:536:LEU:N	2.93	0.42
1:A:146:LEU:HB3	1:A:301:VAL:HG22	2.02	0.41
1:A:748:PHE:HE2	1:A:801:ARG:HG3	1.85	0.41
1:D:380:LYS:HD2	1:D:1257:LEU:HD11	2.01	0.41
1:B:156:PHE:CZ	1:B:189:GLY:C	2.86	0.41
1:B:535:CYS:SG	1:B:536:LEU:N	2.93	0.41
1:C:50:LYS:N	1:C:99:PRO:O	2.53	0.41
1:D:304:VAL:HG12	1:D:327:VAL:HB	2.02	0.41
1:C:705:ILE:HG21	1:C:1080:PHE:HD1	1.85	0.41
1:A:50:LYS:N	1:A:99:PRO:O	2.53	0.41
1:B:634:LYS:HD2	1:B:634:LYS:HA	1.91	0.41
1:D:535:CYS:H	1:D:538:HIS:HD2	1.66	0.41
1:A:176:THR:HG21	1:A:440:ARG:HH11	1.85	0.41
1:A:705:ILE:HG21	1:A:1080:PHE:HD1	1.85	0.41
1:D:1276:TRP:NE1	1:D:1306:ASN:O	2.40	0.41
1:D:603:VAL:HG22	1:D:632:LEU:HD21	2.01	0.41
1:A:317:TYR:HA	1:A:385:ILE:HD11	2.03	0.41
1:B:304:VAL:HG12	1:B:327:VAL:HB	2.03	0.41
1:B:749:ARG:O	1:B:753:ASP:CB	2.69	0.41
1:B:859:ARG:HG2	1:B:1104:HIS:CE1	2.54	0.41
1:C:105:ASP:HA	1:C:117:LYS:HA	2.03	0.41
1:B:146:LEU:HD11	1:B:182:LEU:HB2	2.01	0.41
1:D:749:ARG:O	1:D:753:ASP:CB	2.69	0.41
1:A:603:VAL:HG22	1:A:632:LEU:HD21	2.03	0.41
1:B:134:MET:HA	1:B:138:TRP:CE3	2.56	0.41
1:C:603:VAL:HG22	1:C:632:LEU:HD21	2.03	0.41
1:C:748:PHE:HE2	1:C:801:ARG:HG3	1.85	0.41
1:A:726:ASN:HD22	1:A:746:LEU:HD22	1.85	0.41
1:B:399:GLU:H	1:B:403:TYR:HB2	1.85	0.41
1:C:146:LEU:HB3	1:C:301:VAL:HG22	2.02	0.41
1:D:1399:TYR:HA	1:D:1412:GLU:HG2	2.02	0.41
1:A:662:ILE:HG22	1:A:704:PHE:HD1	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:335:LEU:HD13	1:D:378:TRP:HZ3	1.86	0.40
1:A:823:PHE:HB2	1:A:849:TRP:CE2	2.57	0.40
1:B:1399:TYR:HA	1:B:1412:GLU:HG2	2.02	0.40
1:B:516:VAL:HG21	1:B:534:VAL:HG12	2.03	0.40
1:B:50:LYS:CB	1:B:98:THR:O	2.53	0.40
1:C:317:TYR:HA	1:C:385:ILE:HD11	2.03	0.40
1:C:662:ILE:HG22	1:C:704:PHE:HD1	1.86	0.40
1:A:105:ASP:HA	1:A:117:LYS:HA	2.03	0.40
1:A:1077:ILE:O	1:A:1081:GLN:NE2	2.54	0.40
1:A:834:ASP:OD1	1:A:834:ASP:N	2.54	0.40
1:B:355:ILE:HD13	1:B:379:THR:HA	2.03	0.40
1:C:834:ASP:N	1:C:834:ASP:OD1	2.54	0.40
1:A:1121:HIS:HD2	1:A:1124:PHE:HB2	1.87	0.40
1:A:741:ILE:HD12	1:A:801:ARG:HG2	2.04	0.40
1:D:105:ASP:N	1:D:105:ASP:OD1	2.52	0.40
1:D:516:VAL:HG21	1:D:534:VAL:HG12	2.03	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	1177/1466 (80%)	1102 (94%)	74 (6%)	1 (0%)	53	87
1	B	1208/1466 (82%)	1127 (93%)	80 (7%)	1 (0%)	53	87
1	C	1177/1466 (80%)	1103 (94%)	73 (6%)	1 (0%)	53	87
1	D	1208/1466 (82%)	1128 (93%)	79 (6%)	1 (0%)	53	87
All	All	4770/5864 (81%)	4460 (94%)	306 (6%)	4 (0%)	56	87

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1014	VAL
1	C	1014	VAL
1	B	1024	CYS
1	D	1024	CYS

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	760/1277 (60%)	751 (99%)	9 (1%)	74	88
1	B	743/1277 (58%)	730 (98%)	13 (2%)	63	84
1	C	760/1277 (60%)	751 (99%)	9 (1%)	74	88
1	D	743/1277 (58%)	730 (98%)	13 (2%)	63	84
All	All	3006/5108 (59%)	2962 (98%)	44 (2%)	70	85

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	150	THR
1	B	303	CYS
1	B	334	ARG
1	B	357	ARG
1	B	544	ARG
1	B	859	ARG
1	B	900	ARG
1	B	922	PHE
1	B	925	ARG
1	B	991	TYR
1	B	1001	ASN
1	B	1064	ASN
1	B	1146	ASN
1	A	191	MET
1	A	226	ARG
1	A	314	ASN
1	A	816	ASN
1	A	859	ARG

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Mol	Chain	Res	Type
1	A	900	ARG
1	A	934	ARG
1	A	1073	ASN
1	A	1146	ASN
1	C	191	MET
1	C	226	ARG
1	C	314	ASN
1	C	816	ASN
1	C	859	ARG
1	C	900	ARG
1	C	934	ARG
1	C	1073	ASN
1	C	1146	ASN
1	D	150	THR
1	D	303	CYS
1	D	334	ARG
1	D	357	ARG
1	D	544	ARG
1	D	859	ARG
1	D	900	ARG
1	D	922	PHE
1	D	925	ARG
1	D	991	TYR
1	D	1001	ASN
1	D	1064	ASN
1	D	1146	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (56) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	187	HIS
1	B	259	HIS
1	B	431	GLN
1	B	538	HIS
1	B	707	HIS
1	B	816	ASN
1	B	1001	ASN
1	B	1064	ASN
1	B	1090	HIS
1	B	1104	HIS
1	B	1146	ASN
1	B	1161	HIS

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Mol	Chain	Res	Type
1	B	1329	HIS
1	B	1405	ASN
1	A	129	ASN
1	A	187	HIS
1	A	224	HIS
1	A	256	ASN
1	A	259	HIS
1	A	268	GLN
1	A	314	ASN
1	A	322	ASN
1	A	431	GLN
1	A	816	ASN
1	A	1073	ASN
1	A	1081	GLN
1	A	1104	HIS
1	A	1121	HIS
1	A	1146	ASN
1	C	129	ASN
1	C	187	HIS
1	C	224	HIS
1	C	256	ASN
1	C	259	HIS
1	C	268	GLN
1	C	314	ASN
1	C	431	GLN
1	C	1073	ASN
1	C	1081	GLN
1	C	1104	HIS
1	C	1121	HIS
1	C	1146	ASN
1	D	187	HIS
1	D	259	HIS
1	D	431	GLN
1	D	538	HIS
1	D	707	HIS
1	D	816	ASN
1	D	1001	ASN
1	D	1064	ASN
1	D	1090	HIS
1	D	1104	HIS
1	D	1146	ASN
1	D	1161	HIS

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Mol	Chain	Res	Type
1	D	1329	HIS
1	D	1405	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 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 (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	2

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Mol	Chain	Number of breaks
1	C	2
1	B	1
1	D	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	1209:UNK	C	1246:ASP	N	42.80
1	C	1209:UNK	C	1246:ASP	N	42.80
1	B	1184:VAL	C	1188:UNK	N	10.31
1	D	1184:VAL	C	1188:UNK	N	10.31
1	A	1184:VAL	C	1188:UNK	N	9.14
1	C	1184:VAL	C	1188:UNK	N	9.14