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EMDB ID	:	EMD-20407
Title	:	In situ structure of BTV RNA-dependent RNA polymerase in BTV core
Authors	:	He, Y.; Shivakoti, S.; Ding, K.; Cui, Y.; Roy, P.; Zhou, Z.H.
Deposited on	:	2019-07-03
Resolution	:	3.60 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB 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.

The types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

EMDB validation analysis	:	0.0.1.dev70
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.60 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f EM\ structures}\ (\#{ m Entries})$
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for $\geq=3, 2, 1$ and 0 types of geometric quality criteria respectively. 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 $\leq=5\%$ The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain		
			61%		
1	А	1302	80%	15%	•
			27%		
2	В	901	89%	8%	·
			52%	_	
2	С	901	85%	12%	·
_	-		30%		
2	D	901	86%	10%	·
		0.01	52%		_
2	E	901	86%	12%	·
		0.01	31%		_
2	F'	901	85%	11%	·
	a	0.01	53%		_
2	G	901	87%	12%	·
	тт	0.01	30%		_
2	H	901	84%	12%	•



Mol	Chain	Length	Quality of chain			
			51%			
2	Ι	901	86%	12%	·	
			29%			
2	J	901	85%	12%	•	
			51%			
2	Κ	901	88%	10%	·	



2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 80873 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 RNA-directed RNA polymerase.

Mol	Chain	Residues	Atoms				AltConf	Trace	
1	А	1244	Total 10062	С 6417	N 1720	0 1865	S 60	0	0

• Molecule 2 is a protein called Inner core structural protein VP3.

Mol	Chain	Residues		Α	toms			AltConf	Trace
0	Р	879	Total	С	Ν	Ο	\mathbf{S}	0	0
2	D	012	7046	4496	1222	1287	41	0	0
2	С	885	Total	\mathbf{C}	Ν	Ο	\mathbf{S}	0	0
2	U	000	7151	4561	1239	1310	41	0	0
2	Л	863	Total	\mathbf{C}	Ν	Ο	\mathbf{S}	0	0
2	D	005	6968	4448	1209	1271	40	0	0
2	E	885	Total	\mathbf{C}	Ν	Ο	\mathbf{S}	0	0
2	Ľ	000	7151	4561	1239	1310	41	0	0
2	F	868	Total	\mathbf{C}	Ν	Ο	\mathbf{S}	0	0
2	Ľ	000	6995	4463	1209	1283	40	0	0
2	C	885	Total	\mathbf{C}	Ν	Ο	\mathbf{S}	0	0
2	G	000	7151	4561	1239	1310	41	0	0
2	н	868	Total	\mathbf{C}	Ν	Ο	\mathbf{S}	0	0
2	11	000	7017	4476	1218	1282	41	0	0
2	T	885	Total	\mathbf{C}	Ν	Ο	\mathbf{S}	0	0
2	L	000	7151	4561	1239	1310	41	0	0
9	т	870	Total	С	Ν	Ο	\mathbf{S}	0	0
	J	010	7030	4484	1220	1285	41	0	0
2	K	885	Total	С	Ν	0	S	0	0
		000	7151	4561	1239	1310	41	U	U



3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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 and atom inclusion in map density. 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. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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: RNA-directed RNA polymerase



					_
***** ***	*****			*****	••••
E629 6630 7631 1632 1633 E634 9635 1635 1635 1637	F639 6640 6642 6642 6644 6645 8645 8645 8645 8645	N648 1650 1650 1651 1655 1655 1655 1655 1655	1660 1661 1661 1661 1666 1665 1665 1665	E672 R673 D674 K675 K675 G676 F678 K679 K679 K679 K680 C681 C683 C683	L685 P686 V687
S689 V690 D691 V692 A693 N694 R695 I696 A697 V698	D699 6701 6701 5702 D703 D703 T704 L705 1706	A708 1709 0711 6711 5712 5712 1714 A715 A715 A715 1717 D718	T719 ↔ H720 ↔ L721 ↔ S722 ↔ G723 ↔ S726 ↔ T727 ↔ T726 ↔ T729 ↔ T729 ↔	S732 M733 H734 G743 E745 E745 B748 B748 C752 C752 C752 C753	S758 E759 Q760 ♦
••••	•• • • • •	••••		•••••	
Y761 V762 D763 D765 V769 V769 V769 V777	D795 C794 C794 C794 C794 C794 C794	E797 E797 5799 5801 5801 7803 7803 7803 7803 7803 7803 7803 7813 7813 7813 7813 7813	0819 0826 1827 1828 1828 1830 1831 1831 1831 1833 8833 8833 883	R836 X837 X837 X837 2838 8848 V845 V845 V845 V845 V845 V845 V84	·
M853 1854 1855 1855 1855 1864 1871	K873 1877 G878 A879 W880 K881 M882 K883	R884 1885 K887 K887 E888 A890 M891 Y892 R893 R893 R893	R895 F897 B898 B898 B901 B901 F905 G904 F905 F905	L907 1908 8911 8911 8911 1920 1920 8923 8923 8923	6926
* * * * * *		• ••••	****		
L932 E938 D943 S944 1945 1945 L950 D951	E952 A955 P9566 1957 R959 R959 H962 D963	1964 P965 P966 C967 0968 N969 E970 E970 C17 1971 C171 C171 C17	011 011 111 1112 1112 1112 1112 1113 1113	мочо 1991 1993 1993 1993 1993 1993 1993 1993 1993 1993 1993 1993 1993 1993 1993 1000	
q1003 11004 11005 11005 11007 ↓ 11008 €1009 €1001 ↓ 1012 ↓ 1012 ↓	L1013 G1014 E1015 F1015 S1017 P1018 G1019 R1020 R1020 L11021	81022 R1023 T1024 M1025 H1027 S1028 A1029 L1031 L1031 K1032	E1033 S1034 S1035 A1036 A1036 R1037 T1038 L1040 S1041 S1042 S1042 S1043 S1043 S1043	E1045 L1046 E1047 Y1048 Q1049 A1051 L1052 N1053 S1054 W1055 I1056 T1057	q1058 V1059 S1060 M1061
•••••	• ••••		****	•••••	••
L1065 G1064 E1066 E1066 G1067 U1068 T1076 T1075	K1077 1088 1088 11088 11088 11088 11088 11088	A1065 1100 110	N1111 N1111 S1120 V1122 D1120 R1122 R1122 D1122 V1127	L1125 R1130 V1133 V1133 V1133 V1133 P1133 F1136 F1136 F1136 F1146 F1144	N1142 T1143
11144 L1145 L1145 N1146 V1147 11148 E1149 K1150 L1151 G1152 G1153	N1154 H1155 S1156 V1157 D1159 D1159 V1161 V1161	V1163 F1164 L1166 L1166 M1167 M1168 L1168 E1170 E1171 T1172 C1172	A1174 E1175 E1176 A1177 A1178 A1178 A1178 E1179 F1181 A1181 A1181 S1183 S1183 S1183 S1183 S1183 S1183	11186 R1187 F1187 F1188 A1190 L1191 K1192 K1193 K1193 A1199 A1199	61201 61201 61202 61210
			• •••••	••••• •	
T1211 (1212 (1213 (1213 (1213) (1213) (1213) (1213) (1213) (1213)	L1235 L1235 R1244 K1251 K1253 K1253 M1254 T1253	D1260 D1261 D1261 K1263 K1264 Y1265 Y1265 T1268 R1269 T1268 R1269 R1269	R1272 R1273 R1278 P1278 R1279 T1280 K1281 V1282 K1283 K1283 K1285 K1285 K1285	11287 11285 11285 11285 11292 11293 11293 112998 112998 112998 112998 112998 112998 112998 112088 1120888 1120888 112088 112088 112088 112	
1302					
• Molecule 2: Inn	er core structura	al protein VP3			
Chain B:	27%	89%	8% •	-	
MET ALA ALA ALA GLN GLN GLN PRO GLN FRO GLU TLE LVS	THR PRO PRO CLU GLU GLV ASP SER SER SER	ASP ASP ASP ASP ASC ASS ASS ASS ASS ASS ASS ASS ASS ASS	A40 411 443 443 443 443 152 152 152 152 152 152 152 152 152 152	F50 685 193 193 193 193	

• Molecule 2: Inner core structural protein VP3

Chain F: 85% 11% •

• Molecule 2: Inner core structural protein VP3

• Molecule 2: Inner core structural protein VP3

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	150346	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE	Depositor
	CORRECTION	
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{\AA}^2)$	32.0	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT $(4k \ge 4k)$	Depositor
Maximum map value	0.076	Depositor
Minimum map value	-0.045	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	348.16, 348.16, 348.16	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.36, 1.36, 1.36	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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).

Mal	Chain	Bond	lengths	Bond angles		
10101	Ullaili	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.31	0/10268	0.52	0/13862	
2	В	0.36	0/7203	0.52	0/9782	
2	С	0.33	0/7310	0.50	0/9927	
2	D	0.37	0/7124	0.52	0/9673	
2	Е	0.32	0/7310	0.50	0/9927	
2	F	0.37	0/7151	0.53	0/9712	
2	G	0.33	0/7310	0.52	0/9927	
2	Н	0.37	0/7174	0.53	0/9742	
2	Ι	0.33	0/7310	0.51	0/9927	
2	J	0.37	0/7187	0.53	0/9760	
2	Κ	0.33	0/7310	0.51	0/9927	
All	All	0.34	0/82657	0.52	0/112166	

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 (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	А	10062	0	10106	128	0
2	В	7046	0	7032	56	0
2	С	7151	0	7137	74	0
2	D	6968	0	6955	68	0
2	Е	7151	0	7137	65	0

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes				
2	F	6995	0	6968	68	0				
2	G	7151	0	7137	69	0				
2	Н	7017	0	6996	77	0				
2	Ι	7151	0	7137	74	0				
2	J	7030	0	7010	73	0				
2	Κ	7151	0	7137	77	0				
All	All	80873	0	80752	770	0				

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (770) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:K:438:VAL:HG11	2:K:452:TRP:CZ2	1.57	1.37
2:K:438:VAL:HG11	2:K:452:TRP:CH2	1.65	1.32
2:D:461:GLU:CG	2:D:462:PRO:HD3	1.67	1.23
2:K:438:VAL:CG1	2:K:452:TRP:CZ2	2.23	1.21
2:G:595:VAL:HG22	2:G:891:LYS:NZ	1.60	1.16
2:K:477:ILE:HD11	2:K:524:MET:HE2	1.28	1.15
2:C:475:CYS:SG	2:C:477:ILE:HG12	1.88	1.12
2:K:438:VAL:CG1	2:K:452:TRP:CH2	2.31	1.12
2:D:461:GLU:HG3	2:D:462:PRO:HD3	1.12	1.12
2:K:477:ILE:HD11	2:K:524:MET:CE	1.84	1.07
2:D:461:GLU:HG3	2:D:462:PRO:CD	1.86	1.04
2:G:595:VAL:CG2	2:G:891:LYS:NZ	2.22	1.02
2:G:477:ILE:HD11	2:G:524:MET:HE2	1.49	0.95
2:G:477:ILE:HD11	2:G:524:MET:CE	1.97	0.94
2:F:671:MET:HE3	2:F:671:MET:HA	1.50	0.93
2:E:477:ILE:HD11	2:E:524:MET:CE	2.04	0.88
2:K:141:GLY:HA2	2:K:213:VAL:HG13	1.56	0.88
2:H:475:CYS:SG	2:H:477:ILE:HD11	2.14	0.88
2:D:461:GLU:HG2	2:D:462:PRO:HD3	1.56	0.87
2:K:671:MET:HA	2:K:671:MET:HE3	1.54	0.87
2:G:595:VAL:CG2	2:G:891:LYS:HZ1	1.90	0.84
2:G:595:VAL:HG22	2:G:891:LYS:HZ2	1.40	0.83
2:K:438:VAL:HG11	2:K:452:TRP:HZ2	1.42	0.81
2:D:461:GLU:CG	2:D:462:PRO:CD	2.52	0.80
2:C:101:VAL:C	2:C:102:LEU:HD12	2.02	0.79
2:H:475:CYS:SG	2:H:477:ILE:HG13	2.24	0.78
2:D:475:CYS:SG	2:D:477:ILE:HG13	2.23	0.78

		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:E:141:GLY:HA2	2:E:213:VAL:HG13	1.66	0.77
2:H:475:CYS:SG	2:H:477:ILE:CD1	2.72	0.77
2:E:791:PRO:O	2:E:794:VAL:HG23	1.86	0.76
2:E:477:ILE:HD11	2:E:524:MET:HE2	1.69	0.74
2:K:438:VAL:HG12	2:K:452:TRP:CH2	2.22	0.74
2:C:475:CYS:SG	2:C:477:ILE:CG1	2.72	0.73
2:E:793:ASP:OD1	2:E:793:ASP:N	2.20	0.73
1:A:1160:LEU:O	1:A:1163:VAL:HG22	1.87	0.73
2:H:667:MET:O	2:H:671:MET:HG3	1.89	0.72
2:K:438:VAL:HG11	2:K:452:TRP:HH2	1.54	0.69
2:D:283:ARG:HE	2:D:659:ASN:HB3	1.56	0.69
2:D:474:TYR:O	2:D:475:CYS:SG	2.51	0.69
2:H:475:CYS:SG	2:H:477:ILE:CG1	2.80	0.69
2:F:667:MET:O	2:F:671:MET:HG2	1.92	0.69
2:G:209:CYS:H	2:G:872:ARG:HG3	1.59	0.67
2:D:472:ILE:H	2:D:535:ASN:HD21	1.41	0.67
2:B:671:MET:HE3	2:B:671:MET:HA	1.75	0.67
2:J:461:GLU:HA	2:J:461:GLU:OE1	1.93	0.67
2:F:671:MET:HA	2:F:671:MET:CE	2.23	0.67
2:G:477:ILE:HD11	2:G:524:MET:HE3	1.76	0.67
2:I:793:ASP:O	2:I:797:GLY:HA3	1.95	0.66
2:B:667:MET:O	2:B:671:MET:HG2	1.95	0.66
2:C:475:CYS:HG	2:C:477:ILE:HG12	1.59	0.66
1:A:230:LEU:HD11	1:A:368:ILE:HB	1.78	0.65
2:K:477:ILE:HD11	2:K:524:MET:HE3	1.74	0.65
2:I:793:ASP:O	2:I:797:GLY:CA	2.44	0.65
2:C:102:LEU:HD12	2:C:102:LEU:N	2.12	0.65
2:E:474:TYR:H	2:E:531:ASN:HD21	1.45	0.64
2:E:135:ARG:HD2	2:E:138:ARG:HH21	1.61	0.64
2:G:595:VAL:HG22	2:G:891:LYS:HZ3	1.58	0.64
2:D:474:TYR:H	2:D:531:ASN:HD21	1.46	0.63
2:D:671:MET:HA	2:D:671:MET:HE3	1.78	0.63
2:D:632:ARG:H	2:D:635:HIS:HD2	1.45	0.63
2:H:472:ILE:H	2:H:535:ASN:HD21	1.46	0.63
2:J:667:MET:CE	2:J:671:MET:CE	2.77	0.63
2:F:632:ARG:H	2:F:635:HIS:HD2	1.46	0.62
2:E:201:ASP:OD1	2:E:202:VAL:HG13	1.99	0.62
2:J:474:TYR:H	2:J:531:ASN:HD21	1.47	0.62
2:C:667:MET:SD	2:C:671:MET:CE	2.88	0.62
1:A:499:LYS:HG3	1:A:644:GLY:HA3	1.82	0.62
2:C:384:GLY:HA2	2:C:446:GLY:HA3	1.82	0.62

	juo puge	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:96:GLU:O	1:A:100:ASN:ND2	2.32	0.61
2:E:728:TYR:HB3	2:E:826:LEU:HB3	1.83	0.61
2:J:667:MET:HE3	2:J:671:MET:CE	2.30	0.61
2:K:671:MET:HA	2:K:671:MET:CE	2.29	0.61
1:A:764:ASP:O	1:A:765:ASP:OD1	2.18	0.61
2:E:791:PRO:O	2:E:795:LEU:HD23	2.00	0.61
2:D:526:ARG:HH12	2:D:580:PHE:HA	1.63	0.61
2:H:327:LEU:HG	2:H:372:VAL:HG11	1.82	0.61
2:H:59:PHE:HD2	2:I:317:ARG:HH22	1.49	0.61
2:E:31:LEU:HD13	2:E:345:LEU:HD13	1.82	0.61
2:I:474:TYR:H	2:I:531:ASN:HD21	1.48	0.61
2:J:135:ARG:NH1	2:J:684:GLU:OE2	2.33	0.61
1:A:406:VAL:HG13	1:A:607:ASN:HD22	1.65	0.60
2:D:472:ILE:O	2:D:531:ASN:ND2	2.34	0.60
1:A:995:VAL:HG22	1:A:1168:ASN:HB3	1.83	0.60
2:J:526:ARG:NH2	2:J:580:PHE:O	2.35	0.60
2:C:667:MET:SD	2:C:671:MET:HE3	2.42	0.60
2:F:416:VAL:HG22	2:F:429:ILE:HG13	1.84	0.60
2:K:141:GLY:CA	2:K:213:VAL:HG13	2.30	0.60
2:J:857:ILE:HG12	2:J:858:VAL:HG23	1.84	0.59
2:K:293:ILE:HG23	2:K:297:LEU:HD12	1.82	0.59
2:B:247:ARG:NH1	2:B:536:GLU:OE1	2.35	0.59
2:E:801:SER:HB2	2:E:816:LYS:HB2	1.84	0.59
2:E:667:MET:O	2:E:671:MET:HG2	2.02	0.59
2:E:750:ARG:HH22	2:F:185:ASN:HD21	1.49	0.59
1:A:1265:ARG:NH2	1:A:1301:PHE:O	2.35	0.59
1:A:1281:LYS:HB3	1:A:1285:LYS:HE2	1.84	0.59
2:C:370:ARG:NH2	2:C:404:ASP:OD2	2.36	0.59
2:I:358:LYS:HB2	2:I:570:ASP:HB3	1.84	0.58
2:F:283:ARG:HD3	2:F:659:ASN:HB3	1.86	0.58
2:F:460:ARG:NH1	2:F:478:ASP:OD1	2.35	0.58
2:G:475:CYS:O	2:G:475:CYS:SG	2.62	0.58
2:G:474:TYR:H	2:G:531:ASN:HD21	1.51	0.58
2:D:37:GLN:O	2:D:41:GLN:NE2	2.37	0.58
1:A:397:GLN:OE1	1:A:606:HIS:ND1	2.36	0.58
2:F:460:ARG:HG2	2:F:460:ARG:HH21	1.68	0.58
1:A:884:ARG:HE	1:A:896:LYS:HZ2	1.52	0.58
2:F:791:PRO:HD2	2:F:794:VAL:HG21	1.85	0.58
2:J:209:CYS:H	2:J:872:ARG:HG3	1.69	0.58
2:I:386:ARG:NH2	2:I:454:THR:O	2.37	0.58
2:B:96:GLN:HE22	2:B:830:VAL:H	1.52	0.57

	h i c	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:D:774:PHE:O	2:D:779:ARG:NH2	2.37	0.57
1:A:1160:LEU:CD2	1:A:1178:ALA:HA	2.33	0.57
2:F:437:ASN:OD1	2:F:440:ARG:NH2	2.35	0.57
1:A:1154:ASN:ND2	1:A:1156:SER:O	2.37	0.57
2:B:774:PHE:O	2:B:779:ARG:NH2	2.38	0.57
2:I:370:ARG:NH2	2:I:404:ASP:OD2	2.37	0.57
2:I:475:CYS:O	2:I:475:CYS:SG	2.62	0.57
2:K:200:ARG:NH1	2:K:203:ASP:OD1	2.36	0.57
2:E:477:ILE:HD11	2:E:524:MET:HE1	1.83	0.57
2:G:595:VAL:CG2	2:G:891:LYS:HZ2	2.05	0.57
2:H:141:GLY:HA3	2:H:213:VAL:HG13	1.86	0.57
2:F:472:ILE:H	2:F:535:ASN:HD21	1.53	0.57
2:G:16:PRO:O	2:G:306:ASN:ND2	2.37	0.57
2:H:350:PRO:HG2	2:H:472:ILE:HD13	1.86	0.57
2:J:283:ARG:HE	2:J:659:ASN:HB3	1.69	0.57
2:I:7:GLN:HG3	2:I:8:ARG:HG3	1.87	0.57
2:B:632:ARG:NH2	2:C:484:ASN:OD1	2.37	0.57
1:A:656:ARG:NH2	1:A:712:SER:OG	2.38	0.57
2:E:293:ILE:HG23	2:E:297:LEU:HD12	1.85	0.57
2:H:227:VAL:HA	2:H:231:GLU:HB2	1.86	0.57
2:J:416:VAL:HG22	2:J:429:ILE:HG13	1.87	0.57
2:B:595:VAL:HG12	2:B:595:VAL:O	2.04	0.56
2:C:95:MET:SD	2:C:102:LEU:HD11	2.45	0.56
2:G:384:GLY:HA2	2:G:446:GLY:HA3	1.87	0.56
2:J:259:ARG:NH2	2:J:880:LYS:O	2.38	0.56
2:K:370:ARG:NH2	2:K:404:ASP:OD2	2.38	0.56
2:K:671:MET:HE3	2:K:671:MET:CA	2.27	0.56
2:H:247:ARG:NH1	2:H:536:GLU:OE2	2.37	0.56
2:H:370:ARG:NH2	2:H:404:ASP:OD2	2.38	0.56
2:H:786:TYR:OH	2:H:794:VAL:HG21	2.05	0.56
2:K:793:ASP:OD1	2:K:793:ASP:N	2.38	0.56
2:F:352:GLN:HE21	2:F:544:LEU:HB2	1.70	0.56
2:D:475:CYS:SG	2:D:477:ILE:CG1	2.93	0.56
2:D:259:ARG:NH2	2:D:880:LYS:O	2.39	0.56
2:J:750:ARG:HD3	2:K:254:VAL:HG11	1.87	0.56
1:A:1272:ARG:HH22	1:A:1300:GLN:HE21	1.53	0.56
2:D:526:ARG:NH2	2:D:580:PHE:O	2.38	0.56
2:K:835:THR:HB	2:K:838:SER:HB3	1.87	0.56
2:G:714:ARG:NH2	2:G:836:PRO:O	2.39	0.56
2:K:452:TRP:HD1	2:K:452:TRP:O	1.89	0.56
2:K:104:VAL:HG22	2:K:858:VAL:HG22	1.88	0.56

		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:758:SER:HB3	1:A:769:TYR:HB2	1.88	0.56
2:C:729:THR:HG22	2:C:731:MET:H	1.71	0.56
2:J:384:GLY:HA2	2:J:446:GLY:HA3	1.88	0.56
2:B:632:ARG:H	2:B:635:HIS:HD2	1.53	0.55
2:F:247:ARG:NH1	2:F:536:GLU:OE2	2.39	0.55
2:D:475:CYS:SG	2:D:477:ILE:CD1	2.94	0.55
2:F:133:LYS:HG2	2:F:697:LEU:HD22	1.88	0.55
2:G:47:GLN:HG2	2:G:52:THR:HG21	1.88	0.55
2:H:262:ASP:HB2	2:H:881:MET:HG2	1.87	0.55
2:G:454:THR:HG21	2:G:476:GLY:N	2.21	0.55
2:J:172:LEU:O	2:J:180:ARG:NH2	2.39	0.55
2:H:271:LEU:HD22	2:H:890:LEU:HD13	1.88	0.55
2:C:742:VAL:HB	2:C:772:VAL:HG23	1.89	0.55
1:A:1299:ASN:ND2	2:D:315:THR:O	2.40	0.55
2:B:361:PRO:HG3	2:D:901:VAL:HB	1.88	0.55
2:F:85:VAL:HG23	2:F:163:VAL:HA	1.88	0.55
2:I:410:TYR:OH	2:I:512:GLU:OE2	2.23	0.55
2:J:161:PRO:HB3	2:J:187:LEU:HD21	1.88	0.55
1:A:994:ALA:HA	2:H:47:GLN:HE22	1.71	0.55
2:G:632:ARG:H	2:G:635:HIS:HD2	1.54	0.55
2:F:595:VAL:HG12	2:F:595:VAL:O	2.07	0.54
1:A:1155:HIS:O	2:H:308:ARG:NH1	2.41	0.54
2:C:200:ARG:NH1	2:C:202:VAL:O	2.40	0.54
2:C:570:ASP:OD1	2:C:570:ASP:N	2.40	0.54
2:G:570:ASP:N	2:G:570:ASP:OD1	2.38	0.54
1:A:130:PHE:HB2	1:A:683:GLY:HA3	1.90	0.54
2:C:100:ARG:HA	2:C:862:ARG:HA	1.89	0.54
2:E:475:CYS:SG	2:E:475:CYS:O	2.66	0.54
2:E:632:ARG:H	2:E:635:HIS:HD2	1.55	0.54
2:E:664:ARG:NH2	2:F:201:ASP:OD1	2.39	0.54
2:H:475:CYS:SG	2:H:475:CYS:O	2.65	0.54
2:I:201:ASP:OD2	2:I:881:MET:HE2	2.08	0.54
2:K:671:MET:CE	2:K:671:MET:CA	2.86	0.54
1:A:496:LEU:O	1:A:645:ARG:NH1	2.41	0.54
1:A:535:ILE:HG13	1:A:536:VAL:HG13	1.88	0.54
2:F:740:ARG:NH1	2:F:769:ASP:O	2.40	0.54
2:I:141:GLY:CA	2:I:213:VAL:HG13	2.37	0.54
1:A:492:THR:HB	1:A:495:GLU:HB2	1.90	0.54
2:B:350:PRO:HG2	2:B:472:ILE:HD13	1.89	0.54
2:I:384:GLY:HA2	2:I:446:GLY:HA3	1.90	0.54
2:J:350:PRO:HG2	2:J:472:ILE:HD13	1.89	0.54

	had pagemi	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:J:386:ARG:NH2	2:J:454:THR:O	2.41	0.54
2:J:701:ASP:OD2	2:J:773:ARG:NH2	2.40	0.54
1:A:854:ILE:HG21	1:A:1201:ASP:HB2	1.90	0.54
2:E:477:ILE:CD1	2:E:524:MET:HE2	2.38	0.54
2:I:360:ASP:OD1	2:I:360:ASP:N	2.39	0.54
2:I:595:VAL:HG12	2:I:595:VAL:O	2.08	0.54
2:J:667:MET:CE	2:J:671:MET:HE1	2.38	0.54
2:G:51:MET:SD	2:H:78:GLN:NE2	2.75	0.54
2:H:504:LEU:HB3	2:H:513:ALA:HB2	1.88	0.54
2:I:181:ALA:O	2:I:185:ASN:ND2	2.41	0.54
2:K:315:THR:OG1	2:K:316:GLN:N	2.41	0.54
2:K:263:THR:HG22	2:K:882:ARG:HE	1.73	0.54
2:C:209:CYS:H	2:C:872:ARG:HG3	1.73	0.53
2:K:115:GLY:HA3	2:K:129:THR:HG23	1.90	0.53
2:I:201:ASP:OD2	2:I:881:MET:CE	2.56	0.53
2:K:475:CYS:O	2:K:475:CYS:SG	2.66	0.53
2:F:792:ASP:O	2:F:796:GLN:NE2	2.42	0.53
2:G:729:THR:HG22	2:G:731:MET:H	1.73	0.53
2:F:227:VAL:HA	2:F:231:GLU:HB2	1.90	0.53
2:D:98:ARG:HB2	2:D:723:GLN:HE22	1.73	0.53
2:G:784:LYS:HB3	2:G:786:TYR:CE2	2.43	0.53
2:H:302:TYR:HB3	2:H:582:ARG:HB3	1.90	0.53
2:C:595:VAL:HG12	2:C:595:VAL:O	2.09	0.53
2:J:200:ARG:NH2	2:J:263:THR:O	2.42	0.53
1:A:194:ASP:N	1:A:194:ASP:OD1	2.42	0.53
1:A:223:ARG:HH11	2:J:33:VAL:HG22	1.74	0.53
2:J:257:ASP:OD1	2:J:257:ASP:N	2.41	0.53
2:J:264:ILE:HB	2:J:883:ILE:HG12	1.91	0.53
2:K:454:THR:HG21	2:K:476:GLY:N	2.24	0.53
2:C:667:MET:SD	2:C:671:MET:HE1	2.49	0.53
2:D:264:ILE:HB	2:D:883:ILE:HG12	1.91	0.53
2:E:265:TRP:HB3	2:E:886:ILE:HD13	1.91	0.53
2:D:175:LEU:HD11	2:D:179:HIS:HB3	1.91	0.53
1:A:1070:ILE:HB	1:A:1192:LYS:HD2	1.91	0.52
2:B:283:ARG:HE	2:B:659:ASN:HB3	1.73	0.52
2:J:658:HIS:HB2	2:K:309:ILE:HA	1.91	0.52
2:C:158:VAL:HG12	2:C:191:ILE:HG22	1.91	0.52
2:E:762:LEU:HA	2:E:765:ILE:HD12	1.92	0.52
2:G:315:THR:OG1	2:G:316:GLN:N	2.41	0.52
2:H:699:LEU:HD12	2:H:778:LEU:HB3	1.91	0.52
1:A:343:ARG:NH2	1:A:348:GLU:OE2	2.42	0.52

	jue pagem	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:424:ALA:HB1	1:A:429:GLU:HB2	1.91	0.52
2:B:175:LEU:O	2:B:180:ARG:NH2	2.42	0.52
2:D:326:ILE:HA	2:F:31:LEU:HD22	1.91	0.52
2:F:384:GLY:HA2	2:F:446:GLY:HA3	1.90	0.52
2:C:358:LYS:HB2	2:C:570:ASP:HB2	1.91	0.52
2:J:90:PHE:HB2	2:J:166:VAL:HG12	1.91	0.52
2:E:229:LEU:HD21	2:E:257:ASP:HB2	1.91	0.52
2:K:632:ARG:H	2:K:635:HIS:HD2	1.58	0.52
1:A:285:THR:HG23	2:K:317:ARG:HD2	1.91	0.52
1:A:411:ASP:OD2	1:A:414:ARG:NH1	2.43	0.52
2:H:367:PRO:HG3	2:J:309:ILE:HG13	1.92	0.52
2:B:141:GLY:HA3	2:B:213:VAL:HG13	1.92	0.52
2:C:263:THR:HG1	2:C:882:ARG:HH21	1.57	0.52
2:E:454:THR:HG21	2:E:476:GLY:N	2.25	0.52
2:H:283:ARG:HE	2:H:659:ASN:HB3	1.74	0.52
2:H:662:ASN:ND2	2:I:487:THR:O	2.43	0.52
2:J:677:PRO:HA	2:J:681:LEU:HD23	1.90	0.52
2:J:725:GLY:O	2:J:860:ARG:NH2	2.42	0.52
2:E:358:LYS:HB2	2:E:570:ASP:HB3	1.91	0.52
2:E:410:TYR:OH	2:E:512:GLU:OE2	2.28	0.52
2:I:572:SER:OG	2:I:573:TRP:N	2.43	0.52
1:A:280:VAL:HG21	1:A:362:HIS:HD2	1.75	0.51
1:A:552:SER:HB3	1:A:555:TYR:HB2	1.91	0.51
2:C:98:ARG:HG3	2:C:723:GLN:HE22	1.75	0.51
2:I:421:THR:OG1	2:I:426:ASP:OD2	2.28	0.51
1:A:826:ASP:OD1	1:A:826:ASP:N	2.39	0.51
2:B:750:ARG:HD3	2:C:254:VAL:HG11	1.91	0.51
2:H:176:THR:OG1	2:H:177:ALA:N	2.44	0.51
2:J:283:ARG:HH11	2:K:490:ILE:HG12	1.75	0.51
2:B:671:MET:HA	2:B:671:MET:CE	2.40	0.51
2:C:475:CYS:SG	2:C:475:CYS:O	2.68	0.51
2:G:262:ASP:N	2:G:262:ASP:OD1	2.43	0.51
2:B:262:ASP:OD1	2:B:262:ASP:N	2.42	0.51
2:C:835:THR:HB	2:C:838:SER:HB3	1.92	0.51
2:D:267:LEU:HD11	2:D:890:LEU:HD11	1.92	0.51
2:I:741:VAL:HG12	2:I:771:TRP:HB2	1.91	0.51
2:J:667:MET:HE3	2:J:671:MET:HE2	1.93	0.51
2:H:252:GLN:O	2:H:256:THR:OG1	2.25	0.51
1:A:27:ILE:O	1:A:912:ASN:ND2	2.40	0.51
1:A:1159:ASP:OD1	2:H:44:ARG:NH1	2.44	0.51
2:D:211:GLU:OE1	2:D:872:ARG:NH2	2.43	0.51

		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:D:707:ARG:NH2	2:D:767:ASP:OD1	2.38	0.51
2:I:95:MET:HG3	2:I:97:SER:H	1.76	0.51
2:J:44:ARG:HA	2:J:47:GLN:HB2	1.92	0.51
2:B:104:VAL:HG22	2:B:858:VAL:HG22	1.93	0.51
2:C:135:ARG:NH2	2:C:613:ASP:OD2	2.44	0.51
2:F:671:MET:CE	2:F:671:MET:CA	2.86	0.51
2:G:10:GLU:OE1	2:G:529:ARG:NH2	2.44	0.51
2:H:384:GLY:HA2	2:H:446:GLY:HA3	1.91	0.51
2:J:115:GLY:HA3	2:J:129:THR:HG23	1.93	0.51
2:B:40:MET:HA	2:B:43:VAL:HG12	1.92	0.51
2:C:229:LEU:HD21	2:C:257:ASP:HB2	1.92	0.51
2:E:595:VAL:HG12	2:E:595:VAL:O	2.11	0.51
2:E:780:THR:HB	2:E:820:GLU:HG2	1.91	0.51
1:A:594:ILE:HG22	1:A:803:THR:HG23	1.93	0.51
1:A:1018:PRO:HB2	1:A:1169:ILE:HD11	1.93	0.51
2:E:172:LEU:O	2:E:180:ARG:NH2	2.44	0.51
2:I:779:ARG:NH2	2:I:817:TYR:O	2.43	0.51
1:A:985:SER:OG	1:A:986:PHE:N	2.42	0.50
2:B:257:ASP:OD2	2:B:882:ARG:NH1	2.41	0.50
2:C:283:ARG:NH2	2:C:660:PHE:O	2.43	0.50
2:D:695:GLU:OE2	2:D:854:ASN:N	2.45	0.50
2:E:384:GLY:HA2	2:E:446:GLY:HA3	1.92	0.50
2:C:678:SER:OG	2:C:679:LEU:N	2.44	0.50
2:G:410:TYR:OH	2:G:512:GLU:OE2	2.30	0.50
1:A:115:LEU:HD23	1:A:116:ARG:H	1.76	0.50
2:F:135:ARG:NH2	2:F:613:ASP:OD2	2.44	0.50
2:F:633:PRO:HB2	2:F:663:ILE:HG12	1.93	0.50
2:H:430:GLY:O	2:H:433:GLN:NE2	2.45	0.50
2:I:857:ILE:HG22	2:I:858:VAL:HG23	1.92	0.50
1:A:911:ARG:NH2	1:A:966:PRO:O	2.44	0.50
2:G:402:LEU:HD23	2:G:425:LEU:HD21	1.92	0.50
2:H:318:ILE:HG13	2:H:319:THR:HG23	1.94	0.50
2:I:703:VAL:HG23	2:I:851:VAL:HG22	1.94	0.50
1:A:3:ALA:HB3	1:A:6:VAL:HG12	1.93	0.50
1:A:546:ARG:NH2	1:A:559:GLY:O	2.44	0.50
2:H:141:GLY:CA	2:H:213:VAL:HG13	2.41	0.50
2:K:384:GLY:HA2	2:K:446:GLY:HA3	1.94	0.50
2:F:262:ASP:OD1	2:F:262:ASP:N	2.40	0.50
2:I:85:VAL:HG12	2:I:163:VAL:HG12	1.93	0.50
2:C:135:ARG:NH1	2:C:643:ASP:OD2	2.45	0.50
1:A:949:LYS:NZ	2:J:38:GLU:OE2	2.44	0.50

	h a	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:A:1141:ALA:HA	1:A:1144:ILE:HG22	1.94	0.50
2:C:203:ASP:HB2	2:C:876:ALA:HB3	1.93	0.50
2:D:421:THR:HB	2:D:423:GLU:HG3	1.94	0.50
2:F:86:PRO:HD3	2:F:145:LEU:HD21	1.94	0.50
2:G:472:ILE:O	2:G:531:ASN:ND2	2.45	0.50
2:J:654:LEU:HA	2:K:308:ARG:HH22	1.77	0.50
2:E:703:VAL:HG23	2:E:851:VAL:HG12	1.92	0.50
1:A:432:VAL:O	1:A:628:TYR:OH	2.30	0.49
2:C:421:THR:OG1	2:C:426:ASP:OD2	2.28	0.49
2:D:263:THR:HG22	2:D:882:ARG:HG2	1.93	0.49
2:E:529:ARG:NE	2:E:585:GLU:OE2	2.46	0.49
2:H:754:ASN:ND2	2:I:257:ASP:OD1	2.45	0.49
1:A:313:SER:OG	1:A:314:SER:N	2.45	0.49
2:C:700:THR:OG1	2:C:701:ASP:N	2.45	0.49
2:G:708:ASP:HB2	2:G:850:LYS:HZ1	1.76	0.49
2:K:715:LEU:HG	2:K:836:PRO:HB3	1.93	0.49
1:A:35:TYR:HA	1:A:908:ILE:HG12	1.92	0.49
1:A:104:PRO:HB3	1:A:118:TYR:HB3	1.95	0.49
2:D:193:GLU:HB3	2:D:204:VAL:HG23	1.93	0.49
2:H:259:ARG:O	2:H:263:THR:OG1	2.29	0.49
2:J:499:GLU:OE2	2:J:502:ARG:NH2	2.45	0.49
2:K:229:LEU:HD21	2:K:257:ASP:HB2	1.95	0.49
1:A:1120:SER:OG	1:A:1121:TYR:N	2.46	0.49
2:B:658:HIS:HB2	2:C:309:ILE:HA	1.94	0.49
2:C:540:SER:OG	2:C:541:VAL:N	2.45	0.49
2:D:475:CYS:SG	2:D:477:ILE:HD11	2.52	0.49
2:G:379:LEU:HD23	2:G:500:MET:HG2	1.94	0.49
2:I:179:HIS:HA	2:I:182:MET:HB2	1.94	0.49
1:A:273:GLY:O	1:A:819:GLN:NE2	2.45	0.49
2:B:370:ARG:NH2	2:B:404:ASP:OD2	2.44	0.49
2:C:632:ARG:HG2	2:C:634:SER:H	1.78	0.49
2:C:792:ASP:HB3	2:C:796:GLN:HE21	1.77	0.49
2:I:454:THR:HG21	2:I:476:GLY:N	2.28	0.49
2:B:211:GLU:OE1	2:B:872:ARG:NH2	2.46	0.49
2:B:283:ARG:O	2:B:655:SER:OG	2.30	0.49
2:G:665:ASP:OD1	2:G:668:ARG:NH2	2.45	0.49
2:I:710:LEU:HD12	2:I:711:PRO:HD2	1.95	0.49
2:K:382:THR:HG22	2:K:384:GLY:H	1.77	0.49
2:B:701:ASP:OD2	2:B:773:ARG:NH2	2.45	0.49
2:D:284:SER:O	2:D:284:SER:OG	2.31	0.49
1:A:379:ILE:HG13	1:A:380:THR:HG23	1.94	0.49

	had pagemi	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:E:96:GLN:NE2	2:E:830:VAL:O	2.42	0.49
2:K:358:LYS:HB2	2:K:570:ASP:HB2	1.95	0.49
2:C:615:ARG:HH12	2:C:675:LEU:HD21	1.78	0.49
2:C:628:LEU:HB3	2:C:631:ALA:HB2	1.95	0.49
2:H:263:THR:HG23	2:H:882:ARG:HG3	1.94	0.49
2:H:595:VAL:O	2:H:595:VAL:HG12	2.13	0.49
1:A:863:HIS:HE1	1:A:932:LEU:H	1.61	0.48
2:B:662:ASN:HB2	2:C:485:PRO:HG3	1.93	0.48
2:J:293:ILE:HG21	2:K:315:THR:HG22	1.95	0.48
2:K:84:LYS:NZ	2:K:147:ASP:O	2.40	0.48
2:G:365:MET:HE1	2:G:574:ILE:HD12	1.96	0.48
2:H:200:ARG:HB3	2:H:881:MET:HE1	1.94	0.48
2:J:71:ILE:HG21	2:J:599:ILE:HG23	1.95	0.48
2:K:251:SER:OG	2:K:252:GLN:N	2.46	0.48
1:A:224:GLU:O	2:J:44:ARG:NH2	2.40	0.48
2:F:504:LEU:HB3	2:F:513:ALA:HB2	1.95	0.48
2:H:475:CYS:HG	2:H:477:ILE:CG1	2.25	0.48
2:I:801:SER:OG	2:I:802:TYR:N	2.46	0.48
1:A:134:ARG:HE	1:A:138:GLU:HB2	1.79	0.48
2:H:223:TYR:OH	2:H:270:GLN:NE2	2.46	0.48
2:H:724:GLU:HB2	2:H:860:ARG:HH12	1.78	0.48
2:K:354:ILE:CG2	2:K:391:THR:HG23	2.43	0.48
2:K:707:ARG:NH1	2:K:767:ASP:OD1	2.47	0.48
1:A:1132:ASP:HB2	1:A:1135:MET:HB2	1.96	0.48
2:E:27:SER:OG	2:E:28:GLY:N	2.46	0.48
2:F:103:ARG:NH1	2:F:865:GLN:O	2.47	0.48
2:B:293:ILE:HG23	2:B:297:LEU:HD12	1.96	0.48
2:C:54:THR:HB	2:D:882:ARG:HB2	1.94	0.48
2:J:472:ILE:H	2:J:535:ASN:HD21	1.61	0.48
2:K:725:GLY:O	2:K:860:ARG:NH1	2.46	0.48
2:B:653:ASN:O	2:C:308:ARG:NH2	2.47	0.48
2:D:228:GLN:OE1	2:D:265:TRP:N	2.44	0.48
2:F:284:SER:O	2:F:284:SER:OG	2.32	0.48
2:G:284:SER:O	2:G:288:ASN:ND2	2.47	0.48
2:I:743:GLN:OE1	2:I:773:ARG:NH1	2.46	0.48
2:F:133:LYS:HD3	2:F:697:LEU:HB3	1.94	0.48
2:F:754:ASN:ND2	2:G:257:ASP:OD1	2.40	0.48
2:H:112:SER:O	2:H:782:ARG:NH1	2.46	0.48
1:A:572:SER:OG	1:A:573:ARG:N	2.46	0.48
1:A:655:ARG:HH22	1:A:678:PHE:HB3	1.79	0.48
2:C:725:GLY:O	2:C:860:ARG:NH1	2.42	0.48

		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:E:209:CYS:H	2:E:872:ARG:HG3	1.78	0.48
2:E:833:SER:O	2:E:833:SER:OG	2.31	0.48
2:I:202:VAL:HG13	2:I:203:ASP:N	2.29	0.48
2:K:135:ARG:HD2	2:K:138:ARG:HH21	1.78	0.48
2:H:740:ARG:NH1	2:H:769:ASP:O	2.47	0.47
2:I:705:MET:HG3	2:I:848:MET:HB3	1.96	0.47
2:J:393:ASN:OD1	2:K:411:ASN:ND2	2.47	0.47
1:A:1278:PRO:HB2	1:A:1281:LYS:HB2	1.95	0.47
2:F:671:MET:HE3	2:F:671:MET:CA	2.32	0.47
2:G:464:PRO:HG2	2:G:539:HIS:CE1	2.49	0.47
1:A:656:ARG:HH22	1:A:714:LEU:HA	1.78	0.47
2:C:193:GLU:HB3	2:C:204:VAL:HB	1.95	0.47
2:D:722:ARG:NH1	2:D:830:VAL:O	2.46	0.47
2:E:532:GLN:NE2	2:E:536:GLU:OE2	2.48	0.47
2:K:456:ASP:N	2:K:456:ASP:OD1	2.45	0.47
1:A:572:SER:HA	1:A:1202:GLU:HB2	1.96	0.47
1:A:255:LYS:O	1:A:259:ASN:ND2	2.47	0.47
2:E:418:TYR:OH	2:F:481:GLU:OE1	2.33	0.47
2:I:793:ASP:OD1	2:I:793:ASP:N	2.44	0.47
2:J:138:ARG:HA	2:J:216:ILE:HG21	1.96	0.47
2:J:197:VAL:HG13	2:J:225:GLU:HG3	1.97	0.47
1:A:655:ARG:NH2	1:A:679:LYS:O	2.48	0.47
2:J:91:ARG:HG3	2:J:104:VAL:HB	1.96	0.47
2:K:96:GLN:NE2	2:K:830:VAL:O	2.41	0.47
1:A:1201:ASP:OD1	1:A:1201:ASP:N	2.47	0.47
2:D:172:LEU:O	2:D:180:ARG:NH2	2.47	0.47
2:F:200:ARG:HD2	2:F:881:MET:HE1	1.96	0.47
2:F:857:ILE:HG13	2:F:858:VAL:HG23	1.96	0.47
2:H:321:THR:OG1	2:H:322:GLY:N	2.47	0.47
2:I:120:GLU:OE2	2:I:817:TYR:N	2.48	0.47
2:K:354:ILE:HG22	2:K:391:THR:HG23	1.97	0.47
1:A:674:ASP:N	1:A:674:ASP:OD1	2.48	0.47
2:B:470:ARG:NH1	2:B:544:LEU:O	2.44	0.47
2:D:754:ASN:ND2	2:E:257:ASP:OD1	2.48	0.47
2:H:615:ARG:HH12	2:H:675:LEU:HD21	1.80	0.47
2:H:707:ARG:NH1	2:H:767:ASP:OD1	2.42	0.47
1:A:35:TYR:HB3	1:A:907:LEU:HD23	1.96	0.47
2:B:52:THR:O	2:C:317:ARG:NH1	2.48	0.47
2:B:882:ARG:HH21	2:K:47:GLN:HE21	1.62	0.47
2:D:461:GLU:HG3	2:D:462:PRO:N	2.21	0.47
2:E:708:ASP:OD2	2:E:850:LYS:NZ	2.40	0.47

	has pagemi	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:F:197:VAL:HG22	2:F:202:VAL:HG21	1.97	0.47
2:K:141:GLY:HA2	2:K:213:VAL:CG1	2.38	0.47
1:A:335:GLN:HE22	1:A:341:ASP:HA	1.80	0.47
2:E:98:ARG:H	2:E:723:GLN:HE22	1.62	0.47
2:H:345:LEU:HD22	2:I:318:ILE:HD13	1.96	0.47
2:H:416:VAL:HG22	2:H:429:ILE:HG13	1.97	0.47
1:A:267:TRP:HA	1:A:270:LYS:HD2	1.97	0.46
2:F:350:PRO:HG2	2:F:472:ILE:HD13	1.98	0.46
2:F:460:ARG:HH21	2:F:460:ARG:CG	2.25	0.46
2:G:743:GLN:OE1	2:G:773:ARG:NH1	2.42	0.46
2:H:150:THR:OG1	2:H:151:ARG:N	2.48	0.46
2:B:152:ASP:OD1	2:B:152:ASP:N	2.48	0.46
2:D:587:THR:OG1	2:D:588:HIS:N	2.48	0.46
2:H:283:ARG:O	2:H:655:SER:OG	2.31	0.46
1:A:286:ALA:O	2:J:341:ARG:NH1	2.47	0.46
1:A:294:ASP:OD1	1:A:294:ASP:N	2.44	0.46
2:E:22:VAL:HG13	2:E:301:GLU:HB3	1.96	0.46
2:F:293:ILE:HG21	2:G:315:THR:HG22	1.97	0.46
2:J:247:ARG:NH1	2:J:536:GLU:OE2	2.48	0.46
2:J:667:MET:CE	2:J:671:MET:HE2	2.45	0.46
2:J:774:PHE:HB2	2:J:779:ARG:HH22	1.81	0.46
1:A:306:ARG:NH1	2:J:63:ASP:OD2	2.40	0.46
2:I:100:ARG:HH21	2:I:862:ARG:HH22	1.63	0.46
2:I:262:ASP:OD1	2:I:262:ASP:N	2.43	0.46
2:I:745:THR:OG1	2:I:746:TYR:N	2.48	0.46
2:J:627:VAL:HG21	2:J:778:LEU:HG	1.97	0.46
2:F:675:LEU:HD12	2:F:681:LEU:HD11	1.98	0.46
2:G:565:ASP:HB2	2:H:261:GLN:HE21	1.80	0.46
2:K:209:CYS:SG	2:K:210:SER:N	2.88	0.46
1:A:138:GLU:HG2	1:A:139:MET:HG3	1.98	0.46
1:A:226:GLU:HG2	2:J:44:ARG:HH21	1.79	0.46
1:A:995:VAL:HA	1:A:1168:ASN:HD22	1.80	0.46
2:C:799:PRO:HG3	2:C:849:THR:HG23	1.98	0.46
2:E:480:ARG:O	2:E:484:ASN:N	2.46	0.46
2:J:437:ASN:HD22	2:J:440:ARG:HH21	1.62	0.46
2:G:441:ALA:HB2	2:G:449:TYR:HE1	1.80	0.46
2:J:739:ASP:OD1	2:J:739:ASP:N	2.40	0.46
1:A:173:ASP:HA	1:A:176:ASN:HD21	1.80	0.46
1:A:546:ARG:HH12	1:A:563:ILE:HD13	1.81	0.46
2:B:671:MET:CE	2:B:671:MET:CA	2.94	0.46
2:B:740:ARG:NH1	2:B:770:ASP:OD1	2.49	0.46

		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:C:141:GLY:HA2	2:C:213:VAL:HG13	1.98	0.46
2:D:416:VAL:HG22	2:D:429:ILE:HG13	1.98	0.46
2:E:402:LEU:HG	2:E:406:LEU:HD23	1.98	0.46
2:G:866:ILE:HG22	2:G:867:LEU:HD12	1.97	0.46
2:K:257:ASP:N	2:K:257:ASP:OD1	2.40	0.46
1:A:1132:ASP:O	1:A:1136:ARG:N	2.49	0.46
2:F:275:PRO:HB3	2:F:541:VAL:HG12	1.98	0.46
2:G:150:THR:HG22	2:G:159:ALA:HA	1.97	0.46
2:H:352:GLN:HE21	2:H:544:LEU:HD13	1.81	0.46
2:K:699:LEU:HD13	2:K:778:LEU:HD13	1.97	0.46
1:A:431:ILE:HD11	1:A:536:VAL:HA	1.97	0.45
2:B:141:GLY:CA	2:B:213:VAL:HG13	2.47	0.45
2:I:546:ASP:O	2:I:550:ASN:ND2	2.49	0.45
2:K:741:VAL:HG22	2:K:771:TRP:HB2	1.97	0.45
2:K:745:THR:OG1	2:K:746:TYR:N	2.48	0.45
1:A:991:ALA:O	1:A:996:GLN:NE2	2.49	0.45
2:B:700:THR:OG1	2:B:701:ASP:N	2.49	0.45
2:E:79:VAL:HG21	2:E:680:LYS:HG3	1.98	0.45
2:E:235:SER:HB3	2:E:271:LEU:HD23	1.97	0.45
2:G:595:VAL:HG12	2:G:595:VAL:O	2.15	0.45
2:I:671:MET:HE2	2:I:671:MET:HB3	1.73	0.45
1:A:144:ASP:OD1	1:A:144:ASP:N	2.49	0.45
2:E:283:ARG:NH2	2:E:660:PHE:O	2.49	0.45
2:F:426:ASP:OD1	2:F:437:ASN:ND2	2.50	0.45
2:I:158:VAL:HG21	2:I:188:ASP:HA	1.99	0.45
2:K:283:ARG:NH2	2:K:660:PHE:O	2.50	0.45
1:A:684:VAL:HG13	1:A:705:LEU:HB3	1.99	0.45
1:A:1076:LYS:HG3	2:D:33:VAL:HG13	1.98	0.45
2:B:98:ARG:H	2:B:723:GLN:HE22	1.65	0.45
2:I:203:ASP:HB2	2:I:876:ALA:HB3	1.99	0.45
2:K:97:SER:OG	2:K:98:ARG:N	2.49	0.45
2:G:742:VAL:HG23	2:G:772:VAL:HG23	1.98	0.45
1:A:221:ARG:NH2	1:A:225:GLU:OE1	2.45	0.45
2:D:247:ARG:NH1	2:D:536:GLU:OE2	2.50	0.45
2:I:296:CYS:HB2	2:I:538:LEU:HD23	1.98	0.45
2:B:252:GLN:O	2:B:256:THR:OG1	2.34	0.45
2:G:263:THR:HG22	2:G:882:ARG:HE	1.81	0.45
2:H:228:GLN:OE1	2:H:265:TRP:N	2.50	0.45
1:A:1183:SER:O	1:A:1187:ARG:N	2.38	0.45
2:C:148:ILE:HB	2:C:163:VAL:HG11	1.99	0.45
2:H:754:ASN:HA	2:I:256:THR:HG23	1.99	0.45

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Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:A:605:ARG:NH1	1:A:794:CYS:O	2.49	0.45	
2:B:330:SER:O	2:B:330:SER:OG	2.34	0.45	
2:B:662:ASN:ND2	2:C:487:THR:O	2.49	0.45	
2:D:855:LYS:HA	2:D:855:LYS:HD3	1.79	0.45	
2:F:741:VAL:HG12	2:F:771:TRP:HB2	1.98	0.45	
2:I:862:ARG:HG3	2:I:864:GLY:H	1.82	0.45	
1:A:245:GLU:HG3	1:A:344:LEU:HD23	1.98	0.45	
2:B:257:ASP:OD1	2:B:257:ASP:N	2.45	0.45	
2:B:309:ILE:HG13	2:J:367:PRO:HG3	1.99	0.45	
2:F:784:LYS:CE	2:F:786:TYR:OH	2.65	0.45	
1:A:1198:ILE:HD11	1:A:1235:LEU:HB3	1.99	0.44	
2:K:146:HIS:NE2	2:K:881:MET:O	2.51	0.44	
2:K:470:ARG:NH1	2:K:544:LEU:O	2.48	0.44	
2:K:510:ASP:N	2:K:510:ASP:OD1	2.44	0.44	
2:G:728:TYR:HB3	2:G:826:LEU:HB3	1.99	0.44	
2:H:257:ASP:OD1	2:H:257:ASP:N	2.40	0.44	
1:A:242:LEU:HD23	1:A:373:LEU:HD21	1.99	0.44	
1:A:709:THR:OG1	1:A:710:ASP:N	2.51	0.44	
2:C:102:LEU:N	2:C:102:LEU:CD1	2.80	0.44	
2:C:786:TYR:OH	2:C:794:VAL:HG21	2.18	0.44	
2:D:455:ILE:HB	2:D:473:ARG:HH21	1.81	0.44	
2:G:595:VAL:HG23	2:G:891:LYS:NZ	2.22	0.44	
2:I:54:THR:OG1	2:I:55:ARG:N	2.50	0.44	
2:J:227:VAL:HA	2:J:231:GLU:HB2	1.98	0.44	
2:D:381:PHE:HE2	2:D:576:LEU:HD11	1.82	0.44	
2:G:229:LEU:HD11	2:G:257:ASP:HB2	1.99	0.44	
2:K:474:TYR:H	2:K:531:ASN:HD21	1.66	0.44	
1:A:210:MET:HG2	1:A:379:ILE:HA	1.99	0.44	
1:A:680:VAL:HG21	1:A:686:PRO:HB3	1.99	0.44	
2:C:410:TYR:OH	2:C:512:GLU:OE2	2.35	0.44	
2:D:315:THR:O	2:D:315:THR:OG1	2.36	0.44	
2:D:595:VAL:HG12	2:D:595:VAL:O	2.17	0.44	
2:I:293:ILE:HG23	2:I:297:LEU:HD12	2.00	0.44	
2:B:142:SER:O	2:B:142:SER:OG	2.34	0.44	
2:D:900:THR:OG1	2:D:901:VAL:N	2.49	0.44	
2:E:547:ASP:OD1	2:E:547:ASP:N	2.47	0.44	
2:F:257:ASP:OD1	2:F:257:ASP:N	2.39	0.44	
2:G:24:SER:HB3	2:G:302:TYR:HD2	1.81	0.44	
2:I:72:LYS:HD3	2:I:595:VAL:HG11	2.00	0.44	
2:J:98:ARG:HB2	2:J:723:GLN:HE22	1.83	0.44	
1:A:655:ARG:HH12	1:A:678:PHE:HB3	1.83	0.44	

		Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
2:B:169:LYS:HE3	2:B:169:LYS:HB3	1.80	0.44	
2:B:481:GLU:OE1	2:K:418:TYR:OH	2.30	0.44	
2:D:655:SER:O	2:D:659:ASN:N	2.49	0.44	
1:A:109:ASP:OD1	1:A:109:ASP:N	2.30	0.44	
2:B:461:GLU:CB	2:B:462:PRO:HD3	2.48	0.44	
2:H:662:ASN:HB2	2:I:485:PRO:HG2	1.99	0.44	
2:I:141:GLY:HA2	2:I:213:VAL:HG13	1.99	0.44	
2:D:219:ARG:HG2	2:D:686:GLU:HG3	2.00	0.43	
2:F:228:GLN:OE1	2:F:265:TRP:N	2.49	0.43	
2:G:115:GLY:HA3	2:G:129:THR:HG23	2.00	0.43	
2:I:707:ARG:NH1	2:I:767:ASP:OD1	2.51	0.43	
2:J:812:TYR:HE1	2:K:255:LEU:HD12	1.82	0.43	
2:H:80:TYR:OH	2:H:885:ASP:OD2	2.27	0.43	
2:I:115:GLY:HA3	2:I:129:THR:HG23	1.98	0.43	
2:K:452:TRP:CD1	2:K:452:TRP:C	2.90	0.43	
1:A:273:GLY:HA3	1:A:359:PHE:HB3	1.99	0.43	
1:A:395:ASP:N	1:A:395:ASP:OD1	2.52	0.43	
1:A:1032:LYS:HA	1:A:1036:ALA:HB3	2.01	0.43	
2:B:260:ARG:NH2	2:K:565:ASP:OD1	2.51	0.43	
2:B:740:ARG:NH1	2:B:769:ASP:O	2.48	0.43	
2:D:889:SER:O	2:D:889:SER:OG	2.35	0.43	
2:J:774:PHE:O	2:J:779:ARG:NH2	2.51	0.43	
1:A:1295:ARG:HD2	2:F:318:ILE:HD13	2.01	0.43	
2:C:458:GLU:OE2	2:C:460:ARG:NE	2.51	0.43	
2:I:257:ASP:OD1	2:I:257:ASP:N	2.44	0.43	
2:I:298:PRO:HB3	2:I:589:ARG:HA	2.01	0.43	
2:F:100:ARG:HE	2:F:862:ARG:HG2	1.84	0.43	
2:G:158:VAL:HA	2:G:191:ILE:HA	1.99	0.43	
2:G:172:LEU:O	2:G:180:ARG:NH2	2.52	0.43	
2:K:386:ARG:HG2	2:K:457:VAL:HG12	2.01	0.43	
1:A:1295:ARG:HG2	2:F:30:LEU:HG	2.00	0.43	
2:C:284:SER:O	2:C:288:ASN:ND2	2.52	0.43	
2:J:740:ARG:NH1	2:J:769:ASP:O	2.43	0.43	
2:K:200:ARG:HH22	2:K:203:ASP:HA	1.84	0.43	
2:C:54:THR:OG1	2:C:55:ARG:N	2.51	0.43	
2:C:627:VAL:HG22	2:C:777:VAL:HA	2.00	0.43	
2:E:193:GLU:HG3	2:E:194:ASN:HD22	1.83	0.43	
2:E:628:LEU:HD12	2:E:631:ALA:HB2	1.99	0.43	
2:G:283:ARG:NH2	2:G:660:PHE:O	2.52	0.43	
2:I:795:LEU:HD23	2:I:795:LEU:HA	1.84	0.43	
1:A:123:GLU:HB3	1:A:128:GLU:HG3	2.00	0.43	

	has pagem	Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:A:502:SER:HB2	1:A:505:LEU:HD23	2.01	0.43	
1:A:1069:VAL:HG12	1:A:1193:LEU:HB2	2.01	0.43	
2:C:782:ARG:NE	2:C:820:GLU:OE2	2.52	0.43	
2:F:724:GLU:HG3	2:F:860:ARG:HH12	1.83	0.43	
2:G:595:VAL:HG23	2:G:891:LYS:HZ1	1.76	0.43	
2:H:792:ASP:O	2:H:796:GLN:NE2	2.52	0.43	
2:I:379:LEU:HD23	2:I:500:MET:HG2	2.00	0.43	
2:G:627:VAL:HG22	2:G:777:VAL:HA	2.00	0.43	
2:K:552:LEU:HD23	2:K:552:LEU:HA	1.87	0.43	
2:K:787:ASP:OD1	2:K:787:ASP:N	2.48	0.43	
1:A:871:MET:SD	1:A:917:TYR:OH	2.71	0.43	
1:A:1118:ARG:HG3	1:A:1210:ALA:HB1	2.01	0.43	
2:J:97:SER:OG	2:J:98:ARG:N	2.52	0.43	
2:B:293:ILE:HD12	2:C:314:LEU:HD12	2.01	0.42	
2:G:251:SER:OG	2:G:252:GLN:N	2.52	0.42	
2:J:118:ILE:HD12	2:J:126:PHE:HD1	1.84	0.42	
1:A:97:VAL:HG21	1:A:248:ILE:HD11	2.01	0.42	
1:A:211:GLU:HG2	1:A:243:LEU:HD21	2.01	0.42	
1:A:847:ARG:NH1	1:A:926:GLY:O	2.50	0.42	
2:H:664:ARG:NE	2:I:486:THR:O	2.52	0.42	
2:J:386:ARG:HE	2:J:456:ASP:HB2	1.84	0.42	
2:C:297:LEU:HD12	2:C:298:PRO:HD2	2.01	0.42	
2:D:378:HIS:CD2	2:D:402:LEU:HD22	2.53	0.42	
2:F:352:GLN:NE2	2:F:544:LEU:HB2	2.33	0.42	
2:H:587:THR:OG1	2:H:588:HIS:N	2.52	0.42	
2:I:460:ARG:O	2:I:461:GLU:HG3	2.19	0.42	
2:J:43:VAL:HG12	2:J:47:GLN:HG3	2.01	0.42	
1:A:599:TYR:HE2	1:A:731:ASN:HB2	1.84	0.42	
2:C:474:TYR:O	2:C:475:CYS:SG	2.77	0.42	
2:D:816:LYS:HB2	2:D:816:LYS:HE3	1.86	0.42	
2:E:47:GLN:HE21	2:F:882:ARG:HH21	1.66	0.42	
2:H:632:ARG:H	2:H:635:HIS:HD2	1.66	0.42	
2:J:228:GLN:OE1	2:J:265:TRP:N	2.53	0.42	
2:K:333:THR:HG23	2:K:336:GLN:H	1.85	0.42	
2:C:31:LEU:HD13	2:C:345:LEU:HD13	2.02	0.42	
2:E:262:ASP:O	2:E:882:ARG:N	2.51	0.42	
2:F:703:VAL:HG21	2:F:821:THR:HG21	2.01	0.42	
2:G:416:VAL:HB	2:G:429:ILE:HD12	2.00	0.42	
2:I:708:ASP:HB3	2:I:850:LYS:HZ1	1.84	0.42	
2:B:608:SER:HB3	2:B:681:LEU:HD13	2.00	0.42	
2:G:478:ASP:OD2	2:G:480:ARG:NE	2.48	0.42	

		Interatomic	Clash	
Atom-1	Atom-2	distance $(Å)$	overlap (Å)	
2:H:526:ARG:NH2	2:H:580:PHE:O	2.52	0.42	
2:H:743:GLN:HE22	2:H:773:ARG:HH11	1.67	0.42	
2:J:133:LYS:NZ	2:J:697:LEU:O	2.50	0.42	
1:A:314:SER:OG	1:A:781:ASP:OD1	2.30	0.42	
1:A:1023:ARG:O	1:A:1027:HIS:N	2.45	0.42	
2:D:751:LEU:HD23	2:D:751:LEU:HA	1.92	0.42	
2:G:359:ILE:HG23	2:H:894:THR:HG23	2.02	0.42	
1:A:743:GLN:NE2	1:A:759:GLU:OE2	2.36	0.42	
2:B:344:TYR:OH	2:B:582:ARG:O	2.27	0.42	
2:C:383:ALA:HA	2:C:388:THR:HG22	2.01	0.42	
2:D:475:CYS:HG	2:D:477:ILE:HG13	1.81	0.42	
2:E:72:LYS:HE2	2:E:72:LYS:HB3	1.89	0.42	
2:F:289:LEU:HD21	2:F:353:ILE:HD11	2.02	0.42	
2:F:762:LEU:HD23	2:F:762:LEU:HA	1.93	0.42	
2:G:464:PRO:HG2	2:G:539:HIS:HE1	1.84	0.42	
2:I:393:ASN:HD21	2:I:397:GLN:HE21	1.66	0.42	
2:J:257:ASP:OD2	2:J:882:ARG:NH1	2.44	0.42	
2:J:262:ASP:N	2:J:262:ASP:OD1	2.52	0.42	
2:D:257:ASP:N	2:D:257:ASP:OD1	2.53	0.42	
2:E:209:CYS:SG	2:E:210:SER:N	2.93	0.42	
2:F:112:SER:OG	2:F:781:VAL:O	2.33	0.42	
2:G:725:GLY:O	2:G:860:ARG:NH1	2.53	0.42	
2:G:787:ASP:OD1	2:G:787:ASP:N	2.44	0.42	
2:I:194:ASN:O	2:I:200:ARG:HD3	2.20	0.42	
2:K:447:THR:O	2:K:452:TRP:CD2	2.73	0.42	
2:C:779:ARG:NH2	2:C:817:TYR:O	2.53	0.42	
2:D:327:LEU:O	2:D:330:SER:OG	2.37	0.42	
2:F:796:GLN:HA	2:F:848:MET:HB2	2.02	0.42	
2:H:701:ASP:OD1	2:H:701:ASP:N	2.50	0.42	
1:A:605:ARG:CZ	1:A:607:ASN:HD21	2.32	0.41	
1:A:1022:SER:O	1:A:1026:MET:N	2.45	0.41	
1:A:1104:ILE:HD12	2:J:39:ILE:HG23	2.02	0.41	
2:D:370:ARG:NH2	2:D:404:ASP:OD2	2.38	0.41	
2:E:487:THR:OG1	2:E:488:TYR:N	2.53	0.41	
2:G:8:ARG:HH22	2:G:589:ARG:HH21	1.68	0.41	
2:K:379:LEU:HD23	2:K:500:MET:HG2	2.01	0.41	
1:A:883:LYS:HA	1:A:883:LYS:HD2	1.93	0.41	
2:F:459:TYR:OH	2:F:550:ASN:OD1	2.37	0.41	
2:H:193:GLU:HB2	2:H:204:VAL:HG13	2.01	0.41	
2:I:202:VAL:CG1	2:I:203:ASP:N	2.82	0.41	
2:C:853:ILE:HG22	2:C:855:LYS:HB2	2.02	0.41	

	juo pugom	Interatomic	Clash	
Atom-1	Atom-2	distance $(Å)$	overlap (Å)	
2:D:350:PRO:HG2	2:D:472:ILE:HD13	2.01	0.41	
2:E:200:ARG:O	2:E:201:ASP:HB3	2.20	0.41	
2:H:855:LYS:HA	2:H:855:LYS:HD3	1.89	0.41	
1:A:649:THR:OG1	1:A:651:TRP:NE1	2.51	0.41	
1:A:1155:HIS:HB2	2:H:308:ARG:HH12	1.85	0.41	
2:E:54:THR:OG1	2:E:55:ARG:N	2.53	0.41	
2:E:296:CYS:HB2	2:E:538:LEU:HD23	2.02	0.41	
2:G:432:ASN:OD1	2:G:432:ASN:N	2.48	0.41	
2:I:104:VAL:HG22	2:I:858:VAL:HG22	2.02	0.41	
2:I:135:ARG:NH2	2:I:613:ASP:OD2	2.47	0.41	
2:I:209:CYS:H	2:I:872:ARG:HG3	1.85	0.41	
1:A:628:TYR:N	1:A:631:TYR:O	2.54	0.41	
2:B:345:LEU:HD22	2:C:318:ILE:HD13	2.03	0.41	
2:D:461:GLU:HG2	2:D:462:PRO:CD	2.37	0.41	
2:D:662:ASN:OD1	2:D:662:ASN:N	2.45	0.41	
2:F:615:ARG:HH12	2:F:675:LEU:HD21	1.84	0.41	
2:G:133:LYS:HD3	2:G:697:LEU:HB3	2.03	0.41	
2:I:355:LEU:O	2:I:391:THR:OG1	2.31	0.41	
1:A:883:LYS:HB2	1:A:1045:GLU:HG2	2.02	0.41	
1:A:1067:SER:HB3	1:A:1278:PRO:HG3	2.03	0.41	
1:A:1126:ASP:O	1:A:1130:ARG:N	2.53	0.41	
2:C:379:LEU:HD21	2:C:500:MET:HG2	2.03	0.41	
2:E:700:THR:OG1	2:E:701:ASP:N	2.53	0.41	
2:H:71:ILE:HG21	2:H:599:ILE:HG23	2.03	0.41	
2:J:219:ARG:HD2	2:J:219:ARG:HA	1.86	0.41	
1:A:828:MET:HG3	1:A:856:LYS:HD3	2.02	0.41	
2:C:831:GLU:H	2:C:834:ASN:ND2	2.18	0.41	
2:D:552:LEU:HD23	2:D:552:LEU:HA	1.90	0.41	
2:E:71:ILE:HG21	2:E:599:ILE:HG23	2.02	0.41	
2:G:31:LEU:HD13	2:G:345:LEU:HD13	2.03	0.41	
2:H:411:ASN:OD1	2:H:411:ASN:N	2.53	0.41	
2:H:786:TYR:CD1	2:H:790:PRO:HB3	2.55	0.41	
2:J:354:ILE:HD12	2:J:391:THR:HG22	2.01	0.41	
1:A:105:TRP:HD1	1:A:127:VAL:HG11	1.85	0.41	
1:A:846:VAL:HA	1:A:849:GLN:HB3	2.02	0.41	
2:C:95:MET:SD	2:C:102:LEU:CD1	3.08	0.41	
2:D:127:TYR:HD1	2:D:617:LEU:HD22	1.85	0.41	
2:E:264:ILE:HB	2:E:883:ILE:HG12	2.03	0.41	
2:F:167:GLU:HG2	2:F:169:LYS:HG2	2.03	0.41	
2:K:671:MET:HE2	2:K:671:MET:HB3	1.84	0.41	
1:A:280:VAL:HG21	1:A:362:HIS:CD2	2.55	0.41	

		Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:A:828:MET:SD	1:A:855:THR:OG1	2.79	0.41	
1:A:1070:ILE:HD12	1:A:1070:ILE:HA	1.87	0.41	
2:B:504:LEU:HB3	2:B:513:ALA:HB2	2.02	0.41	
2:C:176:THR:HG22	2:C:178:GLU:H	1.86	0.41	
2:C:460:ARG:HH21	2:C:473:ARG:HD2	1.84	0.41	
2:E:379:LEU:HD23	2:E:500:MET:HG2	2.02	0.41	
2:G:740:ARG:NH2	2:G:769:ASP:O	2.54	0.41	
2:H:778:LEU:HD23	2:H:778:LEU:HA	1.89	0.41	
2:J:632:ARG:H	2:J:635:HIS:HD2	1.68	0.41	
2:J:653:ASN:HA	2:J:656:HIS:HB2	2.02	0.41	
2:B:228:GLN:OE1	2:B:265:TRP:N	2.54	0.41	
2:E:843:ASN:HD22	2:E:843:ASN:HA	1.69	0.41	
2:F:431:ARG:HE	2:F:431:ARG:HB3	1.67	0.41	
2:G:835:THR:HB	2:G:838:SER:HB3	2.02	0.41	
2:B:857:ILE:HG22	2:B:858:VAL:HG23	2.03	0.40	
2:C:447:THR:OG1	2:C:448:GLY:N	2.54	0.40	
2:C:629:ILE:HG13	2:C:630:GLN:HG3	2.03	0.40	
2:C:793:ASP:OD1	2:C:793:ASP:N	2.53	0.40	
2:E:623:ARG:NH2	2:E:692:ASN:O	2.40	0.40	
2:H:98:ARG:HG2	2:H:174:VAL:HG12	2.03	0.40	
2:J:638:LYS:HA	2:J:638:LYS:HD2	1.83	0.40	
1:A:1154:ASN:HD22	1:A:1159:ASP:HB3	1.85	0.40	
2:B:717:ASP:HB3	2:B:720:ARG:HB3	2.03	0.40	
2:D:708:ASP:OD2	2:D:850:LYS:NZ	2.40	0.40	
2:F:72:LYS:HE2	2:F:72:LYS:HB3	1.80	0.40	
2:F:774:PHE:O	2:F:779:ARG:NH1	2.54	0.40	
2:G:378:HIS:CD2	2:G:402:LEU:HD22	2.56	0.40	
2:I:297:LEU:HD23	2:I:297:LEU:HA	1.93	0.40	
2:K:378:HIS:CD2	2:K:402:LEU:HD22	2.56	0.40	
1:A:661:THR:O	1:A:704:THR:OG1	2.39	0.40	
2:E:705:MET:HB3	2:E:772:VAL:HG13	2.02	0.40	
2:F:460:ARG:CG	2:F:460:ARG:NH2	2.81	0.40	
2:F:784:LYS:HE3	2:F:786:TYR:OH	2.22	0.40	
2:H:293:ILE:HG21	2:I:315:THR:HG22	2.03	0.40	
2:I:460:ARG:HD3	2:I:460:ARG:HA	1.90	0.40	
2:J:889:SER:O	2:J:889:SER:OG	2.37	0.40	
2:H:487:THR:O	2:H:487:THR:OG1	2.40	0.40	
2:I:22:VAL:HG13	2:I:301:GLU:HB3	2.04	0.40	
2:I:705:MET:HE3	2:I:848:MET:HG2	2.04	0.40	
2:B:671:MET:HE3	2:B:671:MET:CA	2.46	0.40	
2:D:329:GLY:HA3	2:F:31:LEU:HB2	2.03	0.40	

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:10:GLU:HG2	2:G:532:GLN:HE22	1.86	0.40
2:H:191:ILE:HD12	2:H:191:ILE:HA	1.86	0.40
2:H:382:THR:HG22	2:H:384:GLY:H	1.87	0.40
2:I:709:MET:HA	2:I:846:TYR:HA	2.04	0.40
2:K:474:TYR:H	2:K:531:ASN:ND2	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	Perce	ntiles
1	А	1238/1302~(95%)	1153~(93%)	85 (7%)	0	100	100
2	В	870/901~(97%)	829~(95%)	41 (5%)	0	100	100
2	С	881/901 (98%)	825 (94%)	56 (6%)	0	100	100
2	D	859/901~(95%)	828~(96%)	31 (4%)	0	100	100
2	Е	881/901 (98%)	828 (94%)	53 (6%)	0	100	100
2	F	864/901~(96%)	822 (95%)	42~(5%)	0	100	100
2	G	881/901 (98%)	836 (95%)	45 (5%)	0	100	100
2	Н	866/901~(96%)	813 (94%)	53~(6%)	0	100	100
2	Ι	881/901 (98%)	829 (94%)	52 (6%)	0	100	100
2	J	868/901~(96%)	821 (95%)	47 (5%)	0	100	100
2	Κ	881/901 (98%)	830 (94%)	51 (6%)	0	100	100
All	All	9970/10312~(97%)	9414 (94%)	556 (6%)	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 side chain 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 side chain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Perce	ntiles
1	А	1110/1161~(96%)	1099~(99%)	11 (1%)	76	88
2	В	767/792~(97%)	765 (100%)	2(0%)	92	97
2	С	782/792~(99%)	777~(99%)	5 (1%)	86	94
2	D	759/792~(96%)	755 (100%)	4 (0%)	88	95
2	Е	782/792~(99%)	776~(99%)	6 (1%)	81	91
2	F	763/792~(96%)	755~(99%)	8 (1%)	76	88
2	G	782/792~(99%)	778 (100%)	4 (0%)	88	95
2	Н	763/792~(96%)	761 (100%)	2(0%)	92	97
2	Ι	782/792~(99%)	776~(99%)	6 (1%)	81	91
2	J	765/792~(97%)	761 (100%)	4 (0%)	88	95
2	К	782/792~(99%)	777 (99%)	5 (1%)	86	94
All	All	8837/9081 (97%)	8780 (99%)	57 (1%)	86	94

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	109	ASP
1	А	115	LEU
1	А	122	ARG
1	А	142	TYR
1	А	343	ARG
1	А	360	TYR
1	А	546	ARG
1	А	624	ARG
1	А	656	ARG
1	А	727	THR
1	А	1020	ARG
2	В	461	GLU
2	В	671	MET
2	С	101	VAL
2	С	461	GLU

		1	1 5
Mol	Chain	Res	Type
2	С	475	CYS
2	С	529	ARG
2	С	671	MET
2	D	271	LEU
2	D	386	ARG
2	D	537	ASP
2	D	671	MET
2	Е	201	ASP
2	Е	386	ARG
2	Е	698	MET
2	Е	745	THR
2	Е	793	ASP
2	Е	794	VAL
2	F	271	LEU
2	F	386	ARG
2	F	391	THR
2	F	460	ARG
2	F	471	TYR
2	F	671	MET
2	F	750	ARG
2	F	794	VAL
2	G	201	ASP
2	G	386	ARG
2	G	460	ARG
2	G	856	ARG
2	Н	52	THR
2	Н	55	ARG
2	Ι	201	ASP
2	Ι	317	ARG
2	Ι	477	ILE
2	Ι	671	MET
2	Ι	792	ASP
2	Ι	793	ASP
2	J	271	LEU
2	J	461	GLU
2	J	487	THR
2	J	671	MET
2	K	354	ILE
2	K	386	ARG
2	K	570	ASP
2	K	671	MET
2	K	794	VAL

Sometimes side chains can be flipped to improve hydrogen bonding and reduce clashes. All (149) such side chains are listed below:

Mol	Chain	Res	Type	
1	А	91	GLN	
1	А	176	ASN	
1	А	259	ASN	
1	А	283	GLN	
1	А	335	GLN	
1	А	377	GLN	
1	А	401	ASN	
1	А	407	GLN	
1	А	507	GLN	
1	А	648	ASN	
1	А	843	GLN	
1	А	863	HIS	
1	А	867	GLN	
1	А	1299	ASN	
1	А	1300	GLN	
2	В	45	GLN	
2	В	96	GLN	
2	В	389	ASN	
2	В	437	ASN	
2	В	450	ASN	
2	В	531	ASN	
2	В	535	ASN	
2	В	550	ASN	
2	В	635	HIS	
2	В	676	GLN	
2	В	702	GLN	
2	В	723	GLN	
2	В	743	GLN	
2	С	92	HIS	
2	С	153	HIS	
2	С	230	GLN	
2	С	288	ASN	
2	С	411	ASN	
2	С	531	ASN	
2	С	532	GLN	
2	С	539	HIS	
2	С	621	GLN	
2	С	635	HIS	
2	С	642	ASN	
2	С	653	ASN	
2	С	676	GLN	

Mol	Chain	Res	Type	
2	С	723	GLN	
2	С	796	GLN	
2	С	834	ASN	
2	С	854	ASN	
2	D	41	GLN	
2	D	196	ASN	
2	D	417	ASN	
2	D	433	GLN	
2	D	437	ASN	
2	D	531	ASN	
2	D	532	GLN	
2	D	535	ASN	
2	D	635	HIS	
2	D	659	ASN	
2	D	676	GLN	
2	D	723	GLN	
2	D	757	GLN	
2	Е	113	GLN	
2	Е	194	ASN	
2	Е	389	ASN	
2	Ε	417	ASN	
2	Е	467	HIS	
2	Ε	531	ASN	
2	Е	635	HIS	
2	Е	653	ASN	
2	Ε	692	ASN	
2	Е	723	GLN	
2	Е	754	ASN	
2	E	843	ASN	
2	F	185	ASN	
2	F	244	HIS	
2	F	450	ASN	
2	F	495	HIS	
2	F	531	ASN	
2	F	532	GLN	
2	F	535	ASN	
2	F	550	ASN	
2	F	635	HIS	
2	F	676	GLN	
2	F	702	GLN	
2	F	743	GLN	
2	F	805	ASN	

Mol	Chain	Res	Type	
2	F	829	ASN	
2	G	218	ASN	
2	G	230	GLN	
2	G	270	GLN	
2	G	288	ASN	
2	G	378	HIS	
2	G	467	HIS	
2	G	531	ASN	
2	G	539	HIS	
2	G	635	HIS	
2	G	642	ASN	
2	G	706	HIS	
2	Н	47	GLN	
2	Н	288	ASN	
2	Н	437	ASN	
2	Н	450	ASN	
2	Н	532	GLN	
2	Н	535	ASN	
2	Н	550	ASN	
2	Н	635	HIS	
2	Н	642	ASN	
2	Н	659	ASN	
2	Н	702	GLN	
2	Н	743	GLN	
2	Н	757	GLN	
2	Н	796	GLN	
2	Н	829	ASN	
2	Ι	47	GLN	
2	Ι	185	ASN	
2	Ι	389	ASN	
2	Ι	393	ASN	
2	Ι	415	GLN	
2	Ι	417	ASN	
2	Ι	531	ASN	
2	Ι	550	ASN	
2	Ι	635	HIS	
2	Ι	653	ASN	
2	Ι	706	HIS	
2	J	179	HIS	
2	J	244	244 HIS	
2	J	288	8 ASN	
2	J	292	ASN	

Mol	Chain	Res	Type
2	J	389	ASN
2	J	417	ASN
2	J	433	GLN
2	J	437	ASN
2	J	531	ASN
2	J	535	ASN
2	J	635	HIS
2	J	659	ASN
2	J	743	GLN
2	J	754	ASN
2	J	829	ASN
2	J	834	ASN
2	Κ	47	GLN
2	Κ	65	GLN
2	Κ	92	HIS
2	Κ	228	GLN
2	K	276	GLN
2	Κ	378	HIS
2	Κ	433	GLN
2	K	635	HIS
2	K	653	ASN
2	K	706	HIS
2	Κ	723	GLN
2	K	834	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-20407. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

6.1.1 Primary map

The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

6.2.1 Primary map

X Index: 128

Y Index: 128

Z Index: 128

The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map

X Index: 114

Y Index: 132

Z Index: 149

The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

6.4.1 Primary map

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

6.5.1 Primary map

The images above show the 3D surface view of the map at the recommended contour level 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.6 Mask visualisation (i)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis (i)

This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)

The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

7.2 Volume estimate (i)

The volume at the recommended contour level is 474 nm^3 ; this corresponds to an approximate mass of 428 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)

*Reported resolution corresponds to spatial frequency of 0.278 \AA^{-1}

8 Fourier-Shell correlation (i)

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-20407 and PDB model 6PO2. Per-residue inclusion information can be found in section 3 on page 5.

9.1 Map-model overlay (i)

The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model (i)

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.02).

9.4 Atom inclusion (i)

At the recommended contour level, 58% of all backbone atoms, 43% of all non-hydrogen atoms, are inside the map.

Map-model fit summary (i) 9.5

The table lists the average atom inclusion at the recommended contour level (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score	
All	0.4340	0.4970	1.0
А	0.3050	0.4370	
В	0.5430	0.5230	
С	0.3780	0.4900	
D	0.5320	0.5200	
E	0.3720	0.4890	
F	0.5140	0.5160	
G	0.3700	0.4880	
Н	0.5190	0.5150	
I	0.3790	0.4930	0.0 <
J	0.5410	0.5240	
K	0.3820	0.4920	

