



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

Feb 21, 2018 – 02:31 PM EST

PDB ID : 6FBV  
EMDB ID: : EMD-4230  
Title : Single particle cryo em structure of Mycobacterium tuberculosis RNA polymerase in complex with Fidaxomicin  
Authors : Das, K.; Lin, W.; Ebright, E.  
Deposited on : 2017-12-19  
Resolution : 3.50 Å(reported)

This is a Full wwPDB/EMDataBank EM Map/Model Validation Report  
for a publicly released PDB/EMDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
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

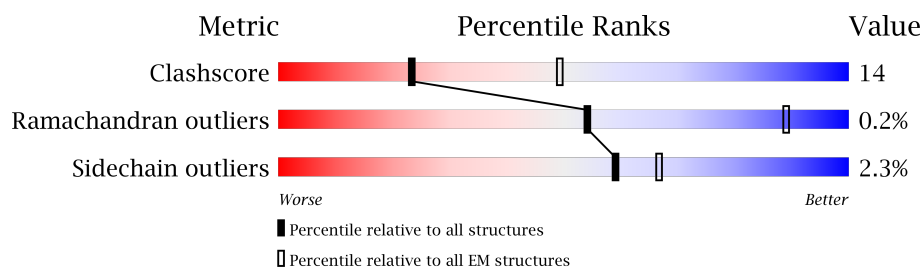
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	A	347	
1	B	347	
2	C	1178	
3	D	1316	
4	E	110	
5	F	528	

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 25146 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 DNA-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	223	Total	C	N	O	S	0	0
			1700	1068	294	336	2		
1	B	230	Total	C	N	O	S	0	0
			1749	1099	301	347	2		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	3	LEU	ILE	conflict	UNP P9WGZ1
B	3	LEU	ILE	conflict	UNP P9WGZ1

- Molecule 2 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	1118	Total	C	N	O	S	0	0
			8671	5427	1521	1684	39		

- Molecule 3 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	1270	Total	C	N	O	S	0	0
			9951	6224	1808	1878	41		

- Molecule 4 is a protein called DNA-directed RNA polymerase subunit omega.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	E	83	Total	C	N	O	0	0
			654	417	108	129		

- Molecule 5 is a protein called RNA polymerase sigma factor SigA.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	293	Total	C	N	O	S	0	0
			2343	1465	424	445	9		

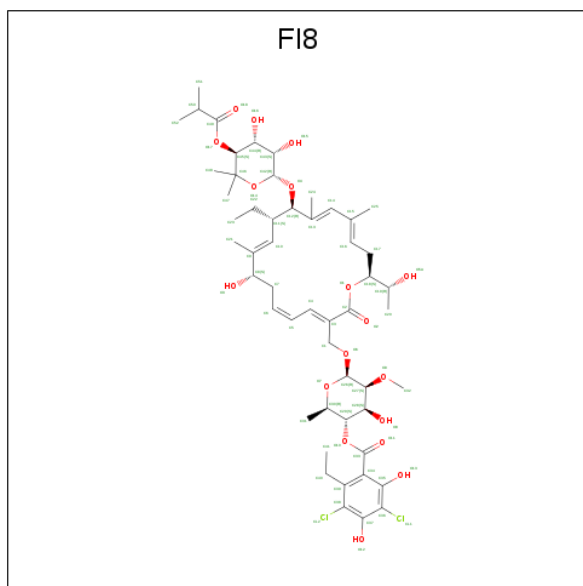
- Molecule 6 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
6	D	2	Total	Zn	0
			2	2	

- Molecule 7 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
7	D	1	Total	Mg	0
			1	1	

- Molecule 8 is Fidaxomicin (three-letter code: FI8) (formula: C<sub>52</sub>H<sub>74</sub>Cl<sub>2</sub>O<sub>18</sub>).

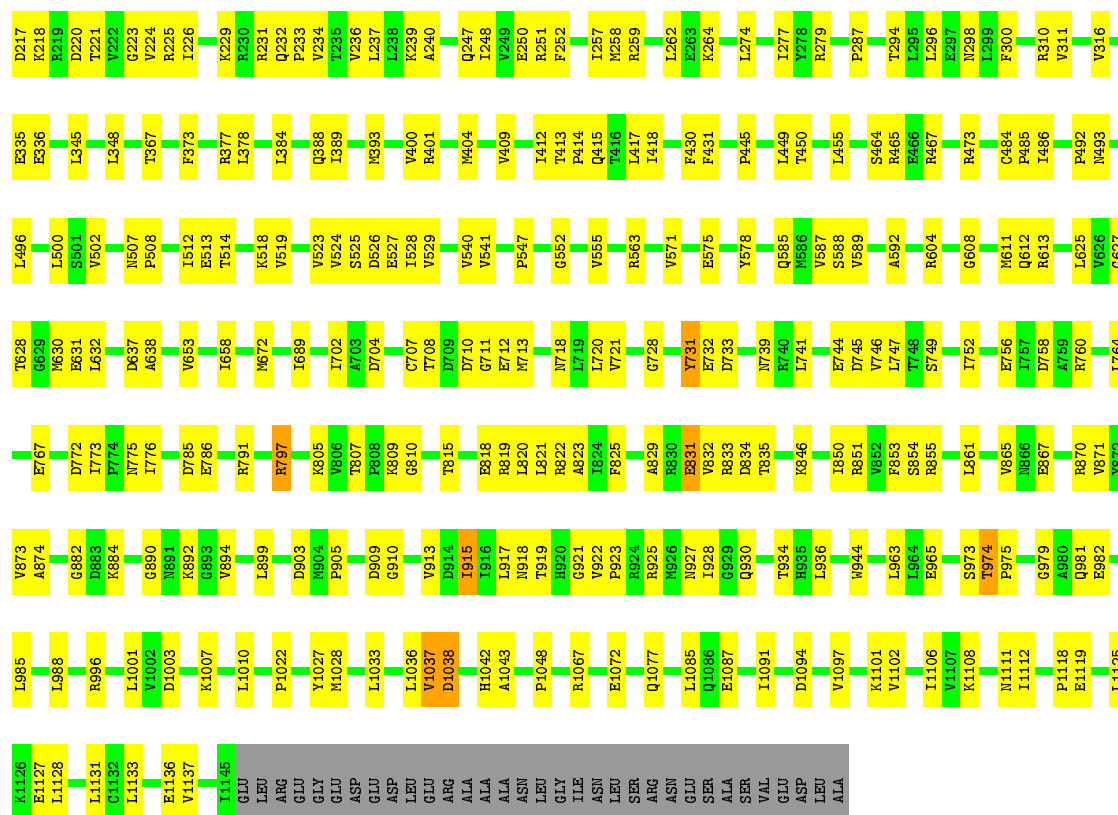


Mol	Chain	Residues	Atoms				AltConf
8	D	1	Total	C	Cl	O	0
			72	52	2	18	

- Molecule 9 is water.

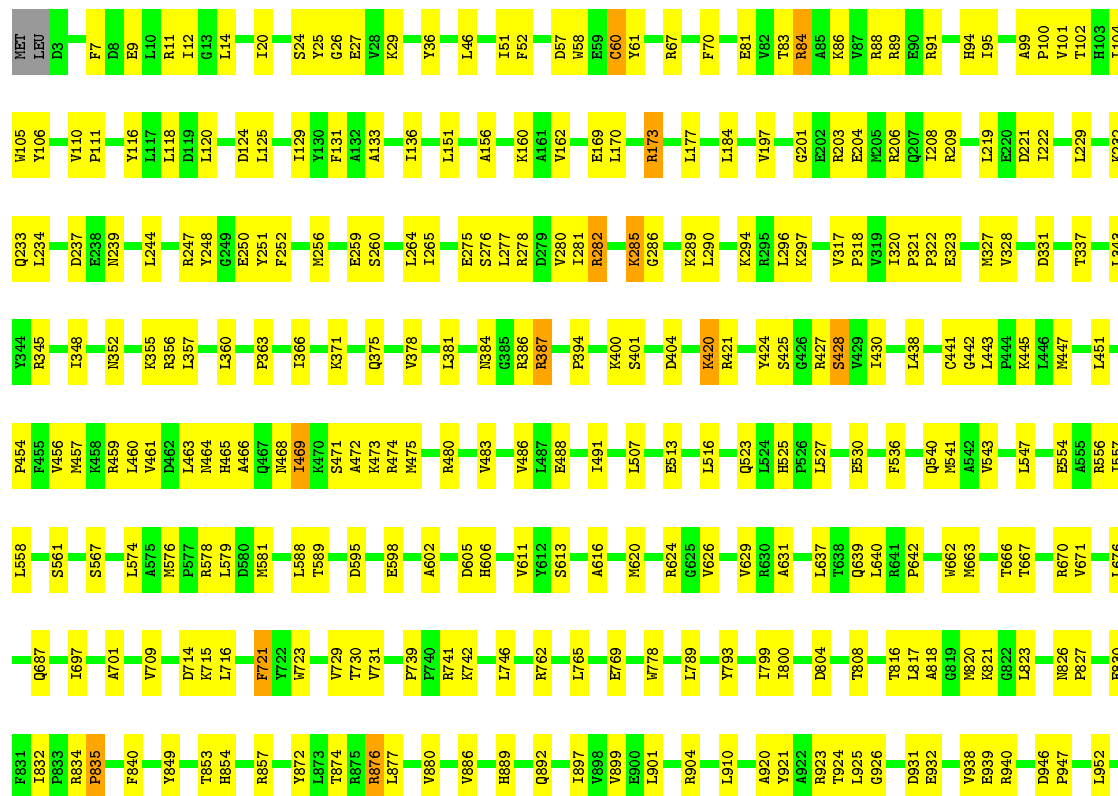
Mol	Chain	Residues	Atoms		AltConf
9	D	3	Total	O	0
			3	3	

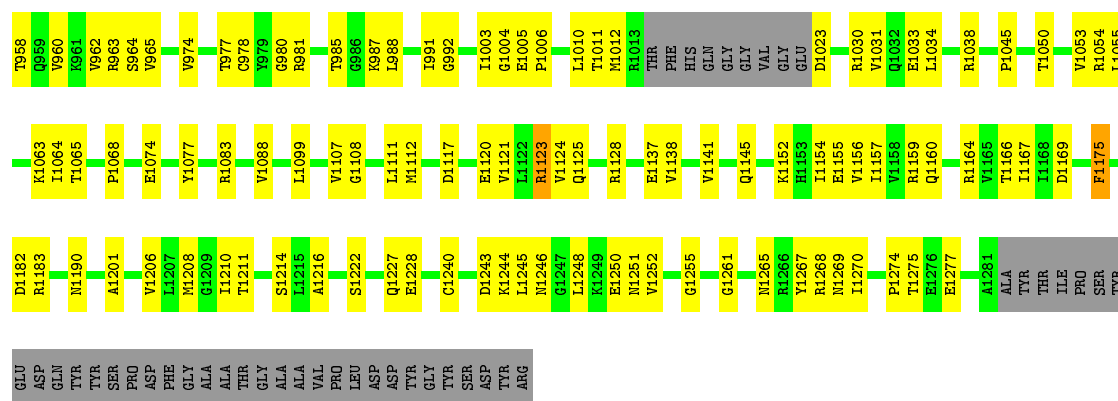




• Molecule 3: DNA-directed RNA polymerase subunit beta'

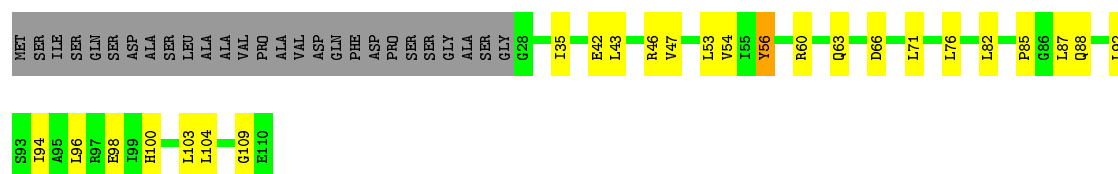
Chain D: 67% 28%





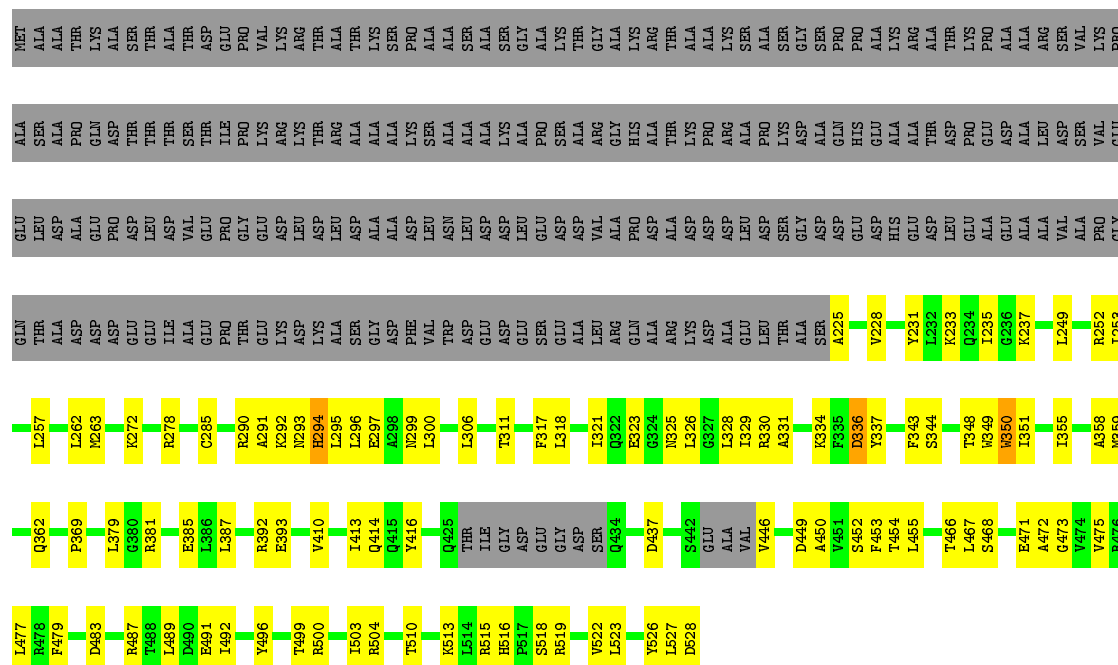
• Molecule 4: DNA-directed RNA polymerase subunit omega

Chain E: 53% 22% 25%



• Molecule 5: RNA polymerase sigma factor SigA

Chain F: 37% 18% 45%



## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	68895	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	1.4	Depositor
Minimum defocus (nm)	-1.0	Depositor
Maximum defocus (nm)	-2.0	Depositor
Magnification	130000	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: MG, ZN, FI8

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	0.37	0/1726	0.61	0/2348
1	B	0.33	0/1775	0.58	0/2414
2	C	0.37	0/8830	0.61	0/11972
3	D	0.34	0/10116	0.58	0/13673
4	E	0.33	0/667	0.58	0/908
5	F	0.27	0/2371	0.52	0/3193
All	All	0.35	0/25485	0.59	0/34508

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1700	0	1734	46	0
1	B	1749	0	1781	52	0
2	C	8671	0	8610	239	0
3	D	9951	0	10024	315	0
4	E	654	0	648	20	0
5	F	2343	0	2377	87	0
6	D	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	D	1	0	0	0	0
8	D	72	0	0	7	0
9	D	3	0	0	0	0
All	All	25146	0	25174	700	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 14.

All (700) 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)
3:D:282:ARG:HH21	3:D:282:ARG:CB	1.28	1.43
3:D:282:ARG:HB2	3:D:282:ARG:NH2	1.08	1.40
3:D:285:LYS:HA	3:D:285:LYS:HE3	1.29	1.10
3:D:282:ARG:NH2	3:D:282:ARG:CB	2.04	0.96
3:D:277:LEU:O	3:D:281:ILE:HG13	1.67	0.95
1:B:98:ARG:HG2	1:B:135:GLU:HG2	1.53	0.91
2:C:226:ILE:HD12	2:C:229:LYS:HZ3	1.35	0.89
2:C:1106:ILE:HG13	2:C:1112:ILE:HD11	1.59	0.84
3:D:762:ARG:NH1	3:D:762:ARG:HB2	1.93	0.84
5:F:471:GLU:HB3	5:F:510:THR:HG21	1.57	0.84
2:C:232:GLN:HE22	2:C:277:ILE:HG12	1.42	0.83
2:C:819:ARG:O	2:C:823:ALA:HB2	1.79	0.83
3:D:281:ILE:CD1	3:D:296:LEU:HD22	2.09	0.83
3:D:282:ARG:HB2	3:D:282:ARG:CZ	2.08	0.81
4:E:42:GLU:OE1	4:E:100:HIS:NE2	2.13	0.80
1:B:170:PRO:HB2	1:B:202:ILE:HG21	1.64	0.79
3:D:899:VAL:HG11	3:D:920:ALA:HB2	1.64	0.79
2:C:850:ILE:HG22	2:C:871:VAL:HG22	1.63	0.78
3:D:101:VAL:HG21	3:D:378:VAL:HG11	1.65	0.78
3:D:285:LYS:HA	3:D:285:LYS:CE	2.12	0.78
5:F:379:LEU:HD23	5:F:413:ILE:HG21	1.66	0.77
3:D:102:THR:HG22	3:D:375:GLN:HE22	1.47	0.77
1:B:95:MET:HE1	1:B:116:VAL:HG11	1.66	0.77
3:D:877:LEU:HD22	3:D:1157:ILE:HD13	1.66	0.76
3:D:278:ARG:HA	3:D:281:ILE:HD12	1.66	0.75
2:C:628:THR:HG23	2:C:975:PRO:HA	1.68	0.75
3:D:356:ARG:NH1	5:F:330:ARG:HH22	1.84	0.75
5:F:235:ILE:HD12	5:F:300:LEU:HD13	1.68	0.75
1:A:71:GLU:HG2	1:A:75:GLU:HG2	1.70	0.74
2:C:116:LYS:HE2	2:C:132:PRO:HD3	1.68	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:486:ILE:HD11	3:D:849:TYR:HE2	1.53	0.74
3:D:457:MET:SD	3:D:473:LYS:HB2	2.28	0.73
1:B:24:GLU:HB3	1:B:191:LYS:HG3	1.69	0.73
3:D:556:ARG:HG3	4:E:35:ILE:HD11	1.71	0.73
3:D:366:ILE:HD13	5:F:325:ASN:HB3	1.69	0.73
3:D:286:GLY:HA2	3:D:289:LYS:HB3	1.69	0.73
3:D:924:THR:HG23	3:D:980:GLY:HA2	1.69	0.72
1:A:175:THR:HG22	2:C:910:GLY:HA3	1.71	0.72
2:C:1007:LYS:HB3	2:C:1022:PRO:HB2	1.70	0.72
1:A:33:THR:HG21	1:B:37:SER:HA	1.72	0.72
2:C:930:GLN:HB2	2:C:1028:MET:HE1	1.71	0.72
3:D:762:ARG:HH11	3:D:762:ARG:CB	2.03	0.72
2:C:486:ILE:HD11	3:D:849:TYR:CE2	2.25	0.72
1:B:14:LEU:HD23	1:B:19:SER:HB3	1.72	0.70
3:D:463:LEU:HD11	3:D:486:VAL:HG22	1.70	0.70
2:C:1087:GLU:OE2	3:D:547:LEU:HB2	1.91	0.70
2:C:547:PRO:HB2	2:C:555:VAL:HB	1.74	0.70
3:D:469:ILE:O	3:D:469:ILE:HD13	1.92	0.70
3:D:981:ARG:O	3:D:1152:LYS:NZ	2.25	0.70
2:C:919:THR:HG21	3:D:729:VAL:HG12	1.73	0.70
3:D:20:ILE:HD13	3:D:318:PRO:HD3	1.74	0.69
3:D:1222:SER:HB2	3:D:1250:GLU:HG3	1.73	0.69
2:C:191:ILE:HG13	2:C:198:THR:HG22	1.74	0.69
3:D:430:ILE:HD13	3:D:541:MET:HE3	1.73	0.69
2:C:1094:ASP:OD2	3:D:420:LYS:NZ	2.24	0.69
5:F:344:SER:O	5:F:348:THR:HB	1.93	0.69
1:A:53:SER:OG	1:A:161:ARG:NH2	2.26	0.69
3:D:762:ARG:NH1	3:D:762:ARG:CB	2.55	0.69
2:C:1119:GLU:OE1	2:C:1119:GLU:HA	1.91	0.68
2:C:807:THR:HG23	2:C:835:THR:HG21	1.74	0.68
3:D:281:ILE:HD11	3:D:296:LEU:HD22	1.75	0.68
5:F:299:ASN:HB2	5:F:328:LEU:HD21	1.76	0.68
3:D:384:ASN:HB2	3:D:401:SER:HB3	1.75	0.68
3:D:285:LYS:CA	3:D:285:LYS:HE3	2.17	0.68
5:F:515:ARG:HD3	5:F:518:SER:HB3	1.76	0.67
3:D:459:ARG:O	3:D:463:LEU:HG	1.95	0.67
3:D:892:GLN:HG3	3:D:892:GLN:O	1.94	0.67
3:D:102:THR:HG21	3:D:129:ILE:HD13	1.77	0.67
5:F:336:ASP:OD1	5:F:336:ASP:N	2.28	0.67
2:C:232:GLN:NE2	2:C:277:ILE:HG12	2.11	0.66
3:D:1227:GLN:HG3	3:D:1228:GLU:HG3	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:259:ARG:NH1	2:C:259:ARG:HG2	2.11	0.66
3:D:1053:VAL:HG11	3:D:1099:LEU:HD11	1.78	0.66
3:D:248:TYR:HB3	3:D:251:TYR:HB2	1.78	0.66
2:C:226:ILE:HD12	2:C:229:LYS:NZ	2.11	0.66
2:C:797:ARG:HD2	2:C:797:ARG:H	1.59	0.66
2:C:981:GLN:HG2	2:C:982:GLU:H	1.60	0.66
3:D:463:LEU:O	3:D:464:ASN:HB2	1.94	0.66
3:D:876:ARG:HD2	3:D:1211:THR:HG22	1.78	0.65
2:C:465:ARG:HH11	2:C:492:PRO:HB2	1.60	0.65
3:D:290:LEU:C	3:D:290:LEU:HD23	2.17	0.65
3:D:469:ILE:C	3:D:469:ILE:HD13	2.16	0.65
3:D:278:ARG:HA	3:D:281:ILE:CD1	2.25	0.65
3:D:567:SER:HB2	3:D:574:LEU:HG	1.78	0.65
5:F:290:ARG:O	5:F:294:HIS:HB3	1.97	0.65
3:D:286:GLY:HA2	3:D:289:LYS:HD3	1.78	0.65
3:D:60:CYS:SG	3:D:61:TYR:N	2.70	0.65
5:F:452:SER:HA	5:F:455:LEU:HD12	1.78	0.64
2:C:259:ARG:HH11	2:C:259:ARG:HG2	1.61	0.64
2:C:311:VAL:HG11	2:C:377:ARG:HD2	1.78	0.64
2:C:611:MET:SD	2:C:892:LYS:HG2	2.37	0.64
3:D:89:ARG:HB3	3:D:323:GLU:HB2	1.79	0.64
3:D:356:ARG:CZ	5:F:330:ARG:NH2	2.60	0.64
1:A:10:SER:HB3	1:A:23:ILE:HG12	1.79	0.64
1:B:15:THR:HG22	1:B:16:ASP:H	1.62	0.64
3:D:589:THR:HG23	3:D:670:ARG:HG2	1.80	0.63
2:C:915:ILE:HD11	2:C:917:LEU:HD21	1.80	0.63
2:C:764:LEU:HD13	2:C:810:GLY:HA2	1.81	0.63
1:A:68:GLY:HA3	1:A:132:GLY:HA3	1.80	0.63
3:D:1088:VAL:HB	3:D:1099:LEU:HA	1.80	0.63
3:D:666:THR:OG1	3:D:667:THR:N	2.32	0.63
1:A:40:ARG:NH1	2:C:903:ASP:OD1	2.27	0.62
3:D:800:ILE:O	3:D:804:ASP:HB2	1.99	0.62
5:F:350:TRP:CE3	5:F:350:TRP:HA	2.34	0.62
5:F:249:LEU:HD11	5:F:343:PHE:HZ	1.64	0.62
3:D:1034:LEU:HD11	3:D:1137:GLU:HB3	1.81	0.62
2:C:83:VAL:HG21	2:C:310:ARG:HH22	1.65	0.62
1:B:104:GLU:OE2	1:B:124:HIS:ND1	2.32	0.61
2:C:294:THR:O	2:C:298:ASN:HB2	2.00	0.61
3:D:118:LEU:HD11	3:D:265:ILE:HG13	1.82	0.61
3:D:357:LEU:HD21	3:D:366:ILE:HG22	1.82	0.61
2:C:95:PRO:HB3	2:C:106:SER:HB3	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:57:ASP:HB3	3:D:58:TRP:CE3	2.36	0.61
2:C:1097:VAL:HG22	8:D:1904:FI8:C31	2.31	0.60
2:C:746:VAL:HG12	2:C:747:LEU:HG	1.83	0.60
3:D:177:LEU:HD13	3:D:201:GLY:HA3	1.83	0.60
3:D:598:GLU:HB2	3:D:631:ALA:HB1	1.82	0.60
2:C:1072:GLU:N	2:C:1072:GLU:OE1	2.33	0.60
2:C:1067:ARG:HA	3:D:421:ARG:HA	1.82	0.60
2:C:525:SER:OG	2:C:527:GLU:HG2	2.01	0.60
1:B:10:SER:HA	1:B:22:VAL:O	2.01	0.60
2:C:1091:ILE:HD12	2:C:1102:VAL:HG21	1.84	0.60
3:D:876:ARG:HD2	3:D:1211:THR:CG2	2.32	0.60
2:C:134:PHE:CE1	2:C:153:PHE:HD1	2.20	0.60
3:D:1108:GLY:HA3	3:D:1125:GLN:NE2	2.16	0.60
3:D:27:GLU:HB2	3:D:94:HIS:CE1	2.36	0.60
5:F:306:LEU:HD12	5:F:351:ILE:HD11	1.84	0.60
2:C:1136:GLU:OE1	3:D:11:ARG:NE	2.35	0.59
3:D:965:VAL:O	3:D:1159:ARG:HD2	2.02	0.59
3:D:463:LEU:CD1	3:D:486:VAL:HG22	2.30	0.59
2:C:1133:LEU:HD13	3:D:12:ILE:HD11	1.83	0.59
3:D:765:LEU:HD22	3:D:769:GLU:HB3	1.84	0.59
4:E:47:VAL:HG11	4:E:53:LEU:HB2	1.84	0.59
1:B:8:THR:HG21	1:B:26:LEU:HD23	1.85	0.59
2:C:157:PHE:CE1	2:C:389:ILE:HD11	2.38	0.59
2:C:815:THR:HB	2:C:818:GLU:HB3	1.83	0.59
3:D:169:GLU:HB3	3:D:208:ILE:HD13	1.85	0.59
2:C:653:VAL:HG13	2:C:658:ILE:HD11	1.85	0.59
2:C:884:LYS:HD3	2:C:1033:LEU:HD12	1.85	0.59
4:E:87:LEU:HG	4:E:88:GLN:HG3	1.84	0.59
2:C:732:GLU:HB3	3:D:536:PHE:HD2	1.68	0.59
2:C:760:ARG:HB3	2:C:865:VAL:HG22	1.83	0.58
3:D:290:LEU:O	3:D:290:LEU:HD23	2.03	0.58
2:C:157:PHE:HE1	2:C:389:ILE:HD11	1.68	0.58
5:F:231:TYR:CZ	5:F:235:ILE:HD11	2.38	0.58
5:F:489:LEU:HD13	5:F:504:ARG:HH21	1.69	0.58
2:C:741:LEU:HD22	2:C:746:VAL:HG11	1.86	0.58
2:C:188:ASP:OD1	2:C:189:GLU:N	2.35	0.58
2:C:775:ASN:HB3	5:F:528:ASP:O	2.02	0.58
3:D:925:LEU:HD11	3:D:960:VAL:HG21	1.84	0.58
3:D:95:ILE:HB	3:D:317:VAL:HG22	1.86	0.58
1:A:79:ASN:ND2	1:A:125:ILE:O	2.37	0.58
2:C:882:GLY:O	2:C:1037:VAL:HG13	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:202:ILE:HD13	1:B:207:ALA:HB2	1.86	0.58
2:C:115:VAL:HG11	2:C:129:TYR:CE2	2.39	0.58
2:C:233:PRO:HB2	2:C:236:VAL:HG23	1.86	0.58
2:C:833:ARG:HG3	2:C:833:ARG:HH11	1.69	0.57
3:D:232:LYS:HG2	3:D:264:LEU:HD21	1.86	0.57
5:F:317:PHE:HE1	5:F:321:ILE:HD11	1.69	0.57
3:D:356:ARG:CZ	5:F:330:ARG:HH22	2.17	0.57
3:D:327:MET:HG3	3:D:337:THR:HB	1.86	0.57
1:A:119:HIS:ND1	1:A:201:SER:HA	2.19	0.57
2:C:540:VAL:HG22	2:C:563:ARG:HG3	1.85	0.57
3:D:420:LYS:HD2	3:D:420:LYS:N	2.19	0.57
3:D:963:ARG:HG2	3:D:978:CYS:HB2	1.85	0.57
5:F:249:LEU:O	5:F:253:ILE:HG12	2.05	0.57
1:B:50:ALA:HB2	1:B:167:ILE:O	2.03	0.57
2:C:819:ARG:O	2:C:823:ALA:CB	2.51	0.57
1:A:71:GLU:HB3	1:A:75:GLU:HB3	1.86	0.57
2:C:187:PHE:HB3	2:C:348:LEU:HD22	1.87	0.57
3:D:156:ALA:O	3:D:160:LYS:CB	2.53	0.57
3:D:872:TYR:HE2	3:D:876:ARG:HH21	1.52	0.57
2:C:855:ARG:HD3	2:C:861:LEU:HD12	1.87	0.57
1:A:153:ARG:NE	1:A:153:ARG:HA	2.20	0.57
1:A:213:LYS:HD2	1:B:223:ARG:HG3	1.87	0.57
2:C:168:ILE:HB	2:C:173:ARG:HD2	1.87	0.57
2:C:833:ARG:HG2	2:C:834:ASP:H	1.68	0.57
2:C:921:GLY:O	2:C:925:ARG:HG2	2.05	0.57
3:D:762:ARG:HH11	3:D:762:ARG:HB3	1.69	0.57
2:C:721:VAL:HG21	2:C:917:LEU:HD12	1.87	0.56
2:C:226:ILE:HD11	2:C:237:LEU:HD22	1.86	0.56
2:C:464:SER:HB3	2:C:467:ARG:HB2	1.87	0.56
5:F:326:LEU:O	5:F:330:ARG:HG3	2.06	0.56
3:D:513:GLU:HB2	4:E:35:ILE:HG21	1.86	0.56
3:D:530:GLU:HB2	3:D:578:ARG:HD2	1.87	0.56
2:C:141:ASN:HD21	2:C:409:VAL:HG13	1.70	0.56
3:D:832:ILE:HG22	3:D:834:ARG:H	1.69	0.56
3:D:427:ARG:HA	3:D:541:MET:O	2.05	0.56
2:C:851:ARG:HH11	2:C:851:ARG:HG2	1.71	0.56
2:C:413:THR:HG22	2:C:415:GLN:H	1.71	0.56
2:C:541:VAL:HG12	2:C:578:TYR:HB2	1.88	0.56
2:C:884:LYS:HE2	2:C:892:LYS:HB3	1.88	0.56
3:D:778:TRP:HB2	3:D:823:LEU:HD21	1.88	0.56
2:C:168:ILE:HG12	2:C:431:PHE:HB3	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:226:ILE:H	2:C:229:LYS:HG2	1.70	0.55
2:C:625:LEU:HG	2:C:718:ASN:ND2	2.21	0.55
2:C:853:PHE:O	2:C:867:GLU:HA	2.05	0.55
5:F:331:ALA:CB	5:F:350:TRP:HD1	2.19	0.55
2:C:922:VAL:HB	2:C:923:PRO:HD3	1.87	0.55
8:D:1904:FI8:C24	8:D:1904:FI8:C25	2.84	0.55
2:C:918:ASN:OD1	2:C:919:THR:N	2.40	0.55
3:D:173:ARG:HD3	3:D:204:GLU:HB3	1.87	0.55
3:D:554:GLU:O	3:D:558:LEU:HB2	2.06	0.55
2:C:388:GLN:HG3	2:C:430:PHE:HB2	1.89	0.55
2:C:1128:LEU:HD22	2:C:1133:LEU:HD12	1.89	0.55
3:D:1246:ASN:OD1	3:D:1246:ASN:N	2.40	0.55
2:C:251:ARG:HH11	2:C:251:ARG:HG3	1.71	0.55
3:D:428:SER:O	3:D:540:GLN:HA	2.07	0.55
5:F:235:ILE:HG23	5:F:300:LEU:HB2	1.88	0.55
2:C:105:LEU:HD12	2:C:138:GLU:O	2.07	0.55
2:C:93:LEU:HD22	2:C:393:MET:HG3	1.89	0.55
2:C:502:VAL:HG23	2:C:587:VAL:O	2.07	0.55
3:D:889:HIS:HB2	3:D:991:ILE:HD11	1.88	0.55
5:F:293:ASN:O	5:F:297:GLU:HG2	2.07	0.55
2:C:400:VAL:HG13	2:C:417:LEU:HB3	1.88	0.55
3:D:507:LEU:HD12	3:D:574:LEU:HD12	1.88	0.54
3:D:992:GLY:O	3:D:1261:GLY:N	2.36	0.54
2:C:1043:ALA:HB2	3:D:447:MET:HG3	1.90	0.54
3:D:1050:THR:HB	3:D:1107:VAL:HB	1.89	0.54
5:F:297:GLU:HA	5:F:300:LEU:HD12	1.89	0.54
2:C:731:TYR:CE1	3:D:579:LEU:HB3	2.42	0.54
5:F:410:VAL:O	5:F:414:GLN:HG2	2.08	0.54
3:D:151:LEU:HD13	3:D:248:TYR:HE2	1.72	0.54
3:D:1265:ASN:OD1	3:D:1268:ARG:NH2	2.29	0.54
3:D:156:ALA:O	3:D:160:LYS:HB3	2.07	0.54
3:D:184:LEU:HD11	3:D:197:VAL:HG11	1.90	0.54
3:D:162:VAL:HG21	3:D:219:LEU:HD11	1.90	0.54
3:D:676:LEU:HD22	3:D:715:LYS:HB3	1.89	0.54
2:C:185:VAL:HG23	2:C:316:VAL:HG22	1.88	0.54
3:D:1003:ILE:HD11	3:D:1154:ILE:HG13	1.88	0.54
3:D:343:LEU:HD13	3:D:381:LEU:HA	1.90	0.54
1:B:171:VAL:HA	1:B:198:THR:HG22	1.90	0.54
2:C:767:GLU:HG2	2:C:807:THR:HA	1.90	0.54
8:D:1904:FI8:C33	8:D:1904:FI8:C41	2.86	0.54
2:C:240:ALA:O	2:C:274:LEU:HD21	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:53:LEU:HD12	2:C:637:ASP:HB2	1.90	0.53
3:D:1245:LEU:O	3:D:1251:ASN:ND2	2.41	0.53
5:F:381:ARG:NH1	5:F:385:GLU:OE2	2.41	0.53
3:D:889:HIS:O	3:D:977:THR:OG1	2.21	0.53
2:C:348:LEU:HD11	2:C:367:THR:HG22	1.89	0.53
1:A:197:GLU:OE2	2:C:996:ARG:NH2	2.41	0.53
3:D:173:ARG:HA	3:D:173:ARG:HE	1.74	0.53
3:D:239:ASN:OD1	3:D:239:ASN:N	2.41	0.53
3:D:442:GLY:HA3	3:D:523:GLN:HB2	1.90	0.53
3:D:111:PRO:HB2	3:D:116:TYR:CE2	2.44	0.53
3:D:1269:ASN:O	4:E:109:GLY:HA2	2.09	0.53
1:B:183:VAL:HG12	1:B:184:GLU:HG3	1.89	0.53
1:A:210:SER:HB2	1:B:228:GLU:HG2	1.90	0.53
3:D:461:VAL:HG21	3:D:469:ILE:HA	1.91	0.53
5:F:228:VAL:HA	5:F:318:LEU:HD21	1.91	0.53
1:A:15:THR:HB	1:A:18:ARG:O	2.09	0.52
3:D:789:LEU:HD21	3:D:818:ALA:HB3	1.90	0.52
8:D:1904:FI8:C21	8:D:1904:FI8:C22	2.85	0.52
2:C:102:SER:HA	2:C:142:ASN:HB2	1.90	0.52
2:C:756:GLU:HB3	2:C:870:ARG:HG2	1.92	0.52
3:D:530:GLU:HG3	3:D:574:LEU:HD22	1.92	0.52
2:C:758:ASP:N	2:C:758:ASP:OD1	2.40	0.52
2:C:739:ASN:HB2	2:C:899:LEU:O	2.09	0.52
3:D:116:TYR:HE1	3:D:294:LYS:HB3	1.73	0.52
3:D:52:PHE:CD1	3:D:322:PRO:HD3	2.44	0.52
3:D:778:TRP:CE2	3:D:835:PRO:HG3	2.44	0.52
3:D:356:ARG:NH1	5:F:330:ARG:NH2	2.54	0.52
3:D:965:VAL:HG11	3:D:1156:VAL:HG22	1.91	0.52
3:D:387:ARG:NH2	5:F:225:ALA:O	2.43	0.52
1:A:152:ASN:HB3	1:A:163:PRO:HG3	1.92	0.52
2:C:217:ASP:HB2	2:C:231:ARG:HH12	1.74	0.52
3:D:762:ARG:CZ	3:D:762:ARG:HB2	2.39	0.52
3:D:360:LEU:HD21	5:F:329:ILE:CG2	2.40	0.52
5:F:231:TYR:O	5:F:235:ILE:HG12	2.10	0.52
2:C:449:LEU:HD23	2:C:589:VAL:HG11	1.92	0.51
2:C:820:LEU:HD11	5:F:475:VAL:HG13	1.93	0.51
1:A:191:LYS:HE2	1:A:193:ILE:HD11	1.91	0.51
2:C:56:VAL:HG21	2:C:500:LEU:HD21	1.91	0.51
5:F:446:VAL:HG22	5:F:449:ASP:H	1.75	0.51
5:F:477:LEU:HD11	5:F:496:TYR:HB2	1.92	0.51
2:C:974:THR:OG1	2:C:979:GLY:HA3	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:60:ARG:NE	4:E:98:GLU:OE2	2.43	0.51
2:C:39:VAL:HG12	2:C:963:LEU:HG	1.91	0.51
3:D:602:ALA:HB1	3:D:606:HIS:O	2.11	0.51
3:D:925:LEU:HD11	3:D:960:VAL:CG2	2.40	0.51
1:A:10:SER:HA	1:A:22:VAL:O	2.10	0.51
2:C:822:ARG:CZ	2:C:829:ALA:HB2	2.40	0.51
3:D:1275:THR:HG22	3:D:1277:GLU:H	1.76	0.51
5:F:317:PHE:CE1	5:F:321:ILE:HD11	2.46	0.51
2:C:54:LEU:HD21	2:C:449:LEU:HD12	1.92	0.51
2:C:604:ARG:CZ	2:C:925:ARG:HD2	2.41	0.51
2:C:107:PHE:HB3	2:C:137:ALA:HA	1.92	0.51
3:D:285:LYS:CA	3:D:285:LYS:CE	2.86	0.51
3:D:926:GLY:O	3:D:940:ARG:NH1	2.44	0.51
5:F:468:SER:HB3	5:F:471:GLU:HG2	1.93	0.51
2:C:389:ILE:O	2:C:393:MET:HB2	2.10	0.51
2:C:56:VAL:HG21	2:C:500:LEU:CD2	2.41	0.51
2:C:731:TYR:HE1	3:D:579:LEU:HB3	1.75	0.51
3:D:938:VAL:HG23	3:D:952:LEU:HD13	1.93	0.51
5:F:262:LEU:HD12	5:F:263:MET:N	2.26	0.51
5:F:477:LEU:HD11	5:F:496:TYR:CG	2.46	0.51
1:B:149:ALA:HB2	1:B:164:VAL:C	2.32	0.50
2:C:1077:GLN:HE21	2:C:1085:LEU:HD21	1.76	0.50
2:C:821:LEU:HD12	5:F:523:LEU:HD23	1.93	0.50
2:C:981:GLN:HG2	2:C:982:GLU:N	2.26	0.50
3:D:1182:ASP:OD1	3:D:1183:ARG:N	2.44	0.50
3:D:525:HIS:CE1	3:D:527:LEU:HB2	2.45	0.50
3:D:778:TRP:CD2	3:D:835:PRO:HG3	2.46	0.50
3:D:84:ARG:HB3	3:D:86:LYS:HG2	1.92	0.50
5:F:510:THR:HG22	5:F:513:LYS:HB2	1.94	0.50
1:B:182:ARG:NH1	3:D:488:GLU:HG2	2.26	0.50
2:C:507:ASN:HB2	2:C:508:PRO:HD2	1.94	0.50
1:A:18:ARG:HB3	1:A:197:GLU:HG3	1.93	0.50
3:D:170:LEU:HD21	3:D:209:ARG:HB2	1.93	0.50
3:D:124:ASP:HB3	3:D:234:LEU:HD11	1.92	0.50
3:D:12:ILE:O	3:D:1240:CYS:HA	2.11	0.50
2:C:689:ILE:CD1	2:C:710:ASP:HA	2.42	0.50
2:C:744:GLU:O	2:C:745:ASP:HB2	2.11	0.50
3:D:1003:ILE:HD11	3:D:1154:ILE:HA	1.93	0.50
5:F:350:TRP:HE3	5:F:350:TRP:HA	1.76	0.50
3:D:701:ALA:HA	3:D:709:VAL:HG21	1.94	0.50
5:F:334:LYS:HD2	5:F:350:TRP:HE1	1.75	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:8:THR:O	1:B:221:LEU:HD11	2.11	0.50
2:C:224:VAL:HG12	2:C:234:VAL:HA	1.93	0.50
5:F:344:SER:O	5:F:348:THR:CB	2.60	0.50
2:C:226:ILE:HG23	2:C:300:PHE:HZ	1.77	0.50
2:C:107:PHE:CD2	2:C:107:PHE:N	2.77	0.49
3:D:328:VAL:HG21	8:D:1904:FI8:C20	2.42	0.49
3:D:579:LEU:HD11	3:D:808:THR:HB	1.94	0.49
2:C:936:LEU:HB2	2:C:985:LEU:HD11	1.94	0.49
3:D:1003:ILE:CD1	3:D:1154:ILE:HG13	2.41	0.49
2:C:1087:GLU:HG3	2:C:1091:ILE:HD11	1.94	0.49
3:D:1124:VAL:HG12	3:D:1125:GLN:HG3	1.93	0.49
3:D:27:GLU:HB2	3:D:94:HIS:HE1	1.77	0.49
3:D:554:GLU:HB3	4:E:54:VAL:HG11	1.94	0.49
2:C:928:ILE:CG2	3:D:817:LEU:HD11	2.43	0.49
2:C:239:LYS:HE3	2:C:262:LEU:HD11	1.95	0.49
2:C:252:PHE:CD1	2:C:258:MET:HG2	2.48	0.49
5:F:331:ALA:HA	5:F:350:TRP:HD1	1.78	0.49
5:F:489:LEU:HD23	5:F:489:LEU:H	1.77	0.49
2:C:48:LEU:HD22	2:C:528:ILE:HD12	1.95	0.49
3:D:576:MET:HB2	3:D:697:ILE:HD12	1.93	0.49
3:D:24:SER:HB2	3:D:94:HIS:HB3	1.95	0.49
5:F:291:ALA:O	5:F:295:LEU:HB3	2.12	0.49
1:B:11:GLU:HG2	1:B:12:ASP:N	2.28	0.49
5:F:473:GLY:HA3	5:F:496:TYR:OH	2.13	0.49
2:C:1127:GLU:HG2	3:D:320:ILE:HD11	1.95	0.49
3:D:904:ARG:HA	3:D:910:LEU:HA	1.95	0.49
5:F:489:LEU:HD13	5:F:504:ARG:NH2	2.27	0.49
1:A:96:TYR:CE2	1:A:137:GLU:HB3	2.48	0.49
3:D:1190:ASN:ND2	3:D:1201:ALA:H	2.11	0.49
3:D:595:ASP:HB3	3:D:631:ALA:HB2	1.95	0.49
5:F:355:ILE:O	5:F:359:MET:HB3	2.13	0.49
2:C:104:SER:HB3	2:C:140:ILE:HB	1.94	0.48
2:C:264:LYS:HE3	2:C:264:LYS:HB3	1.64	0.48
2:C:63:TRP:HD1	2:C:70:TRP:CE2	2.31	0.48
3:D:554:GLU:HB2	3:D:558:LEU:HD12	1.95	0.48
3:D:456:VAL:O	3:D:460:LEU:HB2	2.12	0.48
3:D:826:ASN:HD22	3:D:830:GLU:HG3	1.78	0.48
4:E:43:LEU:HD13	4:E:53:LEU:HD11	1.95	0.48
3:D:352:ASN:O	3:D:355:LYS:HG2	2.14	0.48
4:E:92:LEU:HD23	4:E:96:LEU:HD13	1.94	0.48
3:D:897:ILE:HG23	3:D:1128:ARG:NH2	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:33:THR:CG2	1:B:37:SER:HA	2.43	0.48
2:C:220:ASP:HB3	2:C:257:ILE:HD12	1.96	0.48
3:D:460:LEU:HD21	3:D:475:MET:SD	2.53	0.48
5:F:522:VAL:HG23	5:F:523:LEU:HD12	1.94	0.48
2:C:909:ASP:OD1	2:C:1001:LEU:HD11	2.14	0.48
2:C:277:ILE:HD12	2:C:296:LEU:HD11	1.96	0.48
3:D:1166:THR:OG1	3:D:1206:VAL:HG21	2.13	0.48
3:D:1167:ILE:HD13	3:D:1175:PHE:CD2	2.49	0.48
8:D:1904:FI8:C47	8:D:1904:FI8:C49	2.92	0.48
2:C:191:ILE:HA	2:C:198:THR:HA	1.95	0.47
3:D:1244:LYS:N	3:D:1244:LYS:HD2	2.29	0.47
4:E:82:LEU:HB3	4:E:103:LEU:HD13	1.96	0.47
5:F:272:LYS:HD3	5:F:278:ARG:HH22	1.78	0.47
2:C:805:LYS:HE3	2:C:835:THR:HG23	1.96	0.47
3:D:457:MET:SD	3:D:473:LYS:CB	3.00	0.47
2:C:905:PRO:O	2:C:913:VAL:HG13	2.15	0.47
3:D:1010:LEU:HA	3:D:1145:GLN:HG3	1.96	0.47
3:D:26:GLY:HA3	3:D:51:ILE:HG12	1.96	0.47
3:D:491:ILE:HD11	3:D:516:LEU:HG	1.97	0.47
1:A:68:GLY:HA3	1:A:132:GLY:CA	2.44	0.47
5:F:294:HIS:HA	5:F:297:GLU:HG2	1.96	0.47
5:F:331:ALA:HA	5:F:350:TRP:CD1	2.49	0.47
5:F:499:THR:OG1	5:F:500:ARG:N	2.47	0.47
3:D:400:LYS:HD2	3:D:404:ASP:OD1	2.14	0.47
1:A:162:ILE:HG22	1:A:163:PRO:O	2.15	0.47
1:A:13:VAL:O	1:A:19:SER:HB3	2.14	0.47
2:C:523:VAL:HA	2:C:552:GLY:O	2.15	0.47
3:D:118:LEU:HD21	3:D:265:ILE:HG12	1.97	0.47
5:F:311:THR:HG1	5:F:317:PHE:HD2	1.62	0.47
2:C:653:VAL:HG13	2:C:658:ILE:CD1	2.45	0.47
2:C:708:THR:HA	2:C:712:GLU:O	2.15	0.47
2:C:1131:LEU:HD13	3:D:105:TRP:CH2	2.50	0.47
1:B:26:LEU:HD23	1:B:26:LEU:HA	1.70	0.47
2:C:177:SER:HB3	2:C:378:LEU:HD21	1.97	0.47
2:C:493:ASN:HA	2:C:496:LEU:HD12	1.97	0.47
3:D:88:ARG:HG3	3:D:323:GLU:HG2	1.95	0.47
3:D:588:LEU:HD13	3:D:723:TRP:CE2	2.50	0.47
1:B:97:LEU:HB2	1:B:110:ILE:HG12	1.96	0.47
3:D:110:VAL:HA	3:D:111:PRO:HA	1.77	0.47
3:D:1120:GLU:OE1	3:D:1123:ARG:NH1	2.48	0.47
3:D:133:ALA:O	3:D:256:MET:HG3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:363:PRO:HG3	5:F:296:LEU:HD22	1.97	0.47
3:D:466:ALA:HB3	3:D:472:ALA:HB2	1.97	0.47
3:D:741:ARG:HE	3:D:741:ARG:HB2	1.40	0.46
3:D:821:LYS:HD3	3:D:840:PHE:HE1	1.81	0.46
3:D:923:ARG:NH2	3:D:1155:GLU:OE2	2.48	0.46
1:B:158:GLU:HB3	1:B:161:ARG:HB2	1.97	0.46
1:B:72:ASP:H	1:B:75:GLU:HB2	1.80	0.46
2:C:934:THR:HA	2:C:1027:TYR:O	2.15	0.46
3:D:463:LEU:CD1	3:D:486:VAL:CG2	2.93	0.46
3:D:67:ARG:CZ	5:F:483:ASP:HB3	2.45	0.46
2:C:251:ARG:NH1	2:C:251:ARG:HG3	2.30	0.46
2:C:473:ARG:HG2	2:C:496:LEU:HD21	1.97	0.46
3:D:229:LEU:HD12	3:D:233:GLN:OE1	2.15	0.46
3:D:29:LYS:O	3:D:352:ASN:ND2	2.32	0.46
3:D:637:LEU:HD11	3:D:671:VAL:HG22	1.97	0.46
3:D:901:LEU:N	3:D:958:THR:O	2.46	0.46
3:D:963:ARG:HG2	3:D:978:CYS:CB	2.45	0.46
2:C:507:ASN:HB3	2:C:513:GLU:CD	2.36	0.46
3:D:1083:ARG:HH11	3:D:1112:MET:HE1	1.81	0.46
3:D:1164:ARG:NH2	3:D:1216:ALA:O	2.48	0.46
3:D:877:LEU:HD23	3:D:1210:ILE:HD13	1.97	0.46
5:F:358:ALA:O	5:F:362:GLN:HG2	2.15	0.46
2:C:1128:LEU:HD23	2:C:1128:LEU:HA	1.74	0.46
3:D:259:GLU:HG3	3:D:260:SER:N	2.30	0.46
3:D:360:LEU:HD21	5:F:329:ILE:HG22	1.96	0.46
5:F:499:THR:HG21	5:F:500:ARG:HH11	1.81	0.46
1:A:209:ALA:HA	1:B:222:ALA:O	2.16	0.46
3:D:14:LEU:HD23	3:D:14:LEU:HA	1.60	0.46
3:D:793:TYR:CD1	3:D:800:ILE:HG12	2.51	0.46
3:D:9:GLU:OE1	3:D:1244:LYS:NZ	2.42	0.46
5:F:449:ASP:O	5:F:453:PHE:HB2	2.16	0.46
2:C:571:VAL:CG1	2:C:575:GLU:HB2	2.46	0.46
2:C:628:THR:C	2:C:630:MET:H	2.19	0.46
3:D:331:ASP:N	3:D:331:ASP:OD1	2.48	0.46
2:C:296:LEU:HD23	2:C:296:LEU:HA	1.78	0.46
3:D:438:LEU:O	3:D:561:SER:OG	2.32	0.46
3:D:616:ALA:O	3:D:620:MET:HG3	2.16	0.46
3:D:52:PHE:O	3:D:91:ARG:HD2	2.16	0.46
5:F:296:LEU:O	5:F:300:LEU:HG	2.16	0.46
2:C:129:TYR:CE1	2:C:161:THR:HG22	2.51	0.46
2:C:445:PRO:HB2	2:C:713:MET:SD	2.55	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:529:VAL:HG11	2:C:578:TYR:HE2	1.81	0.46
2:C:1137:VAL:HG11	3:D:7:PHE:CD1	2.51	0.46
5:F:257:LEU:CD2	5:F:337:TYR:CE1	2.99	0.46
2:C:213:GLU:HG2	2:C:225:ARG:O	2.16	0.45
1:B:78:LEU:HD21	3:D:611:VAL:HG12	1.98	0.45
2:C:68:PRO:O	2:C:72:GLU:HG2	2.15	0.45
8:D:1904:FI8:C10	8:D:1904:FI8:C6	2.95	0.45
3:D:400:LYS:HD2	3:D:404:ASP:CG	2.36	0.45
5:F:299:ASN:HB2	5:F:328:LEU:CD2	2.45	0.45
1:A:55:ARG:HB3	1:A:137:GLU:HG3	1.97	0.45
2:C:689:ILE:HD11	2:C:710:ASP:HA	1.96	0.45
2:C:752:ILE:HG12	2:C:874:ALA:HB2	1.97	0.45
3:D:1068:PRO:HD3	3:D:1074:GLU:HA	1.97	0.45
3:D:424:TYR:CE2	3:D:547:LEU:HD11	2.51	0.45
2:C:189:GLU:HB3	2:C:200:HIS:ND1	2.30	0.45
2:C:514:THR:OG1	2:C:585:GLN:NE2	2.48	0.45
3:D:579:LEU:CD1	3:D:808:THR:HB	2.47	0.45
3:D:86:LYS:O	3:D:89:ARG:HG2	2.17	0.45
3:D:36:TYR:CD1	5:F:416:TYR:HE1	2.34	0.45
1:B:38:LEU:HA	1:B:38:LEU:HD12	1.69	0.45
2:C:200:HIS:HB3	2:C:348:LEU:HD23	1.98	0.45
2:C:223:GLY:HA3	2:C:231:ARG:NE	2.32	0.45
2:C:592:ALA:HB3	2:C:630:MET:HG2	1.97	0.45
3:D:14:LEU:HD21	3:D:106:TYR:OH	2.16	0.45
4:E:71:LEU:HA	4:E:76:LEU:HD21	1.99	0.45
3:D:131:PHE:HD1	3:D:256:MET:HE3	1.82	0.45
4:E:85:PRO:HB3	4:E:94:ILE:HD13	1.99	0.45
3:D:222:ILE:HD13	3:D:247:ARG:NH2	2.32	0.45
3:D:25:TYR:CD2	3:D:91:ARG:HD3	2.52	0.45
2:C:335:GLU:HG3	2:C:336:GLU:H	1.82	0.45
2:C:378:LEU:HD13	2:C:512:ILE:HD11	1.99	0.45
3:D:1244:LYS:H	3:D:1244:LYS:HD2	1.82	0.45
1:B:27:GLU:HB3	1:B:30:PHE:CD1	2.52	0.45
3:D:36:TYR:CE2	5:F:369:PRO:HD3	2.51	0.45
1:B:215:LEU:HD23	1:B:215:LEU:HA	1.73	0.45
3:D:880:VAL:O	3:D:1160:GLN:HG2	2.17	0.45
3:D:639:GLN:O	3:D:640:LEU:HD23	2.17	0.45
5:F:472:ALA:HA	5:F:475:VAL:HB	1.99	0.45
2:C:1108:LYS:HD3	2:C:1108:LYS:HA	1.72	0.44
2:C:519:VAL:HG22	2:C:524:VAL:HA	1.98	0.44
2:C:152:VAL:HG21	2:C:418:ILE:HD12	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:608:GLY:O	2:C:612:GLN:HG3	2.17	0.44
3:D:1038:ARG:HB2	3:D:1038:ARG:HE	1.57	0.44
3:D:1117:ASP:O	3:D:1121:VAL:HG23	2.18	0.44
3:D:1250:GLU:CD	3:D:1250:GLU:H	2.21	0.44
3:D:605:ASP:OD1	3:D:606:HIS:N	2.51	0.44
3:D:817:LEU:HD12	3:D:817:LEU:HA	1.65	0.44
3:D:985:THR:HG22	3:D:987:LYS:HG3	1.98	0.44
1:A:23:ILE:HD12	1:A:192:LEU:HD23	1.98	0.44
1:A:33:THR:HG21	1:B:37:SER:CA	2.46	0.44
1:B:99:LYS:HG2	1:B:100:GLN:H	1.83	0.44
1:B:129:ASN:HD22	1:B:129:ASN:C	2.21	0.44
1:B:220:GLY:O	1:B:224:GLU:HG3	2.18	0.44
2:C:67:SER:OG	2:C:68:PRO:HD2	2.17	0.44
2:C:809:LYS:H	2:C:832:VAL:HA	1.83	0.44
3:D:1034:LEU:HD13	3:D:1138:VAL:HG23	1.99	0.44
1:B:78:LEU:HD22	3:D:613:SER:HA	1.99	0.44
3:D:926:GLY:H	3:D:962:VAL:HA	1.81	0.44
4:E:46:ARG:HE	4:E:100:HIS:HA	1.82	0.44
4:E:47:VAL:HG21	4:E:53:LEU:N	2.32	0.44
3:D:445:LYS:HA	3:D:516:LEU:HD22	1.99	0.44
4:E:47:VAL:HG23	4:E:56:TYR:HD1	1.83	0.44
1:A:171:VAL:HG12	1:A:172:LEU:H	1.83	0.44
2:C:217:ASP:HB3	2:C:221:THR:H	1.82	0.44
2:C:449:LEU:CD2	2:C:589:VAL:HG11	2.47	0.44
2:C:604:ARG:NH1	2:C:925:ARG:HD2	2.32	0.44
2:C:449:LEU:HB2	2:C:638:ALA:HB2	1.98	0.44
2:C:752:ILE:HG12	2:C:874:ALA:CB	2.47	0.44
3:D:1190:ASN:HD21	3:D:1201:ALA:H	1.66	0.44
3:D:443:LEU:HA	3:D:443:LEU:HD12	1.77	0.44
1:A:144:ARG:HH11	1:A:144:ARG:HG3	1.83	0.44
1:A:61:HIS:HB2	2:C:846:LYS:HD2	2.00	0.44
2:C:882:GLY:HA2	2:C:894:VAL:CG1	2.47	0.44
3:D:1023:ASP:N	3:D:1023:ASP:OD1	2.50	0.44
3:D:1033:GLU:HB2	3:D:1038:ARG:NH2	2.32	0.44
3:D:739:PRO:HG2	3:D:742:LYS:HB2	2.00	0.44
2:C:732:GLU:HB3	3:D:536:PHE:CD2	2.49	0.44
3:D:136:ILE:HD13	3:D:229:LEU:HD11	1.99	0.44
3:D:454:PRO:HA	3:D:457:MET:HE2	2.00	0.44
3:D:827:PRO:HD3	3:D:854:HIS:CD2	2.53	0.44
5:F:292:LYS:HE2	5:F:292:LYS:HB3	1.71	0.44
2:C:1038:ASP:N	2:C:1038:ASP:OD1	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1125:LEU:HA	2:C:1125:LEU:HD23	1.66	0.44
2:C:247:GLN:HA	2:C:250:GLU:HG2	2.00	0.44
2:C:854:SER:HA	2:C:867:GLU:HG3	2.00	0.44
3:D:151:LEU:HD13	3:D:248:TYR:CE2	2.52	0.44
3:D:459:ARG:HA	3:D:459:ARG:HD2	1.83	0.44
3:D:880:VAL:HA	3:D:1214:SER:HB3	1.99	0.44
1:A:119:HIS:CE1	1:A:201:SER:HA	2.52	0.44
3:D:1108:GLY:HA3	3:D:1125:GLN:HE21	1.82	0.44
3:D:120:LEU:HD12	3:D:125:LEU:HD13	1.99	0.44
3:D:250:GLU:HG2	3:D:250:GLU:O	2.17	0.44
3:D:988:LEU:HA	3:D:988:LEU:HD23	1.73	0.44
2:C:445:PRO:HD2	2:C:707:CYS:HB2	1.99	0.43
2:C:631:GLU:HB3	2:C:713:MET:HB2	1.99	0.43
3:D:629:VAL:HG11	3:D:723:TRP:CH2	2.53	0.43
3:D:746:LEU:HD21	3:D:820:MET:HE1	2.00	0.43
3:D:874:THR:OG1	3:D:1004:GLY:HA3	2.18	0.43
1:A:218:LEU:HD23	1:A:218:LEU:HA	1.80	0.43
1:B:96:TYR:O	1:B:110:ILE:HG23	2.18	0.43
2:C:378:LEU:HD11	2:C:455:LEU:HG	2.00	0.43
2:C:39:VAL:CG1	2:C:963:LEU:HG	2.48	0.43
3:D:1033:GLU:HG2	3:D:1033:GLU:O	2.15	0.43
3:D:1267:TYR:O	3:D:1270:ILE:HG13	2.18	0.43
2:C:1118:PRO:HG2	3:D:1255:GLY:HA3	1.99	0.43
2:C:773:ILE:CG2	2:C:776:ILE:HD12	2.49	0.43
2:C:820:LEU:HD12	5:F:479:PHE:CB	2.48	0.43
2:C:485:PRO:HB2	3:D:853:THR:HG21	1.99	0.43
3:D:946:ASP:N	3:D:947:PRO:HD2	2.34	0.43
4:E:103:LEU:HD23	4:E:103:LEU:HA	1.57	0.43
5:F:231:TYR:CE1	5:F:235:ILE:HD11	2.53	0.43
1:A:8:THR:O	1:A:9:LEU:HD23	2.17	0.43
2:C:413:THR:HG23	2:C:414:PRO:HD2	2.00	0.43
3:D:290:LEU:C	3:D:290:LEU:CD2	2.85	0.43
3:D:454:PRO:HA	3:D:457:MET:CE	2.48	0.43
5:F:349:TRP:CZ3	5:F:350:TRP:CZ3	3.07	0.43
1:B:85:VAL:HG11	1:B:140:VAL:HG11	2.01	0.43
2:C:240:ALA:HB1	2:C:274:LEU:HD23	1.99	0.43
2:C:525:SER:OG	2:C:526:ASP:N	2.52	0.43
2:C:925:ARG:HB2	2:C:927:ASN:OD1	2.18	0.43
3:D:425:SER:HA	3:D:543:VAL:O	2.19	0.43
3:D:730:THR:HG22	3:D:731:VAL:N	2.33	0.43
3:D:925:LEU:HD12	3:D:925:LEU:HA	1.63	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:249:LEU:HD11	5:F:343:PHE:CZ	2.49	0.43
1:A:51:VAL:HG11	1:A:138:LEU:HD23	2.00	0.43
2:C:965:GLU:HG3	2:C:965:GLU:O	2.18	0.43
3:D:118:LEU:O	3:D:120:LEU:HG	2.19	0.43
2:C:485:PRO:O	3:D:857:ARG:NH2	2.52	0.43
2:C:613:ARG:HB2	2:C:613:ARG:CZ	2.49	0.43
2:C:632:LEU:HD12	2:C:711:GLY:O	2.18	0.43
2:C:944:TRP:CE2	2:C:988:LEU:HD22	2.54	0.43
3:D:1045:PRO:HG2	3:D:1111:LEU:HB2	2.00	0.43
3:D:363:PRO:HG2	3:D:366:ILE:HG13	2.00	0.43
3:D:931:ASP:OD1	3:D:932:GLU:HG2	2.18	0.43
5:F:503:ILE:HA	5:F:503:ILE:HD12	1.85	0.43
5:F:292:LYS:O	5:F:296:LEU:HB2	2.19	0.43
1:A:12:ASP:OD1	1:A:13:VAL:N	2.52	0.43
1:B:146:TYR:O	3:D:624:ARG:NE	2.49	0.43
1:B:18:ARG:HG2	1:B:197:GLU:HG3	2.01	0.43
1:B:40:ARG:O	1:B:44:SER:HB3	2.19	0.43
2:C:150:GLN:HG2	2:C:151:THR:H	1.84	0.43
2:C:412:ILE:HA	2:C:412:ILE:HD12	1.89	0.43
1:B:97:LEU:HD13	1:B:110:ILE:HG12	2.01	0.43
2:C:627:GLY:O	2:C:973:SER:HA	2.19	0.43
2:C:846:LYS:O	2:C:873:VAL:HA	2.18	0.43
3:D:1030:ARG:HH21	3:D:1137:GLU:HG2	1.84	0.43
3:D:244:LEU:HG	3:D:252:PHE:CZ	2.54	0.43
3:D:463:LEU:HB3	3:D:465:HIS:CE1	2.54	0.43
3:D:716:LEU:HD23	3:D:716:LEU:HA	1.77	0.43
3:D:1034:LEU:HD11	3:D:1137:GLU:CB	2.47	0.42
3:D:746:LEU:HD23	3:D:746:LEU:HA	1.70	0.42
5:F:466:THR:HG21	5:F:516:HIS:CE1	2.54	0.42
2:C:213:GLU:CG	2:C:225:ARG:HB2	2.49	0.42
3:D:1055:LEU:HD12	3:D:1064:ILE:HG12	2.00	0.42
3:D:939:GLU:OE1	3:D:939:GLU:N	2.47	0.42
2:C:400:VAL:HG22	2:C:417:LEU:O	2.19	0.42
3:D:527:LEU:HD23	3:D:527:LEU:HA	1.65	0.42
1:B:98:ARG:HB3	1:B:133:LYS:NZ	2.34	0.42
2:C:116:LYS:HD3	2:C:116:LYS:HA	1.82	0.42
2:C:107:PHE:HB3	2:C:137:ALA:CB	2.49	0.42
2:C:140:ILE:HA	2:C:147:ILE:HG12	2.02	0.42
2:C:224:VAL:HG21	2:C:237:LEU:HD23	2.00	0.42
2:C:279:ARG:HH21	2:C:287:PRO:HB2	1.85	0.42
2:C:348:LEU:HD21	2:C:367:THR:HG22	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1245:LEU:HD23	3:D:1245:LEU:HA	1.79	0.42
3:D:480:ARG:O	3:D:483:VAL:HG22	2.20	0.42
5:F:331:ALA:CA	5:F:350:TRP:HD1	2.32	0.42
1:A:215:LEU:HD23	1:A:215:LEU:HA	1.67	0.42
2:C:202:VAL:HG21	2:C:345:LEU:HB2	2.02	0.42
2:C:218:LYS:H	2:C:218:LYS:HG2	1.71	0.42
2:C:689:ILE:HG22	2:C:702:ILE:O	2.19	0.42
2:C:98:ASP:OD1	2:C:99:PHE:N	2.52	0.42
3:D:276:SER:O	3:D:280:VAL:HG23	2.19	0.42
3:D:731:VAL:HG22	3:D:799:ILE:HD11	2.01	0.42
1:A:65:THR:HG22	1:A:72:ASP:HB3	2.02	0.42
1:B:98:ARG:HG2	1:B:135:GLU:CG	2.38	0.42
2:C:1101:LYS:HA	2:C:1101:LYS:HD3	1.75	0.42
3:D:1274:PRO:HA	4:E:104:LEU:HD23	2.00	0.42
2:C:134:PHE:HE1	2:C:153:PHE:HD1	1.65	0.42
3:D:451:LEU:HD23	3:D:451:LEU:HA	1.65	0.42
3:D:468:ASN:OD1	3:D:468:ASN:N	2.51	0.42
3:D:624:ARG:HG2	3:D:626:VAL:HG23	2.02	0.42
2:C:401:ARG:O	2:C:404:MET:HG2	2.20	0.42
2:C:785:ASP:HA	2:C:791:ARG:NH2	2.34	0.42
3:D:642:PRO:HB3	3:D:662:TRP:CD2	2.55	0.42
1:A:223:ARG:HD2	1:B:213:LYS:HG3	2.01	0.41
2:C:905:PRO:HB2	2:C:1010:LEU:HD13	2.02	0.41
2:C:809:LYS:N	2:C:831:GLU:O	2.53	0.41
3:D:778:TRP:CB	3:D:823:LEU:HD21	2.49	0.41
1:A:89:GLU:HG2	1:A:90:ASP:N	2.36	0.41
1:A:9:LEU:HA	1:B:221:LEU:HD13	2.02	0.41
1:B:71:GLU:HG3	1:B:75:GLU:OE1	2.20	0.41
1:A:129:ASN:OD1	1:A:130:ASP:N	2.52	0.41
2:C:1091:ILE:CD1	2:C:1102:VAL:HG21	2.49	0.41
2:C:384:LEU:HA	2:C:384:LEU:HD23	1.80	0.41
2:C:631:GLU:HG3	2:C:631:GLU:H	1.70	0.41
3:D:156:ALA:O	3:D:160:LYS:HB2	2.20	0.41
3:D:234:LEU:HA	3:D:234:LEU:HD23	1.78	0.41
3:D:57:ASP:HB3	3:D:58:TRP:HE3	1.82	0.41
3:D:816:THR:HG23	3:D:821:LYS:HA	2.01	0.41
5:F:387:LEU:HD13	5:F:393:GLU:HA	2.01	0.41
2:C:450:THR:HG21	2:C:613:ARG:HD2	2.02	0.41
3:D:1005:GLU:HB3	3:D:1006:PRO:HD3	2.02	0.41
5:F:487:ARG:HH21	5:F:491:GLU:HG2	1.85	0.41
3:D:1063:LYS:HG3	3:D:1077:TYR:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:104:ILE:HD11	3:D:386:ARG:HB3	2.02	0.41
3:D:471:SER:O	3:D:474:ARG:HB3	2.21	0.41
1:A:8:THR:HG23	1:A:8:THR:O	2.20	0.41
2:C:455:LEU:HD11	2:C:500:LEU:HB2	2.03	0.41
3:D:99:ALA:HA	3:D:100:PRO:HD3	1.91	0.41
3:D:1164:ARG:HD2	3:D:1208:MET:CE	2.50	0.41
3:D:1248:LEU:O	3:D:1252:VAL:HG23	2.21	0.41
3:D:46:LEU:HD21	3:D:348:ILE:HD11	2.02	0.41
2:C:775:ASN:ND2	5:F:527:LEU:O	2.54	0.41
2:C:277:ILE:HG21	2:C:296:LEU:HD21	2.02	0.41
3:D:1031:VAL:HG23	3:D:1141:VAL:HG11	2.02	0.41
3:D:203:ARG:HD3	3:D:206:ARG:HH21	1.86	0.41
3:D:237:ASP:HB3	3:D:239:ASN:OD1	2.21	0.41
3:D:739:PRO:HD3	3:D:789:LEU:HD13	2.03	0.41
3:D:24:SER:CB	3:D:94:HIS:HB3	2.49	0.41
5:F:450:ALA:O	5:F:454:THR:HG23	2.20	0.41
2:C:720:LEU:HD13	2:C:1027:TYR:CE1	2.55	0.41
2:C:388:GLN:HG3	2:C:430:PHE:CD1	2.55	0.41
3:D:244:LEU:HG	3:D:252:PHE:HZ	1.84	0.41
1:B:182:ARG:HH12	3:D:488:GLU:HG2	1.85	0.41
2:C:197:LYS:HD2	2:C:198:THR:H	1.86	0.41
2:C:248:ILE:CG2	2:C:262:LEU:HD22	2.51	0.41
3:D:131:PHE:CZ	3:D:371:LYS:HB3	2.55	0.41
1:A:89:GLU:HG2	1:A:91:GLU:H	1.85	0.41
1:B:5:GLN:NE2	1:B:6:ARG:O	2.54	0.41
1:B:56:ILE:HG21	1:B:66:VAL:HG21	2.03	0.41
2:C:61:PHE:HE2	2:C:159:MET:HE3	1.86	0.41
2:C:611:MET:CE	2:C:890:GLY:HA2	2.51	0.41
3:D:1011:THR:HG22	3:D:1012:MET:N	2.36	0.41
3:D:1034:LEU:HD11	3:D:1137:GLU:CG	2.51	0.41
5:F:233:LYS:HG2	5:F:237:LYS:HE3	2.03	0.41
2:C:728:GLY:HA3	3:D:721:PHE:CD2	2.57	0.41
3:D:320:ILE:HG12	3:D:321:PRO:HD2	2.02	0.41
3:D:886:VAL:HA	3:D:974:VAL:O	2.21	0.41
5:F:323:GLU:HG2	5:F:358:ALA:HB3	2.03	0.41
1:B:148:PRO:HG3	3:D:626:VAL:HG21	2.03	0.40
2:C:484:CYS:HB2	2:C:588:SER:HB3	2.02	0.40
3:D:557:ILE:HD13	4:E:53:LEU:HG	2.03	0.40
5:F:325:ASN:O	5:F:329:ILE:HG13	2.20	0.40
1:B:96:TYR:HB2	1:B:98:ARG:HH12	1.87	0.40
2:C:760:ARG:CB	2:C:865:VAL:HG22	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1054:ARG:HD3	3:D:1065:THR:HB	2.03	0.40
3:D:203:ARG:HA	3:D:203:ARG:HD2	1.92	0.40
3:D:297:LYS:HB2	3:D:297:LYS:HE2	1.86	0.40
3:D:81:GLU:HG2	3:D:83:THR:HG23	2.02	0.40
2:C:1106:ILE:HG13	2:C:1112:ILE:CD1	2.41	0.40
3:D:793:TYR:HD1	3:D:800:ILE:HG12	1.86	0.40
4:E:63:GLN:O	4:E:66:ASP:N	2.54	0.40
5:F:477:LEU:HB3	5:F:492:ILE:HG23	2.04	0.40
5:F:515:ARG:HG3	5:F:519:ARG:HG3	2.04	0.40
1:B:34:LEU:O	1:B:38:LEU:HB2	2.20	0.40
2:C:1106:ILE:HG21	3:D:454:PRO:HB2	2.03	0.40
1:A:54:ILE:HG22	1:A:138:LEU:HD23	2.02	0.40
3:D:463:LEU:HD12	3:D:486:VAL:CG2	2.52	0.40
3:D:965:VAL:HG22	3:D:974:VAL:HG11	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	221/347 (64%)	203 (92%)	18 (8%)	0	100	100
1	B	228/347 (66%)	214 (94%)	14 (6%)	0	100	100
2	C	1116/1178 (95%)	1036 (93%)	76 (7%)	4 (0%)	38	77
3	D	1266/1316 (96%)	1196 (94%)	68 (5%)	2 (0%)	51	85
4	E	81/110 (74%)	76 (94%)	5 (6%)	0	100	100
5	F	287/528 (54%)	276 (96%)	11 (4%)	0	100	100
All	All	3199/3826 (84%)	3001 (94%)	192 (6%)	6 (0%)	54	85

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	D	835	PRO
2	C	82	PRO
2	C	831	GLU
3	D	394	PRO
2	C	1048	PRO
2	C	206	PRO

### 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	192/297 (65%)	190 (99%)	2 (1%)	80	91
1	B	197/297 (66%)	194 (98%)	3 (2%)	70	88
2	C	947/998 (95%)	926 (98%)	21 (2%)	57	83
3	D	1058/1095 (97%)	1032 (98%)	26 (2%)	53	81
4	E	70/90 (78%)	69 (99%)	1 (1%)	71	89
5	F	249/427 (58%)	240 (96%)	9 (4%)	40	74
All	All	2713/3204 (85%)	2651 (98%)	62 (2%)	59	82

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	146	TYR
1	A	168	TYR
1	B	129	ASN
1	B	166	SER
1	B	169	SER
2	C	83	VAL
2	C	107	PHE
2	C	373	PHE
2	C	518	LYS
2	C	672	MET
2	C	704	ASP
2	C	731	TYR
2	C	733	ASP

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Mol	Chain	Res	Type
2	C	749	SER
2	C	772	ASP
2	C	786	GLU
2	C	797	ARG
2	C	825	PHE
2	C	915	ILE
2	C	974	THR
2	C	1003	ASP
2	C	1036	LEU
2	C	1037	VAL
2	C	1038	ASP
2	C	1042	HIS
2	C	1111	ASN
3	D	60	CYS
3	D	70	PHE
3	D	84	ARG
3	D	173	ARG
3	D	221	ASP
3	D	275	GLU
3	D	282	ARG
3	D	285	LYS
3	D	345	ARG
3	D	387	ARG
3	D	420	LYS
3	D	428	SER
3	D	441	CYS
3	D	469	ILE
3	D	581	MET
3	D	663	MET
3	D	687	GLN
3	D	714	ASP
3	D	721	PHE
3	D	876	ARG
3	D	921	TYR
3	D	964	SER
3	D	1123	ARG
3	D	1169	ASP
3	D	1175	PHE
3	D	1243	ASP
4	E	56	TYR
5	F	252	ARG
5	F	285	CYS

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Mol	Chain	Res	Type
5	F	294	HIS
5	F	336	ASP
5	F	350	TRP
5	F	392	ARG
5	F	437	ASP
5	F	467	LEU
5	F	526	TYR

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

Mol	Chain	Res	Type
1	B	36	ASN
1	B	129	ASN
2	C	141	ASN
2	C	232	GLN
2	C	247	GLN
2	C	1035	HIS
2	C	1062	GLN
3	D	1251	ASN
5	F	299	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, 3 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
8	FI8	D	1904	-	75,75,75	1.19	6 (8%)	89,109,109	1.60	13 (14%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	FI8	D	1904	-	-	0/75/118/118	0/3/4/4

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	D	1904	FI8	C44-C45	-2.95	1.46	1.53
8	D	1904	FI8	C1-C3	2.12	1.53	1.50
8	D	1904	FI8	C4-C3	2.81	1.44	1.36
8	D	1904	FI8	C5-C4	2.96	1.52	1.43
8	D	1904	FI8	C14-C15	3.50	1.53	1.46
8	D	1904	FI8	O17-C49	4.21	1.44	1.34

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	D	1904	FI8	C11-C10-C9	-4.38	116.40	127.66
8	D	1904	FI8	C7-C6-C5	-3.68	120.31	125.40
8	D	1904	FI8	C1-C3-C4	-3.38	121.23	125.10
8	D	1904	FI8	C37-C38-C39	-3.05	119.96	122.55
8	D	1904	FI8	C31-C30-C29	-3.02	108.71	113.36
8	D	1904	FI8	O2-C2-C3	-2.48	120.26	124.20
8	D	1904	FI8	C27-C28-C29	2.02	113.23	109.01
8	D	1904	FI8	C29-O10-C33	2.19	120.82	117.24
8	D	1904	FI8	C36-C37-C38	2.44	120.04	117.71
8	D	1904	FI8	O10-C33-C34	2.46	119.76	113.44
8	D	1904	FI8	O14-C46-C45	3.91	112.38	108.10
8	D	1904	FI8	O17-C49-C50	4.11	119.57	110.95
8	D	1904	FI8	O1-C2-C3	5.42	119.22	111.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	D	1904	FI8	7	0

## 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.