



Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Feb 19, 2018 – 08:02 pm GMT

PDB ID : 6B5B
EMDB ID: : EMD-7055
Title : Cryo-EM structure of the NAIP5-NLRC4-flagellin inflammasome
Authors : Tenthorey, J.L.; Haloupek, N.; Lopez-Blanco, J.R.; Grob, P.; Adamson, E.; Hartenian, E.; Lind, N.A.; Bourgeois, N.M.; Chacon, P.; Nogales, E.; Vance, R.E.
Deposited on : 2017-09-29
Resolution : 5.20 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : trunk30686

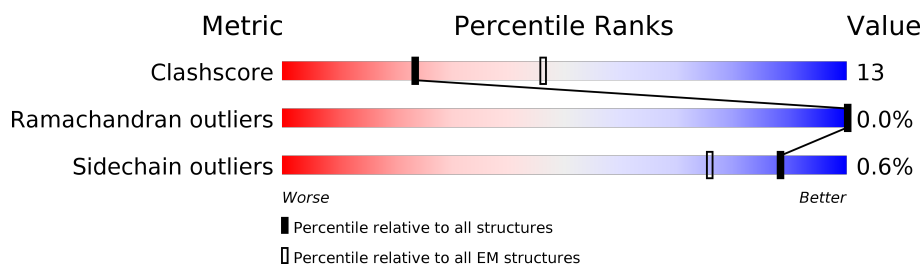
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 5.20 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	136279	1886
Ramachandran outliers	132675	1663
Sidechain outliers	132484	1531

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

Mol	Chain	Length	Quality of chain
1	A	1403	
2	B	1024	
2	C	1024	
3	F	566	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 24555 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 Baculoviral IAP repeat-containing protein 1e.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1199	Total	C	N	O	S	0	0
			9583	6128	1608	1790	57		

- Molecule 2 is a protein called NLR family CARD domain-containing protein 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	903	Total	C	N	O	S	0	0
			7237	4622	1224	1351	40		
2	C	903	Total	C	N	O	S	0	0
			7237	4622	1224	1351	40		

- Molecule 3 is a protein called Flagellin.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	F	68	Total	C	N	O	S	0	0
			498	302	93	98	5		

There are 92 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	-90	MET	-	initiating methionine	UNP G8U UW9
F	-89	GLU	-	expression tag	UNP G8U UW9
F	-88	GLN	-	expression tag	UNP G8U UW9
F	-87	LYS	-	expression tag	UNP G8U UW9
F	-86	LEU	-	expression tag	UNP G8U UW9
F	-85	ILE	-	expression tag	UNP G8U UW9
F	-84	SER	-	expression tag	UNP G8U UW9
F	-83	GLU	-	expression tag	UNP G8U UW9
F	-82	GLU	-	expression tag	UNP G8U UW9
F	-81	ASP	-	expression tag	UNP G8U UW9
F	-80	LEU	-	expression tag	UNP G8U UW9
F	-79	ASN	-	expression tag	UNP G8U UW9
F	-78	GLU	-	expression tag	UNP G8U UW9

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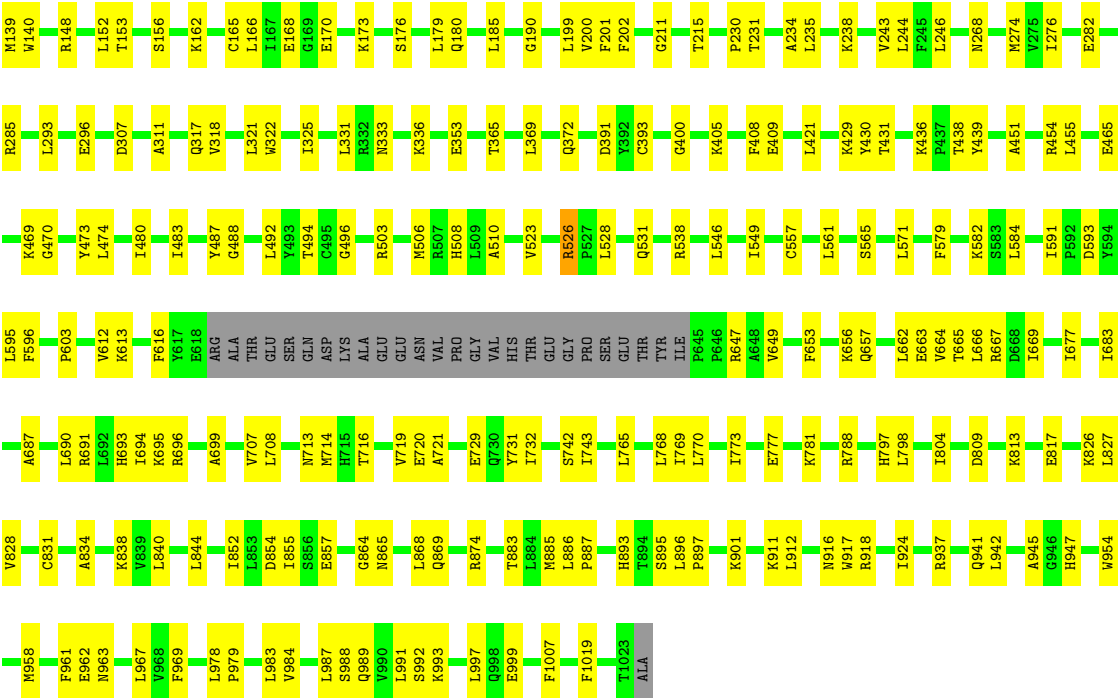
Chain	Residue	Modelled	Actual	Comment	Reference
F	-77	MET	-	expression tag	UNP G8U UW9
F	-76	GLU	-	expression tag	UNP G8U UW9
F	-75	GLN	-	expression tag	UNP G8U UW9
F	-74	LYS	-	expression tag	UNP G8U UW9
F	-73	LEU	-	expression tag	UNP G8U UW9
F	-72	ILE	-	expression tag	UNP G8U UW9
F	-71	SER	-	expression tag	UNP G8U UW9
F	-70	GLU	-	expression tag	UNP G8U UW9
F	-69	GLU	-	expression tag	UNP G8U UW9
F	-68	ASP	-	expression tag	UNP G8U UW9
F	-67	LEU	-	expression tag	UNP G8U UW9
F	-66	ASN	-	expression tag	UNP G8U UW9
F	-65	GLU	-	expression tag	UNP G8U UW9
F	-64	MET	-	expression tag	UNP G8U UW9
F	-63	GLU	-	expression tag	UNP G8U UW9
F	-62	GLN	-	expression tag	UNP G8U UW9
F	-61	LYS	-	expression tag	UNP G8U UW9
F	-60	LEU	-	expression tag	UNP G8U UW9
F	-59	ILE	-	expression tag	UNP G8U UW9
F	-58	SER	-	expression tag	UNP G8U UW9
F	-57	GLU	-	expression tag	UNP G8U UW9
F	-56	GLU	-	expression tag	UNP G8U UW9
F	-55	ASP	-	expression tag	UNP G8U UW9
F	-54	LEU	-	expression tag	UNP G8U UW9
F	-53	ASN	-	expression tag	UNP G8U UW9
F	-52	GLU	-	expression tag	UNP G8U UW9
F	-51	MET	-	expression tag	UNP G8U UW9
F	-50	GLU	-	expression tag	UNP G8U UW9
F	-49	GLN	-	expression tag	UNP G8U UW9
F	-48	LYS	-	expression tag	UNP G8U UW9
F	-47	LEU	-	expression tag	UNP G8U UW9
F	-46	ILE	-	expression tag	UNP G8U UW9
F	-45	SER	-	expression tag	UNP G8U UW9
F	-44	GLU	-	expression tag	UNP G8U UW9
F	-43	GLU	-	expression tag	UNP G8U UW9
F	-42	ASP	-	expression tag	UNP G8U UW9
F	-41	LEU	-	expression tag	UNP G8U UW9
F	-40	ASN	-	expression tag	UNP G8U UW9
F	-39	GLU	-	expression tag	UNP G8U UW9
F	-38	MET	-	expression tag	UNP G8U UW9
F	-37	GLU	-	expression tag	UNP G8U UW9
F	-36	GLN	-	expression tag	UNP G8U UW9

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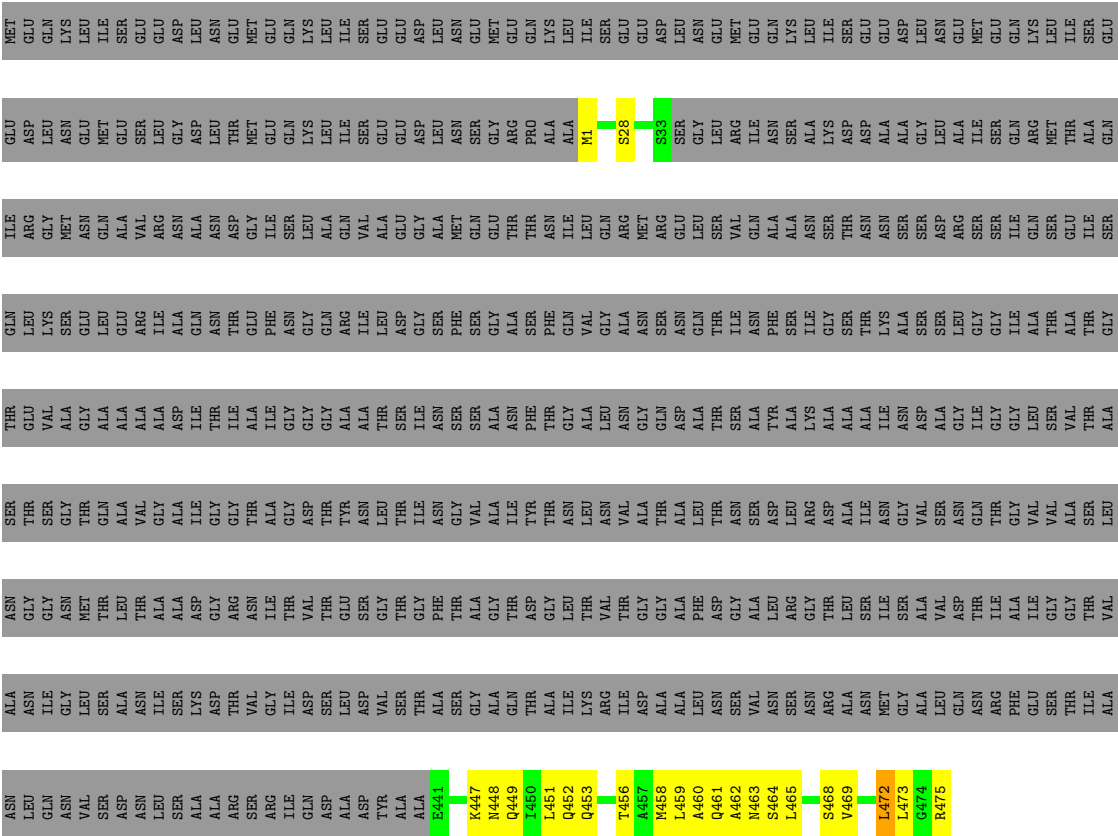
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Chain	Residue	Modelled	Actual	Comment	Reference
F	-35	LYS	-	expression tag	UNP G8U UW9
F	-34	LEU	-	expression tag	UNP G8U UW9
F	-33	ILE	-	expression tag	UNP G8U UW9
F	-32	SER	-	expression tag	UNP G8U UW9
F	-31	GLU	-	expression tag	UNP G8U UW9
F	-30	GLU	-	expression tag	UNP G8U UW9
F	-29	ASP	-	expression tag	UNP G8U UW9
F	-28	LEU	-	expression tag	UNP G8U UW9
F	-27	ASN	-	expression tag	UNP G8U UW9
F	-26	GLU	-	expression tag	UNP G8U UW9
F	-25	MET	-	expression tag	UNP G8U UW9
F	-24	GLU	-	expression tag	UNP G8U UW9
F	-23	SER	-	expression tag	UNP G8U UW9
F	-22	LEU	-	expression tag	UNP G8U UW9
F	-21	GLY	-	expression tag	UNP G8U UW9
F	-20	ASP	-	expression tag	UNP G8U UW9
F	-19	LEU	-	expression tag	UNP G8U UW9
F	-18	THR	-	expression tag	UNP G8U UW9
F	-17	MET	-	expression tag	UNP G8U UW9
F	-16	GLU	-	expression tag	UNP G8U UW9
F	-15	GLN	-	expression tag	UNP G8U UW9
F	-14	LYS	-	expression tag	UNP G8U UW9
F	-13	LEU	-	expression tag	UNP G8U UW9
F	-12	ILE	-	expression tag	UNP G8U UW9
F	-11	SER	-	expression tag	UNP G8U UW9
F	-10	GLU	-	expression tag	UNP G8U UW9
F	-9	GLU	-	expression tag	UNP G8U UW9
F	-8	ASP	-	expression tag	UNP G8U UW9
F	-7	LEU	-	expression tag	UNP G8U UW9
F	-6	ASN	-	expression tag	UNP G8U UW9
F	-5	SER	-	expression tag	UNP G8U UW9
F	-4	GLY	-	expression tag	UNP G8U UW9
F	-3	ARG	-	expression tag	UNP G8U UW9
F	-2	PRO	-	expression tag	UNP G8U UW9
F	-1	ALA	-	expression tag	UNP G8U UW9
F	0	ALA	-	expression tag	UNP G8U UW9
F	1	MET	-	expression tag	UNP G8U UW9





● Molecule 3: Flagellin



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	252214	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 ($e^-/\text{\AA}^2$)	45.8	Depositor
Minimum defocus (nm)	1800	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	22500	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

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	0.31	0/9782	0.63	11/13218 (0.1%)
2	B	0.27	0/7376	0.50	0/9957
2	C	0.27	0/7376	0.50	0/9957
3	F	0.26	0/497	0.63	1/668 (0.1%)
All	All	0.29	0/25031	0.55	12/33800 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	9

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	822	LEU	CA-CB-CG	6.98	131.36	115.30
1	A	1241	LEU	CA-CB-CG	6.70	130.70	115.30
3	F	472	LEU	CA-CB-CG	6.65	130.59	115.30
1	A	719	ASP	CB-CG-OD1	6.64	124.28	118.30
1	A	1356	LEU	CA-CB-CG	6.52	130.29	115.30
1	A	512	ASP	CB-CG-OD1	6.16	123.85	118.30
1	A	1074	LEU	CA-CB-CG	6.10	129.34	115.30
1	A	912	LEU	CA-CB-CG	5.92	128.91	115.30
1	A	1082	LEU	CA-CB-CG	5.73	128.47	115.30
1	A	1107	LEU	CA-CB-CG	5.67	128.33	115.30
1	A	1326	LEU	CA-CB-CG	5.50	127.94	115.30
1	A	193	ASP	CB-CG-OD1	5.08	122.88	118.30

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1107	LEU	Peptide
1	A	1163	LYS	Peptide
1	A	1243	PRO	Peptide
1	A	1248	ILE	Peptide
1	A	1331	ASN	Peptide
1	A	321	CYS	Peptide
1	A	447	GLN	Peptide
1	A	685	PRO	Peptide
1	A	831	TYR	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	9583	0	9567	310	0
2	B	7237	0	7285	165	0
2	C	7237	0	7285	164	0
3	F	498	0	525	18	0
All	All	24555	0	24662	648	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 13.

All (648) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:313:VAL:O	1:A:321:CYS:HA	1.10	1.25
1:A:313:VAL:O	1:A:321:CYS:CA	2.01	1.07
1:A:785:ALA:O	1:A:789:PHE:HB2	1.58	1.03
1:A:1252:ALA:O	1:A:1256:VAL:HB	1.62	0.98
3:F:459:LEU:O	3:F:463:ASN:HB2	1.64	0.97
2:B:104:ASN:O	2:B:108:LEU:HB2	1.66	0.95
2:C:104:ASN:O	2:C:108:LEU:HB2	1.66	0.95
1:A:786:ILE:O	1:A:790:ASN:HB2	1.64	0.95
1:A:1006:VAL:O	1:A:1035:PHE:HB2	1.67	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1032:PHE:HB3	1:A:1057:LYS:O	1.68	0.93
2:B:616:PHE:HB2	2:B:665:THR:O	1.69	0.93
1:A:550:LEU:O	1:A:579:ILE:HA	1.69	0.92
1:A:1083:GLU:HA	1:A:1107:LEU:O	1.70	0.91
2:C:616:PHE:HB2	2:C:665:THR:O	1.69	0.91
1:A:1160:PHE:O	1:A:1187:GLU:HB3	1.72	0.90
1:A:908:PRO:O	1:A:912:LEU:HB2	1.72	0.90
1:A:1094:LEU:O	1:A:1098:LEU:HB2	1.72	0.90
1:A:1310:TYR:O	1:A:1314:PHE:HB2	1.72	0.90
1:A:1313:PHE:O	1:A:1317:LEU:HB2	1.70	0.90
1:A:1034:LEU:O	1:A:1061:SER:HB3	1.72	0.88
1:A:698:LEU:O	1:A:702:PHE:HB2	1.72	0.88
2:C:840:LEU:O	2:C:844:LEU:HB2	1.75	0.87
1:A:195:VAL:O	1:A:203:SER:HA	1.75	0.86
1:A:1223:THR:O	1:A:1227:PHE:HB2	1.74	0.86
1:A:1314:PHE:O	1:A:1318:ASP:HB2	1.75	0.86
1:A:789:PHE:O	1:A:793:LEU:HB2	1.76	0.85
2:B:840:LEU:O	2:B:844:LEU:HB2	1.75	0.85
1:A:1253:LYS:O	1:A:1257:ARG:HB2	1.76	0.85
2:B:584:LEU:O	2:B:612:VAL:HA	1.77	0.85
1:A:988:GLY:O	1:A:992:LEU:HB2	1.77	0.84
2:C:584:LEU:O	2:C:612:VAL:HA	1.77	0.84
2:C:408:PHE:HB2	2:C:439:TYR:O	1.77	0.84
2:C:666:LEU:O	2:C:695:LYS:HB3	1.78	0.83
2:B:408:PHE:HB2	2:B:439:TYR:O	1.77	0.83
2:B:666:LEU:O	2:B:695:LYS:HB3	1.78	0.83
2:B:234:ALA:O	2:B:238:LYS:HB2	1.79	0.83
1:A:1070:GLN:O	1:A:1074:LEU:HB2	1.79	0.82
2:B:139:MET:HB2	2:B:152:LEU:O	1.79	0.81
2:C:139:MET:HB2	2:C:152:LEU:O	1.79	0.81
1:A:516:ALA:O	1:A:520:CYS:HB2	1.80	0.81
2:C:234:ALA:O	2:C:238:LYS:HB2	1.79	0.81
1:A:501:VAL:HA	1:A:547:LEU:O	1.81	0.81
3:F:461:GLN:O	3:F:465:LEU:HB2	1.83	0.79
2:C:98:LEU:O	2:C:102:ALA:HB3	1.84	0.78
2:B:98:LEU:O	2:B:102:ALA:HB3	1.84	0.78
2:C:987:LEU:O	2:C:991:LEU:HB2	1.84	0.78
2:B:987:LEU:O	2:B:991:LEU:HB2	1.84	0.77
1:A:1147:LEU:O	1:A:1151:ILE:HB	1.83	0.77
3:F:456:THR:O	3:F:460:ALA:HB2	1.85	0.76
3:F:448:ASN:O	3:F:452:GLN:HB2	1.87	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1251:VAL:O	1:A:1255:ILE:HB	1.86	0.75
2:B:941:GLN:HA	2:B:969:PHE:O	1.88	0.74
2:C:834:ALA:O	2:C:838:LYS:HB2	1.88	0.74
2:C:166:LEU:HB2	2:C:293:LEU:O	1.88	0.73
1:A:38:GLN:O	1:A:42:GLU:HB3	1.88	0.72
2:C:199:LEU:O	2:C:244:LEU:HB3	1.89	0.72
2:C:365:THR:O	2:C:369:LEU:HB2	1.89	0.72
2:C:941:GLN:HA	2:C:969:PHE:O	1.88	0.72
2:C:99:ASN:O	2:C:103:GLN:HB2	1.89	0.72
2:B:834:ALA:O	2:B:838:LYS:HB2	1.88	0.72
2:B:166:LEU:HB2	2:B:293:LEU:O	1.88	0.72
2:B:365:THR:O	2:B:369:LEU:HB2	1.89	0.72
2:B:99:ASN:O	2:B:103:GLN:HB2	1.90	0.71
1:A:1224:SER:O	1:A:1228:ALA:HB2	1.90	0.71
1:A:548:PHE:O	1:A:578:LEU:HB2	1.91	0.71
2:B:199:LEU:O	2:B:244:LEU:HB3	1.89	0.71
2:C:912:LEU:O	2:C:942:LEU:HA	1.91	0.71
1:A:608:VAL:O	1:A:612:ARG:HB2	1.91	0.71
1:A:34:VAL:O	1:A:38:GLN:HB2	1.90	0.71
1:A:1374:ILE:O	1:A:1378:LYS:HB2	1.91	0.70
1:A:1170:CYS:O	1:A:1174:MET:HB2	1.92	0.70
2:B:912:LEU:O	2:B:942:LEU:HA	1.91	0.69
3:F:447:LYS:O	3:F:451:LEU:HB3	1.91	0.69
2:B:243:VAL:O	2:B:274:MET:HB2	1.93	0.69
2:B:408:PHE:O	2:B:439:TYR:HB2	1.93	0.68
1:A:918:LYS:HA	1:A:1003:GLU:HB3	1.75	0.68
1:A:1148:VAL:O	1:A:1152:GLN:HB2	1.94	0.68
2:C:243:VAL:O	2:C:274:MET:HB2	1.93	0.68
2:C:408:PHE:O	2:C:439:TYR:HB2	1.93	0.67
1:A:665:VAL:O	1:A:669:GLN:HB2	1.94	0.67
2:C:690:LEU:HB3	2:C:714:MET:HA	1.77	0.67
2:B:690:LEU:HB3	2:B:714:MET:HA	1.77	0.67
1:A:187:VAL:HB	1:A:196:GLN:O	1.94	0.67
1:A:1157:LEU:HD12	1:A:1182:LYS:H	1.60	0.67
1:A:95:VAL:O	1:A:103:ILE:HA	1.93	0.67
1:A:441:ILE:HB	1:A:598:GLU:HB3	1.76	0.66
3:F:449:GLN:O	3:F:453:GLN:HB2	1.95	0.66
2:B:230:PRO:O	2:B:234:ALA:HB3	1.96	0.66
2:C:916:ASN:HD22	2:C:918:ARG:HH12	1.44	0.66
2:C:230:PRO:O	2:C:234:ALA:HB3	1.96	0.66
1:A:1329:CYS:SG	1:A:1330:ARG:N	2.69	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:202:PHE:HA	2:C:246:LEU:O	1.96	0.66
2:B:694:ILE:O	2:B:720:GLU:HB3	1.96	0.66
2:C:694:ILE:O	2:C:720:GLU:HB3	1.96	0.66
1:A:1212:ASN:HA	1:A:1241:LEU:HB2	1.79	0.65
2:B:916:ASN:HD22	2:B:918:ARG:HH12	1.44	0.65
1:A:478:THR:O	1:A:482:ARG:HB2	1.96	0.65
1:A:517:ASN:O	1:A:521:ALA:HB2	1.96	0.65
2:B:958:MET:O	2:B:962:GLU:HB2	1.97	0.65
1:A:1296:ASN:HA	1:A:1325:GLU:HB3	1.78	0.65
1:A:399:GLU:O	1:A:403:LEU:HB2	1.97	0.65
2:B:202:PHE:HA	2:B:246:LEU:O	1.96	0.65
1:A:503:TYR:HA	1:A:549:LEU:HB2	1.79	0.64
1:A:97:CYS:SG	1:A:98:PHE:N	2.70	0.64
2:C:958:MET:O	2:C:962:GLU:HB2	1.97	0.64
1:A:483:ILE:O	1:A:487:TRP:HB2	1.98	0.64
2:B:798:LEU:HB2	2:B:827:LEU:HG	1.80	0.64
2:C:798:LEU:HB2	2:C:827:LEU:HG	1.80	0.64
1:A:1093:GLN:O	1:A:1097:ASN:HB2	1.97	0.64
1:A:1106:GLU:HG3	1:A:1133:LYS:HD3	1.79	0.64
1:A:894:LEU:O	1:A:917:LEU:HA	1.98	0.64
1:A:1286:ALA:HB1	1:A:1320:LEU:HD11	1.80	0.63
1:A:39:GLU:O	1:A:43:HIS:HB3	1.97	0.63
2:B:465:GLU:O	2:B:469:LYS:HB2	1.99	0.63
2:C:465:GLU:O	2:C:469:LYS:HB2	1.99	0.63
2:B:201:PHE:O	2:B:246:LEU:HB2	1.99	0.62
1:A:772:GLY:O	1:A:776:LEU:HB2	1.98	0.62
1:A:770:ASP:O	1:A:774:TYR:HB2	1.99	0.62
2:C:201:PHE:O	2:C:246:LEU:HB2	1.99	0.62
1:A:88:HIS:HB2	1:A:95:VAL:HG12	1.81	0.62
1:A:1084:VAL:O	1:A:1108:CYS:O	2.18	0.62
2:C:116:ASN:ND2	2:C:128:PHE:O	2.33	0.62
1:A:440:ILE:O	1:A:452:ALA:HA	1.99	0.62
1:A:1002:LEU:O	1:A:1031:GLU:HB3	1.99	0.62
1:A:398:GLN:O	1:A:402:SER:HB3	2.00	0.62
2:B:769:ILE:HA	2:B:797:HIS:HB2	1.82	0.61
1:A:1198:PHE:O	1:A:1202:LEU:HB2	2.00	0.61
2:C:200:VAL:HG22	2:C:244:LEU:HD23	1.82	0.61
2:C:430:TYR:HB2	2:C:438:THR:HB	1.82	0.61
2:C:769:ILE:HA	2:C:797:HIS:HB2	1.82	0.61
2:B:985:ARG:HD3	2:C:656:LYS:HG2	1.83	0.61
1:A:1080:GLN:HE21	1:A:1105:LYS:HD2	1.66	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1235:ARG:HA	1:A:1262:LEU:HD22	1.83	0.61
2:B:864:GLY:O	2:B:868:LEU:HB2	2.01	0.61
1:A:718:VAL:O	1:A:723:LYS:NZ	2.34	0.60
2:B:116:ASN:ND2	2:B:128:PHE:O	2.33	0.60
1:A:337:LYS:HD2	1:A:361:GLN:HB2	1.83	0.60
2:C:997:LEU:HB3	2:C:1019:PHE:HB3	1.82	0.60
1:A:1094:LEU:O	1:A:1098:LEU:CB	2.49	0.60
3:F:458:MET:O	3:F:462:ALA:HB3	2.02	0.60
1:A:505:SER:HA	1:A:551:ASP:HB3	1.83	0.60
2:C:854:ASP:HA	2:C:885:MET:HB2	1.84	0.60
1:A:1318:ASP:O	1:A:1352:ARG:NH1	2.35	0.60
2:C:864:GLY:O	2:C:868:LEU:HB2	2.00	0.60
1:A:1084:VAL:O	1:A:1108:CYS:C	2.40	0.60
2:B:430:TYR:HB2	2:B:438:THR:HB	1.82	0.60
2:B:997:LEU:HB3	2:B:1019:PHE:HB3	1.82	0.60
2:B:200:VAL:HG22	2:B:244:LEU:HD23	1.82	0.60
3:F:468:SER:O	3:F:472:LEU:HB3	2.02	0.60
1:A:506:LEU:HD13	1:A:556:LEU:HD22	1.84	0.59
1:A:825:MET:O	1:A:831:TYR:OH	2.19	0.59
2:B:719:VAL:HB	2:B:743:ILE:HA	1.84	0.59
3:F:468:SER:O	3:F:472:LEU:CB	2.49	0.59
1:A:1004:VAL:HB	1:A:1032:PHE:HA	1.84	0.59
2:B:231:THR:O	2:B:235:LEU:HB2	2.03	0.59
1:A:1312:ASN:O	1:A:1316:ALA:HB3	2.03	0.59
2:C:719:VAL:HB	2:C:743:ILE:HA	1.84	0.58
1:A:1148:VAL:O	1:A:1152:GLN:CB	2.50	0.58
1:A:1308:GLU:OE1	1:A:1311:ARG:NH2	2.35	0.58
1:A:499:GLN:HG2	1:A:500:LEU:HG	1.85	0.58
2:C:231:THR:O	2:C:235:LEU:HB2	2.03	0.58
2:C:244:LEU:HA	2:C:274:MET:O	2.03	0.58
1:A:1085:SER:HB2	1:A:1110:ARG:HD2	1.83	0.58
2:B:854:ASP:HA	2:B:885:MET:HB2	1.84	0.58
1:A:33:GLN:O	1:A:37:SER:HB3	2.03	0.58
2:B:144:HIS:HD2	2:C:127:ILE:HD13	1.68	0.58
1:A:971:ILE:O	1:A:975:GLU:HB2	2.03	0.58
2:B:579:PHE:HA	2:B:582:LYS:HD2	1.86	0.58
2:C:770:LEU:HB2	2:C:797:HIS:O	2.04	0.58
2:C:579:PHE:HA	2:C:582:LYS:HD2	1.86	0.58
2:B:244:LEU:HA	2:B:274:MET:O	2.03	0.58
2:B:667:ARG:HG2	2:B:695:LYS:HD2	1.86	0.58
2:B:770:LEU:HB2	2:B:797:HIS:O	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:834:LEU:O	1:A:838:THR:N	2.37	0.57
1:A:708:PHE:HB2	1:A:741:TYR:HB2	1.86	0.57
1:A:1113:GLY:HA2	1:A:1139:SER:H	1.69	0.57
1:A:1034:LEU:HB2	1:A:1059:SER:O	2.04	0.57
2:B:989:GLN:NE2	2:C:656:LYS:O	2.37	0.57
2:C:613:LYS:HA	2:C:663:GLU:HB3	1.86	0.57
1:A:651:ASP:HA	1:A:655:ASN:HB2	1.86	0.57
1:A:1382:PRO:O	1:A:1385:LYS:NZ	2.38	0.57
1:A:695:GLN:HG3	1:A:715:GLU:HB3	1.86	0.57
2:C:667:ARG:HG2	2:C:695:LYS:HD2	1.86	0.57
1:A:278:GLU:HA	1:A:281:ARG:HB2	1.86	0.57
1:A:116:ARG:HA	1:A:119:LYS:HG2	1.86	0.56
1:A:1310:TYR:O	1:A:1314:PHE:CB	2.51	0.56
2:B:911:LYS:HG3	2:B:941:GLN:HG2	1.87	0.56
1:A:548:PHE:HB2	1:A:577:LEU:HA	1.87	0.56
1:A:790:ASN:O	1:A:794:TYR:CB	2.52	0.56
2:B:199:LEU:HB2	2:B:243:VAL:HA	1.87	0.56
2:C:451:ALA:O	2:C:455:LEU:HB2	2.06	0.56
1:A:1135:SER:HA	1:A:1161:HIS:O	2.04	0.56
2:C:911:LYS:HG3	2:C:941:GLN:HG2	1.86	0.56
1:A:501:VAL:HG12	1:A:547:LEU:HB3	1.87	0.56
1:A:665:VAL:O	1:A:669:GLN:CB	2.54	0.56
2:B:451:ALA:O	2:B:455:LEU:HB2	2.06	0.56
1:A:1238:GLU:HA	1:A:1265:LEU:HA	1.88	0.56
1:A:1309:GLY:O	1:A:1313:PHE:HB2	2.05	0.56
2:C:199:LEU:HB2	2:C:243:VAL:HA	1.87	0.56
2:B:613:LYS:HA	2:B:663:GLU:HB3	1.86	0.56
1:A:782:PRO:HB3	1:A:815:LEU:HB3	1.87	0.56
2:B:168:GLU:O	2:B:296:GLU:HA	2.06	0.56
2:C:168:GLU:O	2:C:296:GLU:HA	2.06	0.56
2:C:179:LEU:HD22	2:C:246:LEU:HD22	1.88	0.56
1:A:465:VAL:HG23	1:A:577:LEU:HD22	1.88	0.55
1:A:834:LEU:HD23	1:A:837:GLN:HG2	1.88	0.55
1:A:1157:LEU:HB2	1:A:1182:LYS:HB2	1.88	0.55
1:A:757:LEU:O	1:A:761:LEU:HB2	2.07	0.55
2:B:649:VAL:O	2:B:653:PHE:HB2	2.07	0.55
2:B:687:ALA:O	2:B:713:ASN:ND2	2.39	0.55
1:A:283:ASP:OD1	1:A:286:LYS:NZ	2.37	0.55
2:C:788:ARG:NH1	2:C:817:GLU:OE2	2.40	0.55
1:A:1033:ARG:HA	1:A:1059:SER:HB3	1.88	0.55
1:A:1307:GLU:OE1	1:A:1311:ARG:NH1	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:649:VAL:O	2:C:653:PHE:HB2	2.07	0.55
2:B:179:LEU:HD22	2:B:246:LEU:HD22	1.88	0.55
2:B:391:ASP:OD1	2:B:454:ARG:NH1	2.39	0.55
1:A:1109:VAL:O	1:A:1137:ARG:HB3	2.07	0.55
1:A:1297:LEU:O	1:A:1325:GLU:O	2.24	0.55
2:B:826:LYS:HA	2:B:854:ASP:HB3	1.89	0.54
2:C:826:LYS:HA	2:C:854:ASP:HB3	1.89	0.54
2:C:864:GLY:O	2:C:868:LEU:CB	2.56	0.54
1:A:1003:GLU:HA	1:A:1031:GLU:HB3	1.88	0.54
3:F:449:GLN:O	3:F:453:GLN:CB	2.55	0.54
3:F:459:LEU:HA	3:F:462:ALA:HB3	1.89	0.54
1:A:38:GLN:O	1:A:42:GLU:CB	2.54	0.54
1:A:987:GLU:O	1:A:991:LYS:HB3	2.07	0.54
2:B:788:ARG:NH1	2:B:817:GLU:OE2	2.40	0.54
2:B:864:GLY:O	2:B:868:LEU:CB	2.56	0.54
2:C:687:ALA:O	2:C:713:ASN:ND2	2.39	0.54
2:B:603:PRO:HB2	2:B:657:GLN:HG3	1.90	0.54
2:B:865:ASN:OD1	2:B:895:SER:OG	2.26	0.54
1:A:550:LEU:HB2	1:A:578:LEU:O	2.08	0.54
1:A:608:VAL:O	1:A:612:ARG:CB	2.55	0.54
1:A:284:MET:HG3	1:A:306:TYR:HB3	1.89	0.54
1:A:1040:PHE:O	1:A:1044:ILE:N	2.38	0.54
1:A:200:CYS:SG	1:A:201:GLY:N	2.81	0.53
2:B:365:THR:O	2:B:369:LEU:CB	2.56	0.53
1:A:1148:VAL:HG23	1:A:1176:VAL:HB	1.89	0.53
1:A:1227:PHE:O	1:A:1231:LEU:HB2	2.08	0.53
2:B:649:VAL:HG22	2:B:683:ILE:HD11	1.91	0.53
2:B:852:ILE:HA	2:B:883:THR:HB	1.91	0.53
2:C:391:ASP:OD1	2:C:454:ARG:NH1	2.39	0.53
1:A:735:GLN:HB2	2:B:126:ILE:HG12	1.90	0.53
2:C:603:PRO:HB2	2:C:657:GLN:HG3	1.90	0.53
1:A:1235:ARG:NH1	1:A:1236:ASN:OD1	2.42	0.53
1:A:1282:ILE:O	1:A:1286:ALA:CB	2.56	0.53
2:B:409:GLU:HB3	2:B:436:LYS:HE2	1.91	0.53
1:A:838:THR:HA	1:A:841:TRP:HD1	1.73	0.53
2:C:649:VAL:HG22	2:C:683:ILE:HD11	1.91	0.53
2:B:430:TYR:N	2:B:438:THR:O	2.42	0.53
1:A:1031:GLU:HG3	1:A:1057:LYS:HD3	1.92	0.52
1:A:763:SER:H	1:A:769:GLN:HE21	1.56	0.52
2:B:165:CYS:HA	2:B:293:LEU:HB3	1.91	0.52
2:B:528:LEU:O	2:B:531:GLN:NE2	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:865:ASN:OD1	2:C:895:SER:OG	2.26	0.52
1:A:1157:LEU:O	1:A:1184:ARG:NH1	2.42	0.52
1:A:1209:LYS:HA	1:A:1237:LEU:HA	1.89	0.52
1:A:1267:VAL:HG22	1:A:1296:ASN:HD22	1.74	0.52
2:C:409:GLU:HB3	2:C:436:LYS:HE2	1.91	0.52
1:A:601:GLU:HB2	1:A:642:PRO:HD3	1.92	0.52
1:A:1325:GLU:OE1	1:A:1358:ARG:NE	2.42	0.52
2:C:365:THR:O	2:C:369:LEU:CB	2.56	0.52
1:A:216:GLU:O	1:A:220:TRP:N	2.36	0.52
1:A:474:SER:OG	1:A:475:GLY:N	2.41	0.52
1:A:790:ASN:O	1:A:794:TYR:HB2	2.08	0.52
1:A:322:LEU:O	1:A:325:TRP:NE1	2.40	0.52
1:A:711:ASP:OD1	1:A:738:ARG:NE	2.41	0.52
2:C:528:LEU:O	2:C:531:GLN:NE2	2.42	0.52
2:C:664:VAL:O	2:C:693:HIS:HB3	2.10	0.52
1:A:1157:LEU:HD11	1:A:1180:CYS:HB3	1.90	0.52
2:B:317:GLN:O	2:B:321:LEU:HB3	2.10	0.52
1:A:1065:LEU:HD11	1:A:1091:PRO:HB3	1.91	0.51
2:C:480:ILE:HA	2:C:483:ILE:HD12	1.93	0.51
1:A:533:VAL:O	1:A:537:SER:N	2.43	0.51
2:C:317:GLN:O	2:C:321:LEU:HB3	2.10	0.51
1:A:1058:CYS:HB3	1:A:1082:LEU:HD13	1.93	0.51
2:C:165:CYS:HA	2:C:293:LEU:HB3	1.91	0.51
1:A:806:PRO:HA	1:A:809:VAL:HG12	1.92	0.51
2:B:98:LEU:O	2:B:102:ALA:CB	2.58	0.51
1:A:688:ALA:O	1:A:692:SER:CB	2.58	0.51
2:B:664:VAL:O	2:B:693:HIS:HB3	2.10	0.51
2:B:809:ASP:O	2:B:813:LYS:HB2	2.11	0.51
2:C:852:ILE:HA	2:C:883:THR:HB	1.91	0.51
1:A:517:ASN:O	1:A:521:ALA:CB	2.58	0.51
2:C:809:ASP:O	2:C:813:LYS:HB2	2.11	0.51
2:B:318:VAL:O	2:B:322:TRP:HB2	2.11	0.51
2:B:480:ILE:HA	2:B:483:ILE:HD12	1.93	0.51
2:C:430:TYR:N	2:C:438:THR:O	2.42	0.51
1:A:278:GLU:O	1:A:282:MET:HB2	2.11	0.51
1:A:416:PHE:O	1:A:481:LYS:NZ	2.43	0.51
1:A:88:HIS:ND1	1:A:94:GLY:O	2.43	0.51
2:C:318:VAL:O	2:C:322:TRP:HB2	2.11	0.51
1:A:1096:HIS:HA	1:A:1099:HIS:HD2	1.76	0.51
1:A:1096:HIS:NE2	1:A:1117:VAL:O	2.39	0.50
1:A:1224:SER:O	1:A:1228:ALA:CB	2.57	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:831:TYR:O	1:A:835:HIS:ND1	2.44	0.50
2:B:897:PRO:O	2:B:901:LYS:HB2	2.11	0.50
1:A:1374:ILE:O	1:A:1378:LYS:CB	2.58	0.50
1:A:987:GLU:O	1:A:991:LYS:CB	2.60	0.50
2:C:496:GLY:HA2	2:C:565:SER:HA	1.93	0.50
1:A:1017:LEU:HD23	1:A:1020:LEU:HD12	1.93	0.50
1:A:999:ILE:HG13	1:A:1026:ALA:HB1	1.93	0.50
1:A:1350:VAL:HG11	1:A:1359:LEU:HD22	1.94	0.50
1:A:476:LYS:HD3	1:A:580:ALA:HB1	1.94	0.50
2:C:99:ASN:O	2:C:103:GLN:CB	2.59	0.50
2:B:123:ASP:OD2	2:B:372:GLN:NE2	2.45	0.50
2:B:285:ARG:NH1	2:C:123:ASP:O	2.45	0.50
1:A:399:GLU:O	1:A:403:LEU:CB	2.60	0.50
1:A:438:VAL:HG21	1:A:599:ILE:HG23	1.93	0.50
2:B:483:ILE:HA	2:B:487:TYR:HB2	1.94	0.50
3:F:456:THR:O	3:F:460:ALA:CB	2.56	0.50
1:A:865:LEU:O	1:A:869:LEU:HB2	2.11	0.50
2:C:165:CYS:HB3	2:C:276:ILE:HG12	1.93	0.50
2:C:465:GLU:O	2:C:469:LYS:CB	2.60	0.50
1:A:33:GLN:O	1:A:37:SER:CB	2.59	0.50
1:A:832:MET:SD	1:A:832:MET:N	2.85	0.50
1:A:908:PRO:HA	1:A:911:LEU:HB2	1.93	0.50
2:B:855:ILE:HG13	2:B:887:PRO:HD3	1.94	0.50
2:C:855:ILE:HG13	2:C:887:PRO:HD3	1.94	0.50
1:A:685:PRO:O	1:A:689:THR:OG1	2.19	0.50
1:A:834:LEU:HB3	1:A:837:GLN:HB3	1.93	0.50
2:C:797:HIS:CE1	2:C:826:LYS:HD2	2.47	0.50
1:A:786:ILE:O	1:A:790:ASN:CB	2.51	0.49
2:B:165:CYS:HB3	2:B:276:ILE:HG12	1.93	0.49
2:B:506:MET:O	2:B:510:ALA:HB2	2.12	0.49
2:C:123:ASP:OD2	2:C:372:GLN:NE2	2.45	0.49
2:C:897:PRO:O	2:C:901:LYS:HB2	2.11	0.49
1:A:1090:LEU:HD12	1:A:1091:PRO:HD2	1.93	0.49
1:A:39:GLU:O	1:A:43:HIS:CB	2.59	0.49
2:B:496:GLY:HA2	2:B:565:SER:HA	1.93	0.49
2:C:483:ILE:HA	2:C:487:TYR:HB2	1.94	0.49
1:A:1256:VAL:O	1:A:1260:LEU:HB2	2.11	0.49
2:B:99:ASN:O	2:B:103:GLN:CB	2.59	0.49
1:A:1381:HIS:HD2	1:A:1383:GLN:HB2	1.76	0.49
1:A:109:LEU:HD13	1:A:626:ILE:HG12	1.93	0.49
2:C:593:ASP:OD1	2:C:647:ARG:NH2	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:666:LEU:HD22	2:C:669:ILE:HD11	1.94	0.49
1:A:113:PRO:HA	1:A:116:ARG:HB3	1.94	0.49
1:A:512:ASP:HA	1:A:560:PRO:HA	1.95	0.49
2:B:465:GLU:O	2:B:469:LYS:CB	2.60	0.49
1:A:99:CYS:SG	1:A:100:CYS:N	2.86	0.49
1:A:783:LEU:HD22	1:A:822:LEU:HA	1.94	0.49
1:A:88:HIS:NE2	1:A:91:VAL:O	2.40	0.49
1:A:1324:GLN:HA	1:A:1356:LEU:HA	1.95	0.49
1:A:531:SER:O	1:A:535:LEU:N	2.42	0.49
1:A:713:LEU:HB3	1:A:717:GLY:HA2	1.93	0.49
2:B:797:HIS:CE1	2:B:826:LYS:HD2	2.47	0.49
2:C:777:GLU:HG2	2:C:781:LYS:HE3	1.94	0.49
1:A:1218:PHE:HZ	1:A:1251:VAL:HG21	1.77	0.49
2:C:470:GLY:HA2	2:C:473:TYR:HD2	1.78	0.49
1:A:48:LYS:HG2	1:A:49:MET:HG2	1.95	0.49
2:B:199:LEU:HD12	2:B:243:VAL:HG22	1.94	0.49
2:B:455:LEU:HD22	2:B:494:THR:HG21	1.95	0.49
2:B:470:GLY:HA2	2:B:473:TYR:HD2	1.78	0.49
2:B:593:ASP:OD1	2:B:647:ARG:NH2	2.45	0.49
2:C:455:LEU:HD22	2:C:494:THR:HG21	1.95	0.49
1:A:1004:VAL:O	1:A:1033:ARG:HB2	2.13	0.48
1:A:1358:ARG:HD3	1:A:1386:ARG:HH11	1.78	0.48
1:A:1115:PRO:HA	1:A:1142:SER:HA	1.95	0.48
1:A:688:ALA:O	1:A:692:SER:HB3	2.12	0.48
1:A:722:GLU:O	1:A:726:THR:OG1	2.26	0.48
2:C:317:GLN:HE22	2:C:353:GLU:HA	1.78	0.48
1:A:1218:PHE:HB3	1:A:1245:GLY:HA3	1.95	0.48
2:B:317:GLN:HE22	2:B:353:GLU:HA	1.78	0.48
2:C:506:MET:O	2:C:510:ALA:HB2	2.12	0.48
3:F:464:SER:O	3:F:468:SER:N	2.42	0.48
1:A:1109:VAL:HB	1:A:1137:ARG:H	1.79	0.48
1:A:215:LYS:O	1:A:219:LYS:HB2	2.13	0.48
2:B:777:GLU:HG2	2:B:781:LYS:HE3	1.94	0.48
1:A:721:ASP:O	1:A:725:THR:CB	2.61	0.48
2:B:961:PHE:HE1	2:B:967:LEU:HD23	1.79	0.48
2:C:961:PHE:HE1	2:C:967:LEU:HD23	1.79	0.48
1:A:1305:ILE:HG13	1:A:1309:GLY:HA3	1.96	0.48
2:B:666:LEU:HD22	2:B:669:ILE:HD11	1.94	0.48
2:C:199:LEU:HD12	2:C:243:VAL:HG22	1.94	0.48
1:A:194:THR:HA	1:A:204:LEU:O	2.13	0.48
2:C:230:PRO:O	2:C:234:ALA:CB	2.62	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:468:SER:O	3:F:472:LEU:HB2	2.13	0.48
2:C:506:MET:O	2:C:510:ALA:CB	2.62	0.48
2:C:616:PHE:O	2:C:667:ARG:HB2	2.14	0.48
1:A:63:ARG:HD2	1:A:82:ALA:HB1	1.96	0.48
1:A:695:GLN:OE1	1:A:756:ARG:NH2	2.47	0.48
2:B:230:PRO:O	2:B:234:ALA:CB	2.62	0.48
1:A:1344:LYS:HD3	1:A:1373:VAL:HG21	1.96	0.47
1:A:732:PHE:HB2	1:A:740:VAL:H	1.79	0.47
2:B:616:PHE:O	2:B:667:ARG:HB2	2.14	0.47
2:B:804:ILE:HD11	2:B:831:CYS:H	1.79	0.47
2:C:669:ILE:HG22	2:C:699:ALA:HB3	1.95	0.47
2:C:989:GLN:O	2:C:993:LYS:HB2	2.14	0.47
1:A:1090:LEU:HD13	1:A:1112:ASP:HB3	1.96	0.47
1:A:313:VAL:O	1:A:321:CYS:CB	2.62	0.47
1:A:468:VAL:HA	1:A:597:LEU:O	2.13	0.47
1:A:512:ASP:HB3	1:A:559:LEU:HG	1.96	0.47
1:A:644:PHE:HB3	1:A:671:TYR:HE1	1.79	0.47
1:A:75:SER:HB3	1:A:608:VAL:HG21	1.96	0.47
2:B:506:MET:O	2:B:510:ALA:CB	2.62	0.47
2:B:886:LEU:HB3	2:B:917:TRP:HZ2	1.79	0.47
2:B:989:GLN:O	2:B:993:LYS:HB2	2.14	0.47
1:A:783:LEU:H	1:A:821:SER:HB2	1.78	0.47
2:C:325:ILE:HA	2:C:331:LEU:HD23	1.97	0.47
2:C:695:LYS:HA	2:C:720:GLU:HB3	1.96	0.47
2:B:696:ARG:HG2	2:B:721:ALA:HB3	1.96	0.47
1:A:1268:LEU:O	1:A:1297:LEU:HA	2.14	0.47
2:B:834:ALA:O	2:B:838:LYS:CB	2.62	0.47
2:C:591:ILE:HG23	2:C:595:LEU:HD22	1.97	0.47
2:C:804:ILE:HD11	2:C:831:CYS:H	1.78	0.47
2:C:886:LEU:HB3	2:C:917:TRP:HZ2	1.79	0.47
2:B:591:ILE:HG23	2:B:595:LEU:HD22	1.96	0.47
2:C:809:ASP:O	2:C:813:LYS:CB	2.63	0.47
1:A:1031:GLU:HA	1:A:1057:LYS:HB3	1.96	0.47
1:A:889:LEU:HD22	1:A:914:LEU:HD21	1.97	0.47
2:B:809:ASP:O	2:B:813:LYS:CB	2.63	0.47
2:B:918:ARG:HA	2:B:947:HIS:HA	1.96	0.47
2:C:893:HIS:HA	2:C:896:LEU:HD23	1.97	0.47
1:A:1314:PHE:O	1:A:1318:ASP:CB	2.56	0.47
1:A:483:ILE:O	1:A:487:TRP:CB	2.63	0.47
1:A:492:CYS:HB3	1:A:495:LEU:HG	1.97	0.47
2:B:185:LEU:HB3	2:B:190:GLY:HA3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:696:ARG:HG2	2:C:721:ALA:HB3	1.96	0.47
2:C:834:ALA:O	2:C:838:LYS:CB	2.62	0.47
2:B:669:ILE:HG22	2:B:699:ALA:HB3	1.95	0.47
1:A:1057:LYS:HA	1:A:1081:SER:HB2	1.97	0.46
1:A:1295:GLU:HA	1:A:1323:LEU:HA	1.97	0.46
2:B:677:ILE:HG23	2:B:707:VAL:HG22	1.98	0.46
1:A:1014:GLN:HA	1:A:1017:LEU:HD12	1.97	0.46
2:B:282:GLU:HA	2:B:429:LYS:HD3	1.97	0.46
1:A:1130:HIS:HA	1:A:1156:ASN:HD21	1.80	0.46
2:B:325:ILE:HA	2:B:331:LEU:HD23	1.97	0.46
2:B:742:SER:HA	2:B:769:ILE:HB	1.97	0.46
2:B:769:ILE:HG12	2:B:797:HIS:CD2	2.51	0.46
2:C:918:ARG:HA	2:C:947:HIS:HA	1.97	0.46
2:B:170:GLU:HB2	2:B:173:LYS:HD3	1.98	0.46
2:B:185:LEU:O	2:B:190:GLY:N	2.48	0.46
1:A:1265:LEU:HD23	1:A:1294:LEU:HD21	1.98	0.46
1:A:275:PHE:HD1	1:A:280:LEU:HB3	1.80	0.46
1:A:509:ILE:HD13	1:A:518:ILE:HD13	1.96	0.46
2:C:185:LEU:HB3	2:C:190:GLY:HA3	1.97	0.46
2:C:742:SER:HA	2:C:769:ILE:HB	1.97	0.46
2:C:769:ILE:HG12	2:C:797:HIS:CD2	2.51	0.46
1:A:100:CYS:HB3	1:A:121:ARG:HG3	1.97	0.46
1:A:1160:PHE:O	1:A:1187:GLU:CB	2.55	0.46
1:A:772:GLY:O	1:A:776:LEU:CB	2.62	0.46
2:B:153:THR:N	2:B:156:SER:OG	2.47	0.46
2:C:153:THR:N	2:C:156:SER:OG	2.47	0.46
2:C:185:LEU:O	2:C:190:GLY:N	2.48	0.46
2:C:98:LEU:O	2:C:102:ALA:CB	2.58	0.46
1:A:424:VAL:HB	1:A:654:GLN:HE22	1.79	0.46
2:B:557:CYS:O	2:B:561:LEU:HB2	2.16	0.46
2:B:695:LYS:HA	2:B:720:GLU:HB3	1.96	0.46
1:A:193:ASP:O	1:A:207:TRP:NE1	2.44	0.46
1:A:475:GLY:O	1:A:479:PHE:N	2.48	0.46
1:A:1281:GLU:O	1:A:1285:ALA:CB	2.65	0.45
1:A:809:VAL:HG23	1:A:812:LEU:HD12	1.98	0.45
2:B:433:GLN:NE2	2:C:127:ILE:HG13	2.31	0.45
2:B:893:HIS:HA	2:B:896:LEU:HD23	1.97	0.45
2:C:954:TRP:HB3	2:C:983:LEU:HD13	1.99	0.45
1:A:1228:ALA:HA	1:A:1255:ILE:HD11	1.98	0.45
1:A:1103:GLY:H	1:A:1128:LEU:HD21	1.82	0.45
1:A:785:ALA:HA	1:A:789:PHE:CD2	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:231:THR:O	2:C:235:LEU:CB	2.64	0.45
3:F:458:MET:O	3:F:462:ALA:CB	2.64	0.45
1:A:1282:ILE:O	1:A:1286:ALA:HB3	2.16	0.45
1:A:985:ILE:O	1:A:989:TYR:HB2	2.16	0.45
1:A:1161:HIS:HA	1:A:1187:GLU:HB3	1.98	0.45
1:A:1173:LEU:HA	1:A:1176:VAL:HG12	1.98	0.45
1:A:478:THR:O	1:A:482:ARG:CB	2.65	0.45
2:B:148:ARG:NE	2:B:296:GLU:OE2	2.50	0.45
2:C:170:GLU:HB2	2:C:173:LYS:HD3	1.98	0.45
2:C:282:GLU:HA	2:C:429:LYS:HD3	1.97	0.45
1:A:821:SER:HA	1:A:824:ASN:HB2	1.99	0.45
2:C:148:ARG:NE	2:C:296:GLU:OE2	2.50	0.45
1:A:560:PRO:HB2	1:A:563:LEU:HB2	1.98	0.45
2:B:333:ASN:HA	2:B:336:LYS:HZ3	1.82	0.45
1:A:1111:LEU:H	1:A:1137:ARG:HD2	1.82	0.45
1:A:1170:CYS:O	1:A:1174:MET:CB	2.64	0.45
2:B:954:TRP:HB3	2:B:983:LEU:HD13	1.99	0.45
3:F:469:VAL:HG13	3:F:473:LEU:HD23	1.99	0.45
1:A:862:GLU:O	1:A:866:ARG:HB2	2.17	0.45
1:A:709:ASN:ND2	1:A:711:ASP:OD2	2.50	0.44
1:A:896:LEU:HD13	1:A:917:LEU:HD21	1.99	0.44
2:C:557:CYS:O	2:C:561:LEU:HB2	2.16	0.44
2:C:677:ILE:HG23	2:C:707:VAL:HG22	1.98	0.44
1:A:1276:ASP:HA	1:A:1279:VAL:HG22	1.99	0.44
1:A:403:LEU:HD22	1:A:530:ILE:HD13	1.98	0.44
2:B:231:THR:O	2:B:235:LEU:CB	2.64	0.44
1:A:1183:LEU:HB3	1:A:1186:ILE:HD11	2.00	0.44
1:A:567:ILE:O	1:A:570:ASN:ND2	2.50	0.44
2:C:317:GLN:O	2:C:321:LEU:CB	2.65	0.44
2:C:538:ARG:HH21	2:C:693:HIS:CE1	2.36	0.44
2:C:503:ARG:HE	2:C:571:LEU:HD21	1.82	0.44
1:A:904:PHE:HD2	1:A:992:LEU:HD11	1.83	0.44
2:B:307:ASP:O	2:B:311:ALA:HB2	2.17	0.44
2:B:503:ARG:HE	2:B:571:LEU:HD21	1.82	0.44
2:C:307:ASP:O	2:C:311:ALA:HB2	2.17	0.44
1:A:1008:ASN:HB3	1:A:1036:ASN:HB3	2.00	0.44
2:B:317:GLN:O	2:B:321:LEU:CB	2.65	0.44
2:B:691:ARG:HG2	2:B:716:THR:HG22	2.00	0.44
1:A:688:ALA:O	1:A:692:SER:OG	2.35	0.44
1:A:850:LEU:O	1:A:1386:ARG:NH2	2.51	0.44
1:A:227:LEU:O	1:A:231:LYS:HB3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:415:THR:O	1:A:418:HIS:ND1	2.36	0.44
1:A:985:ILE:O	1:A:989:TYR:CB	2.66	0.44
2:C:176:SER:O	2:C:180:GLN:HB2	2.18	0.44
1:A:1002:LEU:O	1:A:1031:GLU:CB	2.66	0.44
1:A:1267:VAL:HA	1:A:1296:ASN:HB2	2.00	0.44
1:A:721:ASP:O	1:A:725:THR:HB	2.17	0.44
1:A:49:MET:O	1:A:96:GLN:NE2	2.51	0.43
1:A:869:LEU:HD21	1:A:904:PHE:HB2	2.00	0.43
2:B:176:SER:O	2:B:180:GLN:HB2	2.18	0.43
2:B:828:VAL:HB	2:B:857:GLU:HB2	2.01	0.43
2:B:409:GLU:HG2	2:B:438:THR:HA	2.00	0.43
1:A:430:THR:HG22	1:A:434:LEU:HD23	2.01	0.43
2:C:474:LEU:O	2:C:508:HIS:NE2	2.52	0.43
2:C:828:VAL:HB	2:C:857:GLU:HB2	2.01	0.43
2:C:937:ARG:NH2	2:C:963:ASN:O	2.39	0.43
1:A:1106:GLU:HA	1:A:1133:LYS:HB3	1.99	0.43
1:A:454:THR:H	1:A:457:GLU:HB2	1.83	0.43
1:A:905:ARG:HA	1:A:908:PRO:HG3	2.01	0.43
2:B:120:LEU:HD13	2:B:369:LEU:HD11	2.00	0.43
2:B:546:LEU:HD23	2:B:549:ILE:HD12	1.99	0.43
1:A:1052:LYS:NZ	1:A:1054:SER:OG	2.51	0.43
1:A:1281:GLU:O	1:A:1285:ALA:HB3	2.19	0.43
1:A:790:ASN:O	1:A:794:TYR:HB3	2.18	0.43
2:C:593:ASP:HA	2:C:596:PHE:HD2	1.84	0.43
2:C:978:LEU:HD12	2:C:979:PRO:HD2	2.00	0.43
1:A:823:GLU:HG3	1:A:1382:PRO:HB2	2.00	0.43
1:A:278:GLU:O	1:A:282:MET:CB	2.67	0.43
1:A:889:LEU:HD11	1:A:911:LEU:HD23	2.01	0.43
2:B:474:LEU:O	2:B:508:HIS:NE2	2.51	0.43
2:C:987:LEU:HG	2:C:991:LEU:HD13	2.00	0.43
1:A:871:PHE:O	1:A:875:SER:CB	2.67	0.43
2:B:797:HIS:HE1	2:B:826:LYS:HD2	1.84	0.43
2:B:322:TRP:HA	2:B:325:ILE:HD12	2.01	0.43
2:B:729:GLU:HA	2:B:732:ILE:HD12	2.01	0.43
1:A:1032:PHE:CB	1:A:1057:LYS:O	2.53	0.43
1:A:499:GLN:HE22	1:A:542:LEU:HD13	1.84	0.43
1:A:813:LEU:HD12	1:A:888:PHE:HB2	2.01	0.43
2:B:538:ARG:HH21	2:B:693:HIS:CE1	2.36	0.43
2:C:129:ASN:O	2:C:133:THR:N	2.52	0.43
2:C:333:ASN:HA	2:C:336:LYS:HZ3	1.84	0.43
2:C:409:GLU:HG2	2:C:438:THR:HA	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:691:ARG:HG2	2:C:716:THR:HG22	2.00	0.43
1:A:1312:ASN:O	1:A:1316:ALA:CB	2.67	0.42
1:A:398:GLN:O	1:A:402:SER:CB	2.66	0.42
1:A:87:TYR:CZ	1:A:96:GLN:HB2	2.53	0.42
2:C:988:SER:O	2:C:992:SER:CB	2.67	0.42
1:A:214:TRP:HE1	1:A:231:LYS:HD3	1.84	0.42
2:B:987:LEU:HG	2:B:991:LEU:HD13	2.00	0.42
2:C:318:VAL:O	2:C:322:TRP:CB	2.68	0.42
2:C:546:LEU:HD23	2:C:549:ILE:HD12	1.99	0.42
2:C:729:GLU:HA	2:C:732:ILE:HD12	2.01	0.42
2:C:797:HIS:HE1	2:C:826:LYS:HD2	1.84	0.42
2:B:593:ASP:HA	2:B:596:PHE:HD2	1.84	0.42
2:C:120:LEU:HD13	2:C:369:LEU:HD11	2.00	0.42
1:A:1371:MET:O	1:A:1375:ASN:HB2	2.19	0.42
1:A:464:SER:HA	1:A:576:CYS:HA	2.01	0.42
2:B:393:CYS:HB2	2:B:421:LEU:HD13	2.01	0.42
2:B:978:LEU:HD12	2:B:979:PRO:HD2	2.00	0.42
2:B:988:SER:O	2:B:992:SER:CB	2.67	0.42
2:C:400:GLY:O	2:C:405:LYS:N	2.44	0.42
1:A:1197:THR:HG22	1:A:1201:ILE:HG12	2.01	0.42
2:B:523:VAL:HG21	2:B:549:ILE:HD13	2.02	0.42
2:C:105:LEU:HD23	2:C:108:LEU:HD13	2.00	0.42
2:C:708:LEU:O	2:C:731:TYR:OH	2.37	0.42
2:C:765:LEU:HD21	2:C:768:LEU:HD22	2.02	0.42
1:A:1292:GLN:HE22	1:A:1321:PRO:HG2	1.85	0.42
1:A:554:SER:HA	1:A:585:ARG:HD2	2.02	0.42
1:A:553:TYR:HB2	1:A:579:ILE:HD11	2.02	0.42
1:A:648:VAL:HG13	1:A:667:LEU:HD11	2.01	0.42
2:C:523:VAL:HG21	2:C:549:ILE:HD13	2.02	0.42
1:A:197:CYS:N	1:A:200:CYS:SG	2.90	0.42
2:B:708:LEU:O	2:B:731:TYR:OH	2.37	0.42
2:C:211:GLY:O	2:C:215:THR:N	2.39	0.42
2:C:322:TRP:HA	2:C:325:ILE:HD12	2.01	0.42
2:B:105:LEU:HD23	2:B:108:LEU:HD13	2.00	0.42
2:B:488:GLY:O	2:B:492:LEU:HB2	2.19	0.42
2:C:115:LEU:HG	2:C:130:LEU:HD12	2.02	0.42
2:C:666:LEU:O	2:C:695:LYS:CB	2.61	0.42
2:C:770:LEU:HD12	2:C:773:ILE:HG13	2.00	0.42
3:F:28:SER:HB3	3:F:449:GLN:HE21	1.84	0.42
1:A:837:GLN:NE2	3:F:458:MET:SD	2.90	0.42
1:A:1260:LEU:HD22	1:A:1285:ALA:HB1	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:820:GLU:OE1	1:A:824:ASN:ND2	2.51	0.42
2:C:662:LEU:HG	2:C:687:ALA:HB2	2.00	0.42
2:B:115:LEU:HG	2:B:130:LEU:HD12	2.02	0.41
2:B:662:LEU:HG	2:B:687:ALA:HB2	2.00	0.41
2:C:984:VAL:HG22	2:C:1007:PHE:HE1	1.85	0.41
2:C:924:ILE:HA	2:C:924:ILE:HD12	1.95	0.41
1:A:685:PRO:HA	1:A:688:ALA:HB3	2.02	0.41
2:C:393:CYS:HB2	2:C:421:LEU:HD13	2.01	0.41
2:C:488:GLY:O	2:C:492:LEU:HB2	2.19	0.41
1:A:1096:HIS:HA	1:A:1099:HIS:CD2	2.53	0.41
1:A:413:LYS:HB3	1:A:416:PHE:HB2	2.03	0.41
1:A:873:TYR:HB3	1:A:903:TYR:HD1	1.85	0.41
1:A:897:ARG:HE	1:A:970:ILE:HG21	1.85	0.41
2:B:318:VAL:O	2:B:322:TRP:CB	2.68	0.41
2:B:844:LEU:HB3	2:B:874:ARG:HG2	2.02	0.41
1:A:1253:LYS:O	1:A:1257:ARG:CB	2.57	0.41
2:B:984:VAL:HG22	2:B:1007:PHE:HE1	1.85	0.41
2:B:349:MET:HB3	2:B:349:MET:HE2	1.82	0.41
2:B:523:VAL:HG11	2:B:526:ARG:HB3	2.03	0.41
1:A:1353:LEU:HD12	1:A:1354:PRO:HD2	2.02	0.41
2:B:211:GLY:O	2:B:215:THR:N	2.39	0.41
2:B:916:ASN:H	2:B:945:ALA:HB3	1.85	0.41
1:A:1030:ILE:O	1:A:1056:THR:OG1	2.33	0.41
2:B:982:ALA:HA	2:B:985:ARG:HG2	2.03	0.41
2:B:139:MET:O	2:B:151:GLN:HA	2.21	0.41
2:B:765:LEU:HD21	2:B:768:LEU:HD22	2.02	0.41
2:B:969:PHE:HD1	2:B:999:GLU:HB3	1.86	0.41
2:C:869:GLN:HE21	2:C:895:SER:HA	1.86	0.41
1:A:737:LEU:HD11	2:B:347:ILE:HG12	2.01	0.41
2:C:666:LEU:HB2	2:C:693:HIS:O	2.20	0.41
1:A:1041:LEU:HA	1:A:1044:ILE:HG22	2.02	0.41
1:A:1297:LEU:HB2	1:A:1323:LEU:HD11	2.03	0.41
1:A:226:PHE:HA	1:A:229:SER:HB3	2.03	0.41
2:B:162:LYS:HB2	2:B:293:LEU:HD12	2.03	0.41
2:B:770:LEU:HD12	2:B:773:ILE:HG13	2.00	0.41
2:B:869:GLN:HE21	2:B:895:SER:HA	1.86	0.41
2:C:140:TRP:CE3	2:C:148:ARG:HB3	2.56	0.41
2:C:162:LYS:HB2	2:C:293:LEU:HD12	2.03	0.41
1:A:1109:VAL:HB	1:A:1136:ILE:HA	2.03	0.41
1:A:1279:VAL:HA	1:A:1282:ILE:HG22	2.03	0.41
1:A:735:GLN:HG3	2:B:124:ILE:HG21	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:666:LEU:HB2	2:B:693:HIS:O	2.20	0.41
2:C:523:VAL:HG11	2:C:526:ARG:HB3	2.03	0.41
1:A:444:HIS:HB3	1:A:448:PRO:HD2	2.03	0.40
1:A:487:TRP:HE1	1:A:498:PHE:HB2	1.85	0.40
1:A:689:THR:HG23	1:A:723:LYS:HG2	2.03	0.40
2:C:234:ALA:O	2:C:238:LYS:CB	2.62	0.40
2:C:844:LEU:HB3	2:C:874:ARG:HG2	2.02	0.40
2:C:285:ARG:HD2	2:C:431:THR:HG21	2.03	0.40
1:A:1021:MET:HB2	1:A:1050:LEU:HD13	2.02	0.40
1:A:1079:LEU:HB2	1:A:1101:PHE:CE2	2.56	0.40
1:A:212:ASP:O	1:A:216:GLU:N	2.41	0.40
1:A:342:CYS:O	1:A:346:GLN:N	2.48	0.40
1:A:437:ASP:O	1:A:606:ASN:ND2	2.55	0.40
2:B:285:ARG:HD2	2:B:431:THR:HG21	2.03	0.40
2:C:916:ASN:H	2:C:945:ALA:HB3	1.85	0.40
2:C:969:PHE:HD1	2:C:999:GLU:HB3	1.86	0.40
1:A:109:LEU:HG	1:A:110:ARG:HB2	2.03	0.40
1:A:315:CYS:HB3	1:A:320:GLY:H	1.86	0.40
1:A:312:ILE:HG12	1:A:321:CYS:HB2	2.03	0.40
1:A:432:HIS:HD2	1:A:433:LEU:HD22	1.86	0.40
1:A:615:PHE:HE1	1:A:653:ILE:HB	1.86	0.40
1:A:986:SER:HA	1:A:989:TYR:HB3	2.03	0.40
2:B:254:HIS:CD2	2:B:256:GLN:HB2	2.57	0.40
2:B:924:ILE:HD12	2:B:924:ILE:HA	1.95	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	1187/1403 (85%)	1011 (85%)	175 (15%)	1 (0%)	53 88

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	899/1024 (88%)	839 (93%)	60 (7%)	0	100	100
2	C	899/1024 (88%)	839 (93%)	60 (7%)	0	100	100
3	F	64/566 (11%)	60 (94%)	4 (6%)	0	100	100
All	All	3049/4017 (76%)	2749 (90%)	299 (10%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	193	ASP

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	1080/1258 (86%)	1069 (99%)	11 (1%)	78	89
2	B	807/913 (88%)	805 (100%)	2 (0%)	94	96
2	C	807/913 (88%)	805 (100%)	2 (0%)	94	96
3	F	56/437 (13%)	54 (96%)	2 (4%)	38	65
All	All	2750/3521 (78%)	2733 (99%)	17 (1%)	88	93

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	107	ASN
1	A	110	ARG
1	A	410	ASN
1	A	517	ASN
1	A	633	LYS
1	A	1184	ARG
1	A	1221	LYS
1	A	1234	LEU
1	A	1235	ARG
1	A	1322	ASN

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Mol	Chain	Res	Type
1	A	1356	LEU
2	B	268	ASN
2	B	526	ARG
2	C	268	ASN
2	C	526	ARG
3	F	1	MET
3	F	475	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	117	HIS
1	A	582	HIS
1	A	654	GLN
1	A	669	GLN
1	A	749	GLN
1	A	769	GLN
1	A	976	ASN
1	A	1129	HIS
1	A	1161	HIS
1	A	1312	ASN
1	A	1319	ASN
1	A	1322	ASN
1	A	1327	ASN
1	A	1381	HIS
2	B	144	HIS
2	B	147	HIS
2	B	317	GLN
2	B	797	HIS
2	B	869	GLN
2	B	916	ASN
2	B	963	ASN
2	C	147	HIS
2	C	317	GLN
2	C	797	HIS
2	C	869	GLN
2	C	916	ASN
2	C	963	ASN
3	F	449	GLN

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](#)

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.