



Full wwPDB EM Validation Report ⓘ

May 10, 2026 – 12:17 AM JST

PDB ID : 9K19 / pdb_00009k19
EMDB ID : EMD-61969
Title : A cryo-EM structure of *B. oleracea* RNA polymerase V in complex with 8U scaffold at 4.06 Angstrom
Authors : Xie, G.; Du, X.; Du, J.
Deposited on : 2024-10-16
Resolution : 4.06 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 ⓘ 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 ⓘ](#)) were used in the production of this report:

EMDB validation analysis : **FAILED**
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : **NOT EXECUTED**
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

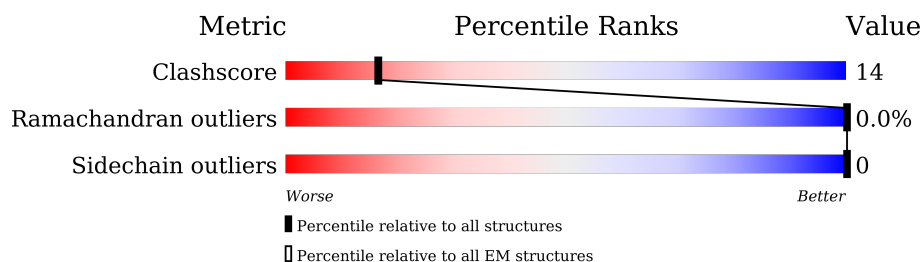
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.06 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	229148	23984
Ramachandran outliers	224038	23583
Sidechain outliers	223484	23102

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 ≥ 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	2032	27% 13% 59%
2	B	1169	60% 25% 14%
3	C	319	69% 25% 6%
4	E	230	60% 30% 10%
5	F	144	40% 15% 44%
6	H	146	53% 45% .
7	I	114	69% 11% 20%
8	J	71	55% 35% 10%
9	K	116	72% 21% 7%

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Mol	Chain	Length	Quality of chain
10	L	51	 69% 22% 10%
11	T	34	 18% 15% 68%
12	N	34	 24% 38% 38%

2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 23378 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 V largest subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	827	Total	C	N	O	S	0	0
			6449	4070	1111	1223	45		

- Molecule 2 is a protein called DNA-directed RNA polymerase IV and V subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1000	Total	C	N	O	S	0	0
			7946	4998	1406	1498	44		

- Molecule 3 is a protein called DNA-directed RNA polymerase RpoA/D/Rpb3-type domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	300	Total	C	N	O	S	0	0
			2340	1463	393	471	13		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	3	THR	SER	conflict	UNP A0A0D3D418

- Molecule 4 is a protein called RNA polymerase subunit H/Rpb5 C-terminal domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	208	Total	C	N	O	S	0	0
			1698	1079	302	315	2		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	101	GLY	SER	conflict	UNP A0A0D3DTU3
E	182	GLN	HIS	conflict	UNP A0A0D3DTU3

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Chain	Residue	Modelled	Actual	Comment	Reference
E	210	ILE	VAL	conflict	UNP A0A0D3DTU3

- Molecule 5 is a protein called DNA-directed RNA polymerase RpoA/D/Rpb3-type domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	80	Total	C	N	O	S	0	0
			660	420	114	122	4		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	51	GLU	ASP	conflict	UNP A0A0D3BZZ8

- Molecule 6 is a protein called DNA-directed RNA polymerase II, IV and V subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	H	142	Total	C	N	O	S	0	0
			1135	732	184	210	9		

- Molecule 7 is a protein called DNA-directed RNA polymerase subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	I	91	Total	C	N	O	S	0	0
			713	436	130	136	11		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	20	ARG	LYS	conflict	UNP A0A0D3A7P5
I	40	ASP	ASN	conflict	UNP A0A0D3A7P5

- Molecule 8 is a protein called DNA-directed RNA polymerase II, IV and V subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	J	64	Total	C	N	O	S	0	0
			514	328	86	93	7		

- Molecule 9 is a protein called DNA-directed RNA polymerase RBP11-like dimerisation domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	K	108	Total	C	N	O	S	0	0
			887	563	154	168	2		

- Molecule 10 is a protein called DNA-directed RNA polymerase II, IV and V subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	L	46	Total	C	N	O	S	0	0
			375	229	71	71	4		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	18	GLU	LYS	conflict	UNP A0A0D2ZPP3
L	32	CYS	ARG	conflict	UNP A0A0D2ZPP3

- Molecule 11 is a DNA chain called DNA (34-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
11	T	11	Total	C	N	O	P	0	0
			222	107	37	67	11		

- Molecule 12 is a DNA chain called DNA (34-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
12	N	21	Total	C	N	O	P	0	0
			431	205	80	125	21		

- Molecule 13 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
13	A	1	Total	Mg	0
			1	1	

- Molecule 14 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
14	A	1	Total	Zn	0
			1	1	
14	C	1	Total	Zn	0
			1	1	

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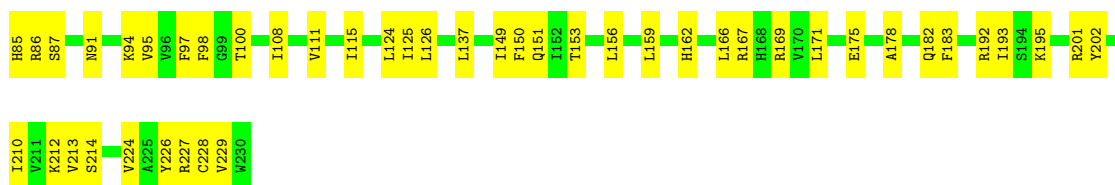
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Mol	Chain	Residues	Atoms		AltConf
14	H	1	Total 1	Zn 1	0
14	I	2	Total 2	Zn 2	0
14	J	1	Total 1	Zn 1	0
14	L	1	Total 1	Zn 1	0

- Molecule 2: DNA-directed RNA polymerase IV and V subunit 2

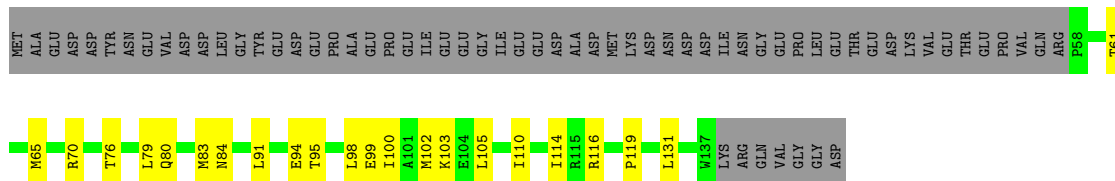
Chain B: 60% 25% 14%

L117	L118	L119	M120	M126	M127	M128	M129	V130	F135	VAL	LYS	LYS	VAL	VAL	G21	E22	F23	F24	L25	PHE	LYS	LYS	THR	GLY	GLN	ASP	GLU	TYR	VAL	GLU	LYS	GLN	ILE	LEU	SER	LYS	LYS	L162	G163	L164	L165	L166	L167	G168	M173	V177	N180	T181	G185	K186	S190	K193
THR	ASP	ASP	GLU	GLU	ILE	ILE	ALA	ALA	GLY	E14	L20	G21	E22	F23	F24	L25	Y40	V43	L47	M51	I54	L58	S65	L69	V70	E71	F72	B85	T88	V89	A90	F91	P99	T100	L101	E107	F110	L111	H114	A115	F116											



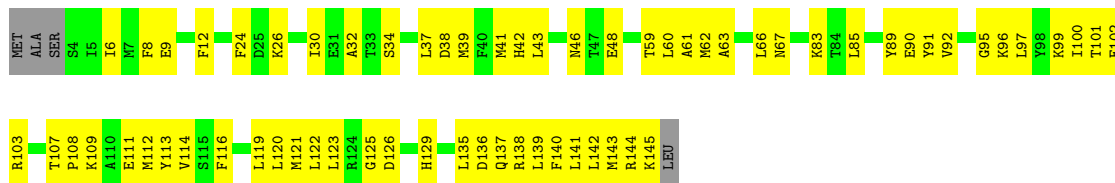
- Molecule 5: DNA-directed RNA polymerase RpoA/D/Rpb3-type domain-containing protein

Chain F: 40% 15% 44%



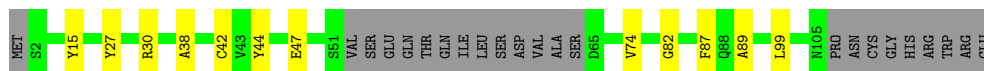
- Molecule 6: DNA-directed RNA polymerase II, IV and V subunit 8

Chain H: 53% 45%



- Molecule 7: DNA-directed RNA polymerase subunit

Chain I: 69% 11% 20%



- Molecule 8: DNA-directed RNA polymerase II, IV and V subunit 10

Chain J: 55% 35% 10%

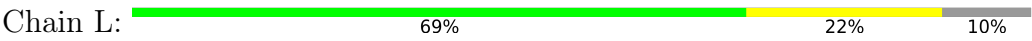


- Molecule 9: DNA-directed RNA polymerase RBP11-like dimerisation domain-containing protein

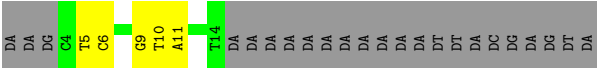
Chain K: 72% 21% 7%



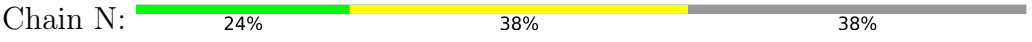
- Molecule 10: DNA-directed RNA polymerase II, IV and V subunit 12



● Molecule 11: DNA (34-MER)



● Molecule 12: DNA (34-MER)



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	27211	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.5625	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MG

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	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.22	0/6560	0.52	0/8856
2	B	0.26	0/8105	0.54	0/10921
3	C	0.24	0/2371	0.52	0/3204
4	E	0.20	0/1724	0.50	0/2321
5	F	0.23	0/673	0.48	0/905
6	H	0.24	0/1161	0.63	0/1565
7	I	0.20	0/726	0.50	0/979
8	J	0.28	0/522	0.55	0/706
9	K	0.25	0/905	0.51	0/1221
10	L	0.23	0/379	0.53	0/506
11	T	0.27	0/247	0.56	0/378
12	N	0.35	0/483	0.48	0/743
All	All	0.24	0/23856	0.53	0/32305

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	A	6449	0	6493	217	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	7946	0	7857	227	0
3	C	2340	0	2337	57	0
4	E	1698	0	1748	58	0
5	F	660	0	669	18	0
6	H	1135	0	1133	56	0
7	I	713	0	651	10	0
8	J	514	0	519	19	0
9	K	887	0	876	20	0
10	L	375	0	371	9	0
11	T	222	0	126	4	0
12	N	431	0	237	16	0
13	A	1	0	0	0	0
14	A	1	0	0	0	0
14	C	1	0	0	0	0
14	H	1	0	0	0	0
14	I	2	0	0	0	0
14	J	1	0	0	0	0
14	L	1	0	0	0	0
All	All	23378	0	23017	656	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 (656) 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:777:THR:HG21	1:A:1166:TYR:HE2	1.22	1.05
4:E:178:ALA:O	4:E:182:GLN:HG3	1.62	0.98
1:A:777:THR:CG2	1:A:1166:TYR:HE2	1.82	0.92
2:B:585:TYR:CZ	2:B:589:ASP:OD2	2.24	0.90
4:E:38:LEU:HD13	4:E:156:LEU:HA	1.54	0.90
2:B:323:HIS:HB2	2:B:326:ASN:HB2	1.53	0.89
1:A:796:THR:HG21	4:E:183:PHE:CE1	2.08	0.87
1:A:1019:ARG:HE	1:A:1020:THR:H	1.24	0.86
1:A:777:THR:CG2	1:A:1166:TYR:CE2	2.59	0.85
6:H:112:MET:SD	6:H:123:LEU:HB3	2.16	0.85
1:A:1050:TRP:HE1	1:A:1054:GLU:HB2	1.43	0.84
1:A:694:LYS:HE2	2:B:951:GLN:HG2	1.60	0.82
1:A:527:PRO:HG2	1:A:530:VAL:HG12	1.62	0.81
1:A:854:SER:HB3	1:A:1138:LYS:HD2	1.64	0.80
1:A:992:ARG:HH21	7:I:42:CYS:HB2	1.47	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:N:14:DC:H2'	12:N:15:DT:H2'	1.62	0.79
2:B:635:LYS:HE3	2:B:652:GLN:HB3	1.66	0.78
1:A:893:GLU:O	1:A:896:ALA:HB3	1.84	0.77
6:H:26:LYS:HD3	6:H:48:GLU:HG2	1.67	0.77
1:A:759:VAL:HG22	2:B:505:PRO:HG2	1.66	0.76
3:C:222:ASP:O	3:C:230:VAL:HA	1.86	0.76
1:A:762:ARG:HD3	1:A:765:ILE:HD11	1.65	0.76
8:J:5:VAL:HG12	8:J:6:ARG:HG3	1.67	0.76
1:A:605:GLN:HG3	1:A:606:PRO:HD3	1.68	0.75
2:B:670:TRP:HD1	2:B:689:LEU:HD21	1.49	0.75
12:N:26:DC:H2'	12:N:27:DT:C6	2.22	0.75
3:C:224:ASP:HB3	3:C:227:THR:HG22	1.68	0.75
1:A:777:THR:HG21	1:A:1166:TYR:CE2	2.13	0.75
2:B:212:VAL:HG21	2:B:486:LEU:HA	1.69	0.75
2:B:168:GLY:H	2:B:441:ALA:HB1	1.49	0.74
4:E:87:SER:HB3	4:E:91:ASN:HB2	1.68	0.74
5:F:61:THR:HG21	5:F:116:ARG:HD3	1.69	0.74
1:A:1017:LEU:HD11	1:A:1021:LEU:HA	1.70	0.74
1:A:626:MET:HE2	1:A:699:ILE:HG22	1.69	0.74
1:A:988:CYS:H	1:A:1003:PRO:HG2	1.50	0.74
1:A:411:PHE:HZ	1:A:469:VAL:HG21	1.52	0.73
2:B:770:VAL:HG12	2:B:940:ILE:HB	1.71	0.72
2:B:784:ILE:HG22	2:B:942:ILE:HG22	1.72	0.71
1:A:1144:LEU:HB2	1:A:1147:HIS:CD2	2.26	0.71
1:A:615:GLN:HE22	2:B:1024:ARG:NH2	1.89	0.70
2:B:352:LEU:HA	2:B:364:LYS:HZ1	1.56	0.70
3:C:206:ASP:HA	3:C:209:LYS:HD2	1.73	0.69
1:A:1017:LEU:O	1:A:1018:GLU:HG3	1.93	0.68
2:B:757:LEU:HD23	2:B:762:LEU:HD11	1.74	0.68
1:A:777:THR:HA	1:A:780:LYS:HG2	1.76	0.68
4:E:178:ALA:O	4:E:182:GLN:CG	2.41	0.68
3:C:204:LEU:HD13	3:C:208:GLU:HB2	1.75	0.68
2:B:963:LYS:HE2	2:B:1006:PHE:CE2	2.29	0.67
1:A:775:PRO:HG2	1:A:844:VAL:HG21	1.76	0.67
2:B:234:SER:HA	2:B:245:ILE:HG22	1.77	0.67
1:A:903:LEU:HB3	1:A:1043:ILE:HG21	1.76	0.67
2:B:331:VAL:HG12	2:B:334:GLN:HE22	1.58	0.67
2:B:886:SER:HB3	10:L:27:ILE:HB	1.76	0.67
2:B:909:LYS:HG3	2:B:1037:LEU:HB2	1.77	0.67
1:A:518:MET:HG3	9:K:62:GLN:HG2	1.77	0.67
3:C:109:LEU:HD23	3:C:165:LEU:HD21	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:154:ILE:HG22	3:C:155:VAL:HG23	1.77	0.66
1:A:1042:ARG:HA	1:A:1078:LYS:HG3	1.76	0.66
6:H:135:LEU:HG	6:H:136:ASP:H	1.60	0.66
4:E:167:ARG:HH12	4:E:169:ARG:HD2	1.60	0.65
1:A:911:THR:HB	1:A:946:LEU:HD21	1.78	0.65
3:C:196:ILE:HG22	3:C:257:ILE:HB	1.79	0.65
4:E:48:ARG:HG2	4:E:54:VAL:HB	1.78	0.65
1:A:908:LEU:HB3	1:A:1033:LEU:HD13	1.79	0.65
1:A:991:PHE:HD2	1:A:992:ARG:HG3	1.60	0.65
1:A:541:PHE:HA	1:A:544:ILE:HD13	1.78	0.65
6:H:101:THR:HB	6:H:111:GLU:H	1.61	0.65
1:A:350:THR:HB	1:A:401:HIS:HB3	1.77	0.65
1:A:1137:ARG:HH12	1:A:1143:VAL:H	1.44	0.65
2:B:540:ILE:HD11	2:B:602:GLN:HB2	1.79	0.65
1:A:411:PHE:CZ	1:A:469:VAL:HG21	2.32	0.65
1:A:777:THR:HG23	1:A:1166:TYR:OH	1.96	0.65
2:B:229:SER:HB3	2:B:230:PRO:HD3	1.79	0.65
4:E:153:THR:HA	4:E:156:LEU:HD13	1.79	0.64
1:A:1040:ASP:HB3	1:A:1043:ILE:HG12	1.79	0.64
1:A:901:ASN:HA	1:A:904:LYS:HZ2	1.62	0.64
3:C:141:SER:HB3	3:C:149:GLN:HA	1.78	0.64
9:K:58:PHE:HB3	9:K:76:HIS:HB2	1.77	0.64
2:B:406:GLU:HG3	2:B:410:HIS:CE1	2.33	0.64
2:B:284:VAL:HG21	2:B:290:ALA:HB2	1.79	0.64
6:H:6:ILE:HG12	6:H:63:ALA:HB2	1.80	0.64
12:N:13:DC:H2'	12:N:13:DC:O2	1.97	0.64
11:T:9:DG:H1'	11:T:10:DT:O4'	1.98	0.63
1:A:339:VAL:HG12	1:A:438:ILE:HG12	1.81	0.63
2:B:245:ILE:HG13	2:B:265:THR:HG23	1.78	0.63
2:B:402:LEU:HB3	2:B:457:TRP:NE1	2.13	0.63
4:E:44:LEU:HB3	4:E:59:ILE:HG22	1.80	0.63
1:A:796:THR:HG21	4:E:183:PHE:CZ	2.32	0.63
1:A:998:LYS:HD2	1:A:1000:SER:H	1.62	0.63
2:B:255:GLU:CD	2:B:256:ASP:H	2.06	0.63
10:L:8:VAL:HG23	10:L:39:LYS:HE3	1.81	0.63
1:A:336:VAL:HA	1:A:439:ASN:HD22	1.64	0.63
2:B:301:ALA:HA	2:B:304:THR:HG22	1.78	0.63
3:C:152:ILE:HD13	8:J:16:ASN:HB3	1.81	0.63
5:F:99:GLU:O	5:F:103:LYS:HG2	1.98	0.63
2:B:1039:HIS:HB3	2:B:1044:LYS:HE2	1.82	0.62
1:A:553:LEU:HD21	1:A:588:ILE:HG12	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:371:MET:HA	1:A:403:ARG:HD2	1.79	0.62
1:A:469:VAL:HA	1:A:473:PHE:HD2	1.64	0.62
1:A:879:LEU:HB2	1:A:1072:LEU:HB2	1.80	0.62
2:B:264:LEU:HB2	2:B:275:VAL:HG12	1.82	0.62
2:B:101:LEU:HB2	2:B:110:PHE:HD1	1.65	0.62
4:E:195:LYS:HG2	4:E:201:ARG:HH12	1.64	0.61
1:A:902:LYS:O	1:A:1039:GLY:HA2	1.99	0.61
5:F:94:GLU:HB2	5:F:100:ILE:HD11	1.83	0.61
8:J:25:LEU:HD21	8:J:31:GLU:HG2	1.83	0.61
9:K:39:ASP:HB3	9:K:69:TYR:HE1	1.63	0.61
1:A:928:ILE:HG23	1:A:930:GLY:H	1.66	0.61
2:B:734:CYS:HB3	2:B:895:THR:HG21	1.82	0.61
3:C:6:THR:HG23	3:C:7:TYR:H	1.66	0.61
4:E:75:ASP:HB2	4:E:80:ARG:HH12	1.66	0.61
1:A:890:TYR:HB3	7:I:99:LEU:HD11	1.82	0.60
4:E:48:ARG:HD2	4:E:59:ILE:HG21	1.84	0.60
4:E:34:HIS:HB2	4:E:67:ARG:HH22	1.66	0.60
3:C:60:SER:HB3	10:L:41:ARG:HH22	1.64	0.60
1:A:814:SER:HA	1:A:821:LEU:HD13	1.82	0.60
1:A:838:ASN:OD1	1:A:839:PRO:HD3	2.00	0.60
2:B:101:LEU:HB2	2:B:110:PHE:CD1	2.37	0.60
2:B:128:VAL:O	2:B:164:ASP:HA	2.02	0.59
2:B:512:ARG:HB3	2:B:623:LEU:HD13	1.83	0.59
2:B:784:ILE:HG13	2:B:920:LEU:HA	1.84	0.59
4:E:78:ARG:HB2	4:E:80:ARG:HG2	1.83	0.59
1:A:1019:ARG:NE	1:A:1020:THR:H	1.99	0.59
3:C:15:ILE:HG12	3:C:25:PHE:HB3	1.84	0.59
8:J:9:THR:HG23	8:J:47:ARG:HH21	1.68	0.59
4:E:98:PHE:HB3	4:E:100:THR:HG22	1.84	0.59
2:B:795:MET:HE3	8:J:8:PHE:CD2	2.38	0.58
6:H:30:ILE:HG22	6:H:43:LEU:HB3	1.83	0.58
12:N:26:DC:C6	12:N:27:DT:H72	2.37	0.58
1:A:912:ALA:HA	1:A:941:LEU:HA	1.86	0.58
1:A:698:GLN:O	1:A:746:PHE:HB2	2.04	0.58
1:A:410:VAL:O	1:A:425:ALA:HA	2.04	0.58
2:B:693:LEU:HD11	2:B:989:PHE:HE2	1.68	0.58
6:H:42:HIS:HB2	6:H:122:LEU:HB3	1.84	0.58
3:C:63:LEU:HD13	3:C:67:PHE:CD2	2.39	0.57
4:E:192:ARG:C	4:E:227:ARG:HD2	2.29	0.57
6:H:39:MET:HE1	6:H:125:GLY:HA3	1.85	0.57
9:K:39:ASP:HB3	9:K:69:TYR:CE1	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:739:GLN:HG2	2:B:800:GLN:HG2	1.85	0.57
2:B:165:ILE:HD12	2:B:436:GLU:HG3	1.87	0.57
6:H:144:ARG:HG3	6:H:145:LYS:HG3	1.85	0.57
3:C:60:SER:HB3	10:L:41:ARG:NH2	2.20	0.57
1:A:550:PRO:HB3	1:A:596:GLU:OE1	2.05	0.57
5:F:76:THR:HA	5:F:79:LEU:HD12	1.87	0.57
12:N:15:DT:H6	12:N:16:DA:H1'	1.68	0.57
4:E:40:ARG:CZ	4:E:80:ARG:HB2	2.35	0.57
6:H:113:TYR:CE1	6:H:122:LEU:HD13	2.40	0.56
1:A:959:ARG:HD2	1:A:1037:ILE:HD12	1.87	0.56
1:A:1050:TRP:NE1	1:A:1054:GLU:HB2	2.18	0.56
4:E:86:ARG:H	4:E:86:ARG:HD3	1.70	0.56
1:A:760:ALA:O	1:A:763:GLU:HG3	2.05	0.56
2:B:924:GLU:HB3	2:B:929:PHE:CZ	2.40	0.56
3:C:30:THR:OG1	3:C:34:MET:HG3	2.06	0.56
1:A:503:MET:HE1	6:H:24:PHE:HE2	1.70	0.56
12:N:18:DC:H4'	12:N:19:DA:O5'	2.05	0.56
1:A:741:VAL:HG22	1:A:753:GLU:HB2	1.86	0.56
2:B:43:VAL:HG22	2:B:200:GLN:HE22	1.70	0.56
2:B:331:VAL:HG12	2:B:334:GLN:NE2	2.20	0.56
2:B:960:ALA:O	2:B:1001:LEU:HD21	2.05	0.56
2:B:979:TYR:CE1	8:J:32:GLY:HA3	2.41	0.56
6:H:42:HIS:O	6:H:121:MET:HG2	2.06	0.56
1:A:704:LEU:HA	1:A:740:ILE:HD13	1.87	0.56
2:B:70:VAL:HG23	2:B:72:PRO:HD3	1.87	0.56
6:H:67:ASN:HA	6:H:85:LEU:HB2	1.87	0.56
1:A:639:VAL:HA	1:A:643:SER:HB2	1.87	0.56
2:B:264:LEU:HD13	2:B:278:LEU:HD22	1.87	0.56
2:B:969:MET:HE1	2:B:1003:ARG:HD2	1.87	0.56
6:H:95:GLY:HA3	6:H:116:PHE:CD2	2.41	0.56
4:E:193:ILE:HG22	4:E:229:VAL:HA	1.88	0.56
2:B:111:LEU:HD22	2:B:181:THR:HG22	1.88	0.56
3:C:42:MET:HA	3:C:46:VAL:HG23	1.87	0.56
2:B:338:THR:O	2:B:339:LYS:HG2	2.05	0.55
2:B:969:MET:HG2	2:B:978:ALA:HB1	1.88	0.55
12:N:23:DG:H2'	12:N:23:DG:N3	2.21	0.55
2:B:237:SER:HB3	2:B:243:ARG:HD3	1.89	0.55
5:F:114:ILE:HD13	5:F:131:LEU:HD12	1.87	0.55
2:B:130:VAL:HG11	2:B:435:ILE:HG21	1.88	0.55
4:E:125:ILE:HB	4:E:149:ILE:HG22	1.89	0.55
3:C:11:PRO:HD2	9:K:100:PHE:HD2	1.70	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:79:SER:O	3:C:276:VAL:HG22	2.07	0.55
6:H:96:LYS:HA	6:H:137:GLN:HA	1.89	0.55
2:B:89:VAL:HG11	2:B:418:MET:HE1	1.89	0.55
4:E:37:TYR:CD2	4:E:63:LEU:HD13	2.42	0.55
1:A:796:THR:HG1	4:E:183:PHE:HZ	1.56	0.54
8:J:9:THR:HG21	8:J:44:CYS:HB2	1.90	0.54
6:H:91:TYR:HB3	6:H:143:MET:SD	2.47	0.54
1:A:615:GLN:HE22	2:B:1024:ARG:HH22	1.53	0.54
1:A:1086:ASP:HA	1:A:1089:ARG:HE	1.72	0.54
2:B:212:VAL:HG23	2:B:486:LEU:HD23	1.90	0.54
3:C:209:LYS:HD3	3:C:223:PHE:HE1	1.72	0.54
6:H:32:ALA:HB3	6:H:41:MET:HB3	1.87	0.54
1:A:987:GLU:HA	1:A:1003:PRO:HD2	1.89	0.54
5:F:79:LEU:O	5:F:83:MET:HG3	2.08	0.54
2:B:932:THR:HG23	2:B:934:GLN:H	1.72	0.54
3:C:138:PHE:HD2	3:C:142:SER:HB2	1.73	0.54
2:B:641:PRO:HD2	2:B:644:TYR:HE1	1.71	0.54
2:B:110:PHE:HZ	2:B:115:ALA:HB2	1.72	0.54
2:B:240:LYS:HZ1	2:B:243:ARG:HH11	1.56	0.54
2:B:247:ARG:HG3	2:B:265:THR:HG21	1.90	0.54
2:B:470:VAL:HG12	2:B:471:VAL:H	1.73	0.54
1:A:1036:VAL:HG11	1:A:1041:PRO:HG3	1.90	0.54
3:C:105:VAL:HG11	3:C:134:THR:OG1	2.07	0.54
2:B:924:GLU:HB3	2:B:929:PHE:CE2	2.43	0.53
6:H:109:LYS:HB3	6:H:126:ASP:N	2.23	0.53
1:A:469:VAL:HG13	1:A:473:PHE:HB2	1.91	0.53
5:F:65:MET:HE2	5:F:70:ARG:HG3	1.90	0.53
6:H:95:GLY:HA3	6:H:116:PHE:HD2	1.74	0.53
1:A:914:GLU:HA	7:I:47:GLU:HA	1.90	0.53
1:A:1017:LEU:HG	1:A:1018:GLU:H	1.73	0.53
8:J:9:THR:HG23	8:J:47:ARG:NH2	2.22	0.53
1:A:822:PHE:HB3	1:A:826:ASP:OD2	2.08	0.53
1:A:942:ASN:O	1:A:946:LEU:HD23	2.09	0.53
6:H:59:THR:CG2	6:H:144:ARG:HG2	2.38	0.53
1:A:1086:ASP:HB3	1:A:1089:ARG:NH2	2.23	0.53
2:B:392:ARG:HB2	2:B:661:GLU:HG3	1.89	0.53
1:A:702:LEU:HB2	1:A:741:VAL:HB	1.90	0.53
2:B:213:PHE:CD1	2:B:471:VAL:HB	2.44	0.53
2:B:746:ARG:NH2	8:J:53:VAL:HG12	2.24	0.53
2:B:786:MET:HE3	2:B:787:ASN:N	2.24	0.53
9:K:42:ILE:O	9:K:45:ILE:HG22	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:81:ARG:HD3	3:C:133:VAL:HB	1.91	0.53
7:I:74:VAL:HG21	7:I:82:GLY:O	2.09	0.53
2:B:391:PHE:CD2	2:B:394:LYS:HD2	2.45	0.52
2:B:366:ARG:HH22	2:B:564:LEU:HB2	1.74	0.52
6:H:9:GLU:HA	6:H:60:LEU:O	2.08	0.52
1:A:511:ALA:HB1	9:K:47:ARG:HH22	1.74	0.52
2:B:69:LEU:H	2:B:88:THR:HG22	1.74	0.52
2:B:947:PHE:HB2	2:B:948:PRO:HD3	1.91	0.52
2:B:1016:ASN:HD22	2:B:1019:THR:HG22	1.73	0.52
5:F:65:MET:HB2	5:F:131:LEU:HB3	1.92	0.52
1:A:561:ILE:HG22	1:A:568:LEU:HD12	1.90	0.52
3:C:78:THR:OG1	3:C:135:PRO:HD2	2.09	0.52
4:E:212:LYS:HD3	4:E:226:TYR:CZ	2.45	0.52
6:H:89:TYR:CD2	6:H:144:ARG:HD2	2.45	0.52
1:A:805:ILE:HD11	4:E:183:PHE:CE1	2.45	0.52
1:A:913:VAL:HG23	1:A:914:GLU:HG2	1.91	0.52
2:B:167:ILE:HG13	2:B:167:ILE:O	2.10	0.52
2:B:69:LEU:HD13	2:B:71:GLU:HB3	1.92	0.52
2:B:248:LEU:HB2	2:B:375:LEU:HD21	1.90	0.52
3:C:8:GLN:NE2	9:K:96:LYS:HG2	2.24	0.52
3:C:194:ILE:HG22	3:C:196:ILE:HG23	1.92	0.52
1:A:954:GLN:HA	1:A:957:LEU:HD13	1.90	0.52
2:B:629:VAL:HG21	2:B:656:GLU:HG3	1.91	0.52
4:E:23:SER:N	4:E:64:GLN:HG2	2.25	0.52
1:A:939:ILE:HD12	1:A:1005:LEU:HD23	1.92	0.52
2:B:190:SER:HA	2:B:193:LYS:NZ	2.25	0.52
12:N:25:DA:H1'	12:N:26:DC:N1	2.24	0.52
1:A:945:LEU:O	1:A:946:LEU:HD22	2.09	0.51
1:A:1108:ILE:HD12	1:A:1109:PRO:HD2	1.91	0.51
2:B:1015:TYR:HE1	2:B:1022:MET:HG2	1.75	0.51
8:J:3:ILE:HD12	8:J:4:PRO:HD2	1.92	0.51
12:N:15:DT:H2''	12:N:16:DA:H4'	1.92	0.51
1:A:967:LEU:HD13	1:A:970:LYS:HZ2	1.74	0.51
3:C:157:LEU:HD22	3:C:161:GLN:HB3	1.92	0.51
1:A:938:HIS:HE1	1:A:988:CYS:HB3	1.74	0.51
2:B:700:VAL:HG21	2:B:714:GLN:HG3	1.93	0.51
9:K:14:GLU:HG3	9:K:15:GLY:H	1.75	0.51
2:B:244:PHE:HB3	2:B:267:TYR:HD1	1.75	0.51
2:B:474:LEU:HD11	2:B:482:SER:HA	1.93	0.51
5:F:105:LEU:HA	5:F:110:ILE:HD11	1.93	0.51
1:A:493:LEU:HD12	2:B:945:HIS:CG	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:749:LEU:HB3	1:A:753:GLU:HG3	1.91	0.51
1:A:990:SER:HA	1:A:1000:SER:HB3	1.92	0.51
2:B:51:ASN:HD22	2:B:177:VAL:HG22	1.75	0.51
2:B:425:HIS:HB3	2:B:430:GLY:HA2	1.93	0.51
2:B:553:MET:HG3	2:B:553:MET:O	2.11	0.51
10:L:10:TYR:HD2	10:L:21:LEU:H	1.57	0.51
2:B:737:LEU:HA	2:B:800:GLN:HE21	1.75	0.51
1:A:857:LEU:HD22	1:A:1135:SER:HB2	1.92	0.51
2:B:585:TYR:CE2	2:B:589:ASP:OD2	2.64	0.51
4:E:38:LEU:HD12	4:E:39:ALA:N	2.25	0.50
6:H:114:VAL:HG21	6:H:121:MET:HE3	1.92	0.50
8:J:22:LEU:O	8:J:26:GLN:HG2	2.11	0.50
1:A:991:PHE:CD2	1:A:992:ARG:HG3	2.43	0.50
9:K:61:TYR:CD2	9:K:71:ILE:HD11	2.45	0.50
1:A:928:ILE:HG13	1:A:929:PHE:H	1.76	0.50
2:B:277:VAL:HG11	2:B:330:TYR:HD2	1.76	0.50
3:C:55:GLU:HG2	10:L:47:GLN:HG2	1.92	0.50
9:K:53:ASP:HB3	9:K:56:VAL:HG22	1.93	0.50
12:N:22:DA:H2'	12:N:23:DG:H8	1.76	0.50
1:A:606:PRO:HA	1:A:609:MET:HE2	1.94	0.50
1:A:961:GLU:HA	1:A:964:ILE:HG12	1.93	0.50
1:A:992:ARG:NH2	7:I:42:CYS:HB2	2.22	0.50
1:A:1058:TRP:HE3	1:A:1058:TRP:H	1.58	0.50
4:E:126:LEU:HD13	4:E:150:PHE:HB2	1.92	0.50
6:H:114:VAL:O	6:H:120:LEU:HA	2.12	0.50
7:I:15:TYR:HD2	7:I:30:ARG:HH21	1.58	0.50
1:A:934:CYS:SG	1:A:1010:TYR:HB3	2.51	0.50
2:B:190:SER:HA	2:B:193:LYS:HZ3	1.76	0.50
2:B:745:GLN:HB3	8:J:51:THR:HG22	1.93	0.50
3:C:34:MET:HA	3:C:34:MET:HE2	1.92	0.50
7:I:87:PHE:HE1	7:I:89:ALA:HB2	1.77	0.50
1:A:727:LYS:O	2:B:670:TRP:HH2	1.94	0.50
1:A:333:PHE:CZ	1:A:609:MET:HE3	2.47	0.50
2:B:484:ILE:HD11	2:B:696:SER:HB3	1.94	0.50
2:B:1015:TYR:CE1	2:B:1022:MET:HG2	2.47	0.50
2:B:718:HIS:CE1	2:B:915:GLY:HA2	2.46	0.50
4:E:94:LYS:HD2	4:E:115:ILE:HD12	1.93	0.50
2:B:99:PRO:HG2	2:B:180:ASN:ND2	2.27	0.49
2:B:779:ASN:O	2:B:943:ASN:HB2	2.12	0.49
2:B:786:MET:HE3	2:B:787:ASN:H	1.77	0.49
6:H:67:ASN:HB3	6:H:83:LYS:HE2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:457:TRP:HB2	2:B:470:VAL:HG11	1.94	0.49
5:F:91:LEU:H	5:F:91:LEU:HD23	1.76	0.49
2:B:47:LEU:HD23	2:B:173:MET:SD	2.52	0.49
8:J:14:ILE:HG13	8:J:17:LYS:HD2	1.95	0.49
1:A:762:ARG:HA	1:A:765:ILE:HG12	1.95	0.49
2:B:229:SER:CB	2:B:230:PRO:HD3	2.41	0.49
2:B:433:LYS:HB3	2:B:436:GLU:HB2	1.93	0.49
3:C:243:GLU:HG2	3:C:244:VAL:N	2.28	0.49
9:K:24:ASP:HB3	9:K:30:ALA:HB3	1.94	0.49
9:K:104:GLN:O	9:K:108:GLU:HG2	2.13	0.49
1:A:328:ILE:HG22	1:A:450:PHE:HE1	1.78	0.49
1:A:474:SER:HB2	1:A:477:LYS:HG2	1.95	0.49
1:A:973:LYS:HG3	1:A:976:GLU:HG2	1.95	0.49
2:B:114:HIS:O	2:B:118:GLN:HG3	2.12	0.49
2:B:212:VAL:CG2	2:B:486:LEU:HD23	2.43	0.49
6:H:89:TYR:HD2	6:H:144:ARG:HD2	1.78	0.49
6:H:107:THR:OG1	6:H:108:PRO:HD3	2.13	0.49
6:H:59:THR:HG22	6:H:144:ARG:HG2	1.95	0.48
1:A:915:PHE:HE1	1:A:1007:PHE:HZ	1.60	0.48
2:B:277:VAL:O	2:B:327:ALA:HB1	2.13	0.48
2:B:1038:ILE:HG22	2:B:1039:HIS:N	2.28	0.48
4:E:108:ILE:HA	4:E:111:VAL:HG22	1.95	0.48
1:A:527:PRO:HB2	1:A:529:VAL:O	2.13	0.48
2:B:646:PHE:HE1	2:B:655:LEU:HD13	1.78	0.48
9:K:61:TYR:HA	9:K:72:ILE:O	2.13	0.48
2:B:287:ASP:C	2:B:289:GLU:H	2.21	0.48
2:B:623:LEU:O	2:B:659:GLY:HA2	2.13	0.48
3:C:63:LEU:HD13	3:C:67:PHE:HD2	1.77	0.48
3:C:204:LEU:HD12	3:C:209:LYS:HE3	1.95	0.48
1:A:364:GLN:HA	1:A:367:VAL:HG12	1.94	0.48
1:A:698:GLN:HB3	2:B:951:GLN:OE1	2.13	0.48
1:A:774:GLU:HB3	1:A:775:PRO:HD3	1.95	0.48
1:A:882:ASN:OD1	1:A:1103:ASP:HB3	2.14	0.48
3:C:148:GLU:HG3	3:C:150:ARG:H	1.79	0.48
6:H:46:ASN:OD1	6:H:48:GLU:HG3	2.13	0.48
6:H:114:VAL:CG2	6:H:121:MET:HE3	2.43	0.48
8:J:54:ASP:OD1	8:J:56:ILE:HG22	2.13	0.48
1:A:755:MET:HE1	2:B:505:PRO:HB2	1.94	0.48
1:A:965:ASN:O	1:A:968:VAL:HG12	2.13	0.48
1:A:1019:ARG:HG3	1:A:1020:THR:HG23	1.96	0.48
2:B:671:GLY:O	2:B:675:LEU:HB2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:79:LEU:HD23	4:E:79:LEU:O	2.14	0.48
1:A:979:LYS:HB3	1:A:1010:TYR:CZ	2.48	0.48
2:B:792:GLU:HB3	3:C:177:HIS:NE2	2.29	0.48
6:H:99:LYS:HB3	6:H:113:TYR:HB2	1.96	0.48
1:A:626:MET:HB3	1:A:630:ASP:HB2	1.96	0.48
2:B:721:GLN:O	2:B:1038:ILE:HG13	2.14	0.48
2:B:101:LEU:HD13	2:B:110:PHE:CE1	2.49	0.47
2:B:674:GLN:O	2:B:678:GLN:HG2	2.13	0.47
1:A:882:ASN:HD21	1:A:1106:ARG:NH1	2.12	0.47
1:A:1105:LYS:HA	4:E:162:HIS:HA	1.95	0.47
2:B:779:ASN:HB3	2:B:785:VAL:HG23	1.96	0.47
1:A:375:TYR:CZ	1:A:383:SER:HB3	2.49	0.47
2:B:196:CYS:HB3	2:B:199:ASP:HB2	1.95	0.47
6:H:66:LEU:HD13	6:H:140:PHE:CD1	2.49	0.47
1:A:473:PHE:HA	1:A:478:GLN:NE2	2.30	0.47
3:C:39:ARG:HA	3:C:186:VAL:HG11	1.95	0.47
6:H:97:LEU:HG	6:H:114:VAL:HG12	1.96	0.47
1:A:964:ILE:HD12	1:A:980:LYS:HG3	1.97	0.47
4:E:97:PHE:CD1	4:E:126:LEU:HG	2.49	0.47
2:B:261:GLU:HG3	2:B:313:GLU:OE1	2.14	0.47
1:A:431:HIS:CE1	1:A:437:LYS:HE3	2.50	0.47
1:A:521:SER:HB2	1:A:522:ARG:NH1	2.30	0.47
1:A:569:SER:HB2	6:H:120:LEU:HD21	1.96	0.47
2:B:771:ALA:O	2:B:941:VAL:HA	2.14	0.47
12:N:18:DC:H1'	12:N:19:DA:C8	2.50	0.47
1:A:745:PHE:CE1	2:B:707:HIS:HA	2.50	0.47
1:A:903:LEU:HG	1:A:1043:ILE:HG13	1.96	0.47
1:A:998:LYS:CD	1:A:1000:SER:H	2.28	0.47
2:B:408:ARG:O	2:B:411:LEU:HG	2.15	0.47
2:B:594:ARG:HA	2:B:599:LEU:HB2	1.97	0.47
3:C:86:ARG:HG2	3:C:102:PHE:HB3	1.97	0.47
10:L:27:ILE:HG23	10:L:37:LEU:HD12	1.96	0.47
2:B:848:ALA:HB1	2:B:850:MET:HE3	1.97	0.46
2:B:1019:THR:HG23	2:B:1021:GLU:H	1.79	0.46
3:C:120:ASP:HB3	3:C:156:LYS:HG2	1.96	0.46
1:A:879:LEU:HD23	1:A:1107:SER:HB3	1.98	0.46
2:B:244:PHE:CE2	2:B:371:MET:HE1	2.50	0.46
2:B:470:VAL:HG12	2:B:471:VAL:N	2.30	0.46
4:E:166:LEU:HD13	4:E:213:VAL:HG13	1.97	0.46
7:I:27:TYR:CE2	7:I:38:ALA:HA	2.50	0.46
1:A:458:PHE:HE1	1:A:461:GLN:HE22	1.62	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1092:ILE:HG23	4:E:156:LEU:HD22	1.97	0.46
2:B:334:GLN:HE21	2:B:346:VAL:HG11	1.79	0.46
2:B:542:GLU:O	2:B:542:GLU:HG2	2.16	0.46
12:N:25:DA:H1'	12:N:26:DC:C6	2.51	0.46
1:A:671:ALA:HB2	1:A:692:ILE:HG21	1.97	0.46
1:A:1096:LEU:HB2	4:E:31:GLU:OE2	2.14	0.46
2:B:273:ILE:HG23	2:B:330:TYR:HE2	1.81	0.46
1:A:358:HIS:NE2	5:F:95:THR:HG22	2.30	0.46
6:H:37:LEU:O	6:H:39:MET:HG2	2.14	0.46
1:A:984:SER:HA	1:A:1006:MET:HE2	1.98	0.46
1:A:1000:SER:O	1:A:1003:PRO:HD3	2.16	0.46
2:B:963:LYS:HB2	2:B:1031:PRO:HD2	1.98	0.46
6:H:6:ILE:HG21	6:H:61:ALA:HB1	1.98	0.46
1:A:835:ALA:HB1	1:A:1143:VAL:HG23	1.98	0.46
1:A:1047:ASN:OD1	1:A:1073:ASP:HB3	2.16	0.46
2:B:118:GLN:HB2	2:B:120:MET:HE2	1.98	0.46
6:H:90:GLU:OE1	6:H:144:ARG:HB2	2.15	0.46
1:A:546:GLN:HG2	1:A:567:LEU:H	1.80	0.46
1:A:612:LEU:HD23	1:A:612:LEU:H	1.81	0.46
4:E:169:ARG:NH1	4:E:171:LEU:HD11	2.31	0.46
2:B:14:GLU:HB2	2:B:634:HIS:HB2	1.98	0.46
2:B:240:LYS:NZ	2:B:243:ARG:HH11	2.13	0.46
4:E:210:ILE:HG12	4:E:228:CYS:HB3	1.97	0.46
6:H:92:VAL:HG22	6:H:142:LEU:HG	1.97	0.46
3:C:116:ASP:HA	3:C:158:ARG:NH2	2.31	0.46
4:E:159:LEU:HD21	4:E:202:TYR:CG	2.52	0.45
1:A:931:MET:HE3	1:A:933:ILE:HG12	1.98	0.45
2:B:91:PHE:HE1	2:B:415:ARG:HH21	1.63	0.45
2:B:823:VAL:HG13	2:B:861:THR:HB	1.99	0.45
6:H:101:THR:HA	6:H:103:ARG:CZ	2.46	0.45
2:B:882:VAL:HG22	2:B:896:VAL:HG22	1.97	0.45
1:A:507:PHE:C	1:A:508:LEU:HD12	2.42	0.45
1:A:1144:LEU:HB2	1:A:1147:HIS:HD2	1.75	0.45
2:B:308:VAL:HA	2:B:311:ILE:HD12	1.98	0.45
3:C:109:LEU:HB2	3:C:126:LEU:HD13	1.99	0.45
6:H:144:ARG:HG3	6:H:145:LYS:CG	2.46	0.45
1:A:720:ASP:O	1:A:723:GLN:HG2	2.17	0.45
1:A:749:LEU:H	2:B:704:ASN:HB2	1.81	0.45
2:B:101:LEU:O	2:B:107:GLU:HB2	2.16	0.45
3:C:158:ARG:HA	3:C:158:ARG:CZ	2.46	0.45
3:C:242:GLU:HB3	3:C:245:ILE:HD11	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:627:LEU:HD12	2:B:658:ILE:HD12	1.99	0.45
2:B:799:GLU:HG3	2:B:901:VAL:HG22	1.97	0.45
3:C:58:VAL:HB	10:L:43:ARG:NH2	2.31	0.45
4:E:54:VAL:HG22	4:E:85:HIS:NE2	2.32	0.45
6:H:62:MET:SD	6:H:139:LEU:HD12	2.57	0.45
1:A:367:VAL:HG22	1:A:385:ARG:HH21	1.82	0.45
1:A:842:LYS:HB3	1:A:842:LYS:HE2	1.81	0.45
1:A:967:LEU:HD13	1:A:970:LYS:NZ	2.31	0.45
2:B:257:PHE:O	2:B:258:LYS:HG2	2.17	0.45
2:B:289:GLU:HA	2:B:292:ASP:HB2	1.97	0.45
2:B:823:VAL:HG22	2:B:861:THR:HB	1.99	0.45
1:A:859:LYS:HE2	1:A:863:LEU:HD12	1.99	0.45
2:B:22:GLU:HA	2:B:25:LEU:HB2	1.99	0.45
2:B:750:LYS:HZ3	2:B:984:ARG:HH21	1.64	0.45
2:B:810:SER:HB3	2:B:890:GLY:HA3	1.99	0.45
1:A:408:ASP:O	1:A:427:ARG:HA	2.17	0.44
1:A:698:GLN:HA	1:A:745:PHE:HB2	2.00	0.44
1:A:413:ASN:OD1	1:A:422:SER:HB2	2.17	0.44
1:A:581:ILE:O	1:A:585:VAL:HG12	2.18	0.44
1:A:697:GLN:HB2	2:B:951:GLN:NE2	2.32	0.44
1:A:725:TYR:OH	1:A:733:SER:HB3	2.16	0.44
1:A:981:MET:HG2	1:A:1010:TYR:OH	2.17	0.44
1:A:985:VAL:C	1:A:987:GLU:H	2.25	0.44
2:B:359:LYS:CG	2:B:363:GLN:HG3	2.48	0.44
2:B:479:PRO:HG2	2:B:761:VAL:HB	1.99	0.44
3:C:195:ILE:HG13	3:C:258:GLU:HG2	1.99	0.44
1:A:503:MET:HG2	1:A:577:LEU:HD11	1.99	0.44
1:A:938:HIS:HB3	1:A:940:HIS:CD2	2.52	0.44
2:B:20:LEU:HD12	2:B:24:PHE:HE2	1.83	0.44
2:B:127:LYS:HG2	2:B:166:PRO:HA	1.99	0.44
2:B:415:ARG:HA	2:B:418:MET:HG3	1.99	0.44
6:H:60:LEU:HD11	6:H:141:LEU:HD11	1.99	0.44
1:A:798:ARG:NH1	5:F:119:PRO:HB2	2.32	0.44
2:B:268:PHE:CD2	2:B:342:PRO:HD2	2.52	0.44
2:B:633:LEU:HD12	2:B:635:LYS:HZ3	1.82	0.44
3:C:46:VAL:HG11	3:C:281:LEU:HD23	2.00	0.44
2:B:827:LYS:HD3	2:B:839:ASP:O	2.18	0.44
3:C:39:ARG:HD3	3:C:188:PHE:CE1	2.53	0.44
4:E:171:LEU:HB2	4:E:175:GLU:OE2	2.18	0.44
2:B:398:LEU:HD13	2:B:536:VAL:HG11	1.99	0.44
2:B:553:MET:SD	2:B:578:GLY:HA3	2.58	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:183:PHE:CD2	4:E:183:PHE:O	2.70	0.44
6:H:116:PHE:HB2	6:H:119:LEU:HB2	1.98	0.44
1:A:842:LYS:HA	1:A:845:LEU:HG	1.98	0.44
2:B:231:TRP:HB3	2:B:375:LEU:HD11	1.99	0.44
2:B:670:TRP:CD1	2:B:689:LEU:HD21	2.40	0.44
2:B:880:GLN:OE1	2:B:899:ARG:HD3	2.18	0.44
1:A:487:LEU:HD12	1:A:582:ASN:OD1	2.18	0.44
1:A:577:LEU:HD23	1:A:580:ILE:HD12	2.00	0.44
1:A:880:TYR:HD2	1:A:1106:ARG:HB3	1.83	0.44
2:B:20:LEU:HD12	2:B:24:PHE:CE2	2.52	0.44
2:B:58:LEU:HD21	2:B:126:MET:HE2	1.98	0.44
2:B:222:LYS:NZ	2:B:573:ASN:HB2	2.32	0.44
3:C:43:ILE:HD11	3:C:186:VAL:HB	1.99	0.44
3:C:67:PHE:CE2	3:C:71:ARG:HD2	2.53	0.44
1:A:342:PRO:HB3	1:A:434:ASN:HA	2.00	0.44
2:B:126:MET:HB3	2:B:167:ILE:O	2.17	0.44
2:B:540:ILE:HD13	2:B:600:PRO:HB2	1.99	0.44
4:E:40:ARG:NE	4:E:80:ARG:HB2	2.33	0.44
5:F:61:THR:HG21	5:F:116:ARG:HH11	1.81	0.44
5:F:102:MET:HE3	5:F:103:LYS:NZ	2.33	0.44
1:A:537:PRO:HB2	1:A:539:TRP:CZ3	2.53	0.43
1:A:755:MET:O	1:A:759:VAL:HG23	2.17	0.43
2:B:366:ARG:HH21	2:B:564:LEU:HD22	1.83	0.43
3:C:200:MET:HB2	3:C:256:LEU:HD13	1.99	0.43
10:L:28:GLN:HG3	10:L:35:ARG:NH1	2.33	0.43
2:B:396:ILE:HG22	2:B:398:LEU:HD12	2.00	0.43
1:A:502:MET:HA	1:A:505:GLN:HE21	1.84	0.43
1:A:836:MET:HE3	1:A:836:MET:O	2.18	0.43
2:B:943:ASN:OD1	2:B:944:PRO:HD2	2.18	0.43
4:E:56:LEU:HD12	4:E:57:GLU:N	2.33	0.43
1:A:325:ARG:O	2:B:1045:VAL:HA	2.19	0.43
1:A:499:LEU:HD23	1:A:499:LEU:HA	1.77	0.43
2:B:641:PRO:HD2	2:B:644:TYR:CE1	2.52	0.43
2:B:846:VAL:HG12	2:B:846:VAL:O	2.18	0.43
2:B:900:GLN:HB3	2:B:902:ARG:NH1	2.33	0.43
2:B:968:PRO:HG3	8:J:41:VAL:O	2.17	0.43
2:B:982:VAL:O	2:B:984:ARG:HG2	2.18	0.43
6:H:34:SER:HB3	6:H:38:ASP:HA	2.01	0.43
2:B:185:GLY:O	2:B:186:LYS:HE2	2.19	0.43
2:B:646:PHE:CE1	2:B:655:LEU:HD13	2.52	0.43
1:A:1029:TYR:O	1:A:1033:LEU:HD23	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1088:TRP:HA	1:A:1091:VAL:HG12	2.00	0.43
2:B:280:PHE:HA	2:B:284:VAL:HG12	2.00	0.43
2:B:391:PHE:HE1	2:B:509:HIS:HE2	1.65	0.43
2:B:772:VAL:HG12	2:B:942:ILE:HG13	2.00	0.43
3:C:147:SER:O	8:J:20:THR:HG21	2.17	0.43
4:E:70:TYR:O	4:E:75:ASP:HB3	2.19	0.43
4:E:95:VAL:HG12	4:E:124:LEU:HD12	2.01	0.43
2:B:40:TYR:HE2	2:B:646:PHE:CE2	2.36	0.43
2:B:969:MET:HE1	2:B:1003:ARG:HB3	2.01	0.43
4:E:169:ARG:NE	4:E:171:LEU:HD21	2.34	0.43
11:T:10:DT:H1'	11:T:11:DA:H5'	2.00	0.43
1:A:1111:SER:OG	1:A:1114:GLN:HG2	2.18	0.43
2:B:242:ASN:O	2:B:243:ARG:HD2	2.19	0.43
2:B:771:ALA:HA	2:B:1028:PHE:O	2.19	0.43
3:C:67:PHE:O	3:C:71:ARG:HG3	2.18	0.43
6:H:12:PHE:CE1	6:H:34:SER:HB2	2.54	0.43
1:A:640:ARG:O	1:A:644:PRO:HG2	2.19	0.43
6:H:113:TYR:CE1	6:H:122:LEU:HB2	2.53	0.43
6:H:137:GLN:HG3	6:H:138:ARG:NH1	2.34	0.43
9:K:47:ARG:HD2	9:K:61:TYR:CD1	2.54	0.43
1:A:796:THR:HG22	1:A:808:PHE:O	2.19	0.42
1:A:946:LEU:HD13	1:A:951:ILE:HD12	2.00	0.42
2:B:510:TRP:HH2	2:B:670:TRP:HE1	1.66	0.42
3:C:31:ASP:O	3:C:34:MET:HB2	2.19	0.42
4:E:151:GLN:HG3	4:E:153:THR:H	1.84	0.42
6:H:101:THR:OG1	6:H:111:GLU:HB2	2.19	0.42
12:N:24:DT:H2'	12:N:25:DA:C4	2.53	0.42
1:A:777:THR:HG23	1:A:1166:TYR:CE2	2.53	0.42
1:A:865:LYS:HD3	1:A:1165:ASN:ND2	2.34	0.42
2:B:110:PHE:CZ	2:B:115:ALA:HB2	2.54	0.42
3:C:113:CYS:HB3	3:C:158:ARG:O	2.19	0.42
11:T:5:DT:H2''	11:T:6:DC:C5	2.54	0.42
1:A:415:PRO:HD3	1:A:456:HIS:CD2	2.53	0.42
1:A:789:ILE:HD11	1:A:1150:LEU:HD11	2.00	0.42
2:B:363:GLN:HE22	2:B:556:LEU:HB3	1.83	0.42
2:B:930:ALA:HB1	2:B:1014:VAL:HB	2.02	0.42
1:A:333:PHE:CE2	1:A:609:MET:HE3	2.54	0.42
1:A:336:VAL:HG22	1:A:439:ASN:ND2	2.35	0.42
1:A:643:SER:HA	1:A:646:VAL:HG22	2.00	0.42
1:A:742:LYS:O	1:A:742:LYS:HG2	2.17	0.42
2:B:240:LYS:HB3	2:B:240:LYS:HE3	1.74	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:538:THR:O	2:B:620:ALA:HB2	2.19	0.42
2:B:729:ASN:ND2	2:B:732:ILE:HD11	2.34	0.42
4:E:78:ARG:HG3	4:E:80:ARG:NH1	2.33	0.42
1:A:941:LEU:HD13	1:A:946:LEU:HG	2.01	0.42
2:B:718:HIS:ND1	2:B:915:GLY:HA2	2.35	0.42
2:B:785:VAL:HB	2:B:941:VAL:CG1	2.49	0.42
3:C:293:LEU:HD11	9:K:94:LEU:HB2	2.02	0.42
1:A:555:CYS:HB3	1:A:591:GLU:HG3	2.02	0.42
1:A:624:LEU:O	1:A:699:ILE:HG23	2.20	0.42
1:A:918:GLU:CG	1:A:936:HIS:HB3	2.49	0.42
2:B:65:SER:HB3	2:B:415:ARG:CZ	2.49	0.42
3:C:139:GLY:O	3:C:144:ALA:HB3	2.18	0.42
8:J:49:LEU:HD23	8:J:49:LEU:HA	1.85	0.42
11:T:5:DT:C2	12:N:31:DG:C2	3.07	0.42
1:A:942:ASN:HB3	1:A:945:LEU:HB2	2.00	0.42
2:B:244:PHE:CZ	2:B:371:MET:HE1	2.55	0.42
1:A:334:ARG:HA	1:A:334:ARG:HD3	1.77	0.42
2:B:117:LEU:HD11	2:B:732:ILE:O	2.20	0.42
2:B:571:LEU:HA	2:B:575:ASP:O	2.20	0.42
2:B:750:LYS:NZ	2:B:984:ARG:HH21	2.18	0.42
3:C:107:PHE:HE2	3:C:136:VAL:HG13	1.85	0.42
6:H:96:LYS:O	6:H:114:VAL:HB	2.19	0.42
1:A:343:MET:HG3	1:A:432:GLU:HG3	2.01	0.42
1:A:796:THR:OG1	4:E:183:PHE:HZ	2.01	0.42
1:A:1132:LEU:HD12	1:A:1132:LEU:HA	1.88	0.42
2:B:300:ASP:O	2:B:303:ILE:HG12	2.20	0.42
2:B:540:ILE:HG22	2:B:541:MET:O	2.20	0.42
1:A:557:GLY:HA3	1:A:560:PHE:CE1	2.54	0.41
1:A:751:PRO:HA	1:A:754:GLU:HB2	2.02	0.41
2:B:277:VAL:HG11	2:B:330:TYR:CD2	2.53	0.41
2:B:424:ARG:NE	2:B:424:ARG:HA	2.35	0.41
7:I:87:PHE:CE1	7:I:89:ALA:HB2	2.55	0.41
2:B:289:GLU:CD	2:B:560:THR:HG21	2.45	0.41
5:F:80:GLN:HA	5:F:83:MET:SD	2.60	0.41
12:N:15:DT:O3'	12:N:16:DA:H4'	2.20	0.41
1:A:694:LYS:HZ2	1:A:698:GLN:HE22	1.67	0.41
1:A:727:LYS:HD2	1:A:727:LYS:HA	1.95	0.41
1:A:906:VAL:HG21	1:A:951:ILE:HD11	2.02	0.41
1:A:920:ARG:NH1	1:A:921:LYS:HB2	2.35	0.41
2:B:54:ILE:HD13	2:B:54:ILE:HA	1.92	0.41
9:K:47:ARG:HD2	9:K:61:TYR:HD1	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:N:26:DC:H2'	12:N:27:DT:H6	1.78	0.41
1:A:631:MET:HA	1:A:634:ILE:HG22	2.01	0.41
1:A:961:GLU:HG2	1:A:982:ASN:HD21	1.85	0.41
2:B:585:TYR:CE1	2:B:589:ASP:OD2	2.68	0.41
2:B:723:ILE:HG22	2:B:741:LEU:HG	2.01	0.41
2:B:772:VAL:HG12	2:B:942:ILE:CG1	2.50	0.41
8:J:56:ILE:HD12	8:J:59:LEU:HD12	2.03	0.41
1:A:325:ARG:HA	1:A:455:VAL:O	2.21	0.41
1:A:917:VAL:HG12	7:I:44:TYR:HB2	2.01	0.41
2:B:266:VAL:HG13	2:B:270:SER:N	2.36	0.41
2:B:568:HIS:CE1	2:B:612:LYS:HG3	2.56	0.41
4:E:48:ARG:NH1	4:E:48:ARG:HB3	2.35	0.41
6:H:62:MET:HE2	6:H:62:MET:HB2	1.81	0.41
9:K:49:GLN:HA	9:K:49:GLN:OE1	2.20	0.41
2:B:162:THR:OG1	2:B:435:ILE:HD13	2.21	0.41
2:B:693:LEU:HD11	2:B:989:PHE:CE2	2.51	0.41
1:A:409:VAL:HA	1:A:426:LEU:O	2.20	0.41
1:A:796:THR:OG1	4:E:183:PHE:CZ	2.71	0.41
1:A:943:LYS:HE2	1:A:947:GLU:CD	2.46	0.41
2:B:803:SER:HA	2:B:896:VAL:O	2.20	0.41
2:B:1038:ILE:HG22	2:B:1039:HIS:H	1.86	0.41
4:E:73:ARG:HB3	4:E:74:PRO:HD3	2.02	0.41
1:A:760:ALA:O	1:A:764:VAL:HG23	2.19	0.41
1:A:920:ARG:HB2	1:A:923:GLN:HE22	1.85	0.41
1:A:1096:LEU:HD21	4:E:156:LEU:HD21	2.03	0.41
2:B:222:LYS:HZ2	2:B:619:ASP:HB2	1.85	0.41
2:B:335:ILE:HD11	2:B:346:VAL:HG22	2.03	0.41
2:B:537:SER:HB3	2:B:624:LEU:HD11	2.02	0.41
2:B:737:LEU:HA	2:B:800:GLN:NE2	2.36	0.41
2:B:835:VAL:HA	2:B:838:LEU:HD13	2.03	0.41
1:A:357:VAL:HG22	5:F:84:ASN:OD1	2.20	0.41
1:A:883:GLU:HG3	1:A:892:GLN:OE1	2.21	0.41
1:A:964:ILE:HG13	1:A:965:ASN:N	2.35	0.41
1:A:1042:ARG:HA	1:A:1078:LYS:CG	2.46	0.41
1:A:1086:ASP:HA	1:A:1089:ARG:NE	2.35	0.41
2:B:247:ARG:CZ	2:B:250:GLU:HG3	2.50	0.41
2:B:780:GLN:HA	2:B:943:ASN:ND2	2.36	0.41
3:C:227:THR:HG23	3:C:229:GLN:HB2	2.02	0.41
4:E:137:LEU:HD23	4:E:137:LEU:H	1.86	0.41
6:H:112:MET:HE1	6:H:129:HIS:HB3	2.03	0.41
1:A:470:LEU:HD23	5:F:98:LEU:HD21	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:973:LYS:CG	1:A:976:GLU:HG2	2.51	0.41
2:B:808:VAL:HG21	2:B:824:GLN:HA	2.02	0.41
1:A:463:LEU:HD21	5:F:79:LEU:HD21	2.03	0.40
1:A:761:ALA:O	1:A:765:ILE:HG23	2.21	0.40
1:A:1098:VAL:O	1:A:1102:ILE:HG22	2.22	0.40
2:B:69:LEU:HD12	2:B:69:LEU:O	2.21	0.40
2:B:85:ARG:H	2:B:85:ARG:HG2	1.60	0.40
3:C:138:PHE:CD2	3:C:142:SER:HB2	2.55	0.40
4:E:70:TYR:CZ	4:E:80:ARG:HB3	2.56	0.40
6:H:8:PHE:HB3	6:H:62:MET:HB3	2.03	0.40
9:K:42:ILE:HD13	9:K:42:ILE:HA	1.87	0.40
1:A:376:THR:HG22	1:A:377:GLN:O	2.21	0.40
2:B:197:ALA:HB3	8:J:58:LYS:NZ	2.36	0.40
2:B:571:LEU:HB2	2:B:615:ARG:HG3	2.02	0.40
2:B:538:THR:HG23	2:B:539:GLN:N	2.36	0.40
4:E:214:SER:HA	4:E:224:VAL:HG22	2.04	0.40
6:H:41:MET:SD	6:H:123:LEU:HD13	2.62	0.40
6:H:100:ILE:HG12	6:H:102:GLU:HG3	2.04	0.40
2:B:245:ILE:HG13	2:B:265:THR:CG2	2.48	0.40
6:H:62:MET:SD	6:H:139:LEU:HB3	2.61	0.40
9:K:35:ILE:O	9:K:71:ILE:HG22	2.21	0.40
1:A:908:LEU:HA	1:A:911:THR:OG1	2.22	0.40
2:B:221:THR:O	2:B:222:LYS:HG2	2.21	0.40
2:B:1013:ARG:NH1	3:C:240:TYR:HB3	2.37	0.40
4:E:37:TYR:HB2	4:E:66:PHE:CE2	2.56	0.40
6:H:8:PHE:CE2	6:H:60:LEU:HD22	2.56	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	819/2032 (40%)	716 (87%)	102 (12%)	1 (0%)	48	81
2	B	992/1169 (85%)	876 (88%)	116 (12%)	0	100	100
3	C	298/319 (93%)	270 (91%)	28 (9%)	0	100	100
4	E	206/230 (90%)	185 (90%)	21 (10%)	0	100	100
5	F	78/144 (54%)	75 (96%)	3 (4%)	0	100	100
6	H	140/146 (96%)	115 (82%)	25 (18%)	0	100	100
7	I	87/114 (76%)	73 (84%)	14 (16%)	0	100	100
8	J	62/71 (87%)	53 (86%)	9 (14%)	0	100	100
9	K	106/116 (91%)	99 (93%)	7 (7%)	0	100	100
10	L	44/51 (86%)	33 (75%)	11 (25%)	0	100	100
All	All	2832/4392 (64%)	2495 (88%)	336 (12%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	419	HIS

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	730/1709 (43%)	730 (100%)	0	100	100
2	B	879/1026 (86%)	879 (100%)	0	100	100
3	C	263/276 (95%)	263 (100%)	0	100	100
4	E	189/209 (90%)	189 (100%)	0	100	100
5	F	72/128 (56%)	72 (100%)	0	100	100
6	H	124/127 (98%)	124 (100%)	0	100	100
7	I	77/101 (76%)	77 (100%)	0	100	100
8	J	57/63 (90%)	57 (100%)	0	100	100
9	K	98/105 (93%)	98 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	L	41/46 (89%)	41 (100%)	0	100	100
All	All	2530/3790 (67%)	2530 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	439	ASN
1	A	461	GLN
1	A	478	GLN
1	A	505	GLN
1	A	515	GLN
1	A	615	GLN
1	A	698	GLN
1	A	781	ASN
1	A	969	GLN
1	A	1153	ASN
2	B	51	ASN
2	B	114	HIS
2	B	251	ASN
2	B	252	GLN
2	B	437	HIS
2	B	491	GLN
2	B	634	HIS
2	B	800	GLN
2	B	851	HIS
2	B	892	ASN
4	E	118	GLN
4	E	209	GLN
5	F	107	GLN
6	H	94	HIS
6	H	132	HIS
7	I	11	ASN
7	I	105	ASN

5.3.3 RNA ⓘ

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 8 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.