



Full wwPDB EM Validation Report ⓘ

May 10, 2026 – 12:19 AM JST

PDB ID : 9K14 / pdb_00009k14
EMDB ID : EMD-61964
Title : A cryo-EM structure of *B. oleracea* RNA polymerase V in complex with 3U scaffold at 3.8 Angstrom
Authors : Xie, G.; Du, X.; Du, J.
Deposited on : 2024-10-16
Resolution : 3.80 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

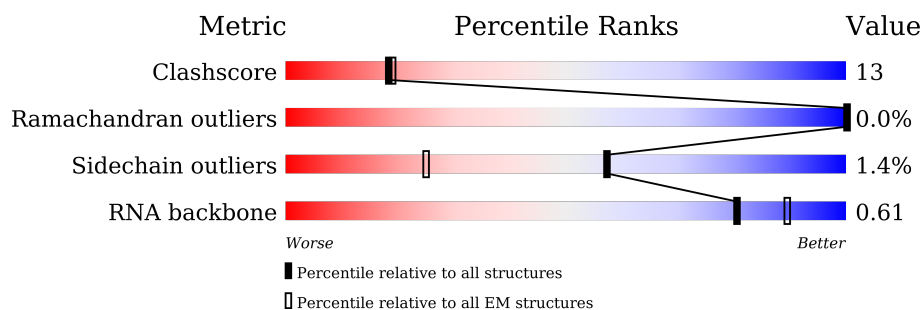
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.80 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	229148	23984
Ramachandran outliers	224038	23583
Sidechain outliers	223484	23102
RNA backbone	8273	3508

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	T	34	6% 29% . 62%
2	N	34	18% 24% 9% 50%
3	P	20	30% 5% 65%
4	A	2032	28% 12% 59%
5	C	319	68% 21% . 10%
6	F	144	38% 17% 44%
7	J	71	68% 21% 11%
8	K	116	68% 24% . 7%

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Mol	Chain	Length	Quality of chain
9	L	51	 73% 16% 12%
10	H	146	 58% 38% • •
11	I	114	 51% 31% • 18%
12	E	230	 50% 40% • 9%
13	B	1169	 65% 17% 17%

2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 23198 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 DNA chain called DNA (34-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
1	T	13	Total	C	N	O	P	0	0
			265	126	48	78	13		

- Molecule 2 is a DNA chain called DNA (34-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
2	N	17	Total	C	N	O	P	0	0
			349	166	62	104	17		

- Molecule 3 is a RNA chain called RNA (5'-R(*UP*AP*UP*AP*UP*GP*CP*AP*GP*AP*AP*AP*GP*CP*GP*AP*CP*UP*UP*U)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
3	P	7	Total	C	N	O	P	0	0
			150	67	28	48	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	A	832	Total	C	N	O	S	0	0
			6506	4113	1120	1229	44		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	C	287	Total	C	N	O	S	0	0
			2256	1418	380	445	13		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	2	THR	SER	conflict	UNP A0A0D3D418

- Molecule 6 is a protein called DNA-directed RNA polymerase RpoA/D/Rpb3-type domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	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 7 is a protein called DNA-directed RNA polymerase II, IV and V subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	J	63	Total	C	N	O	S	0	0
			507	324	85	91	7		

- Molecule 8 is a protein called DNA-directed RNA polymerase RBP11-like dimerisation domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	K	108	Total	C	N	O	S	0	0
			890	565	156	167	2		

- Molecule 9 is a protein called DNA-directed RNA polymerase II, IV and V subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	L	45	Total	C	N	O	S	0	0
			365	224	70	67	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 10 is a protein called DNA-directed RNA polymerase II, IV and V subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	H	141	Total	C	N	O	S	0	0
			1129	729	183	208	9		

- Molecule 11 is a protein called DNA-directed RNA polymerase subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	I	94	Total	C	N	O	S	0	0
			763	467	145	139	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	E	209	Total	C	N	O	S	0	0
			1706	1085	303	316	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
E	210	ILE	VAL	conflict	UNP A0A0D3DTU3

- Molecule 13 is a protein called DNA-directed RNA polymerase IV and V subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	B	965	Total	C	N	O	S	0	0
			7645	4816	1355	1430	44		

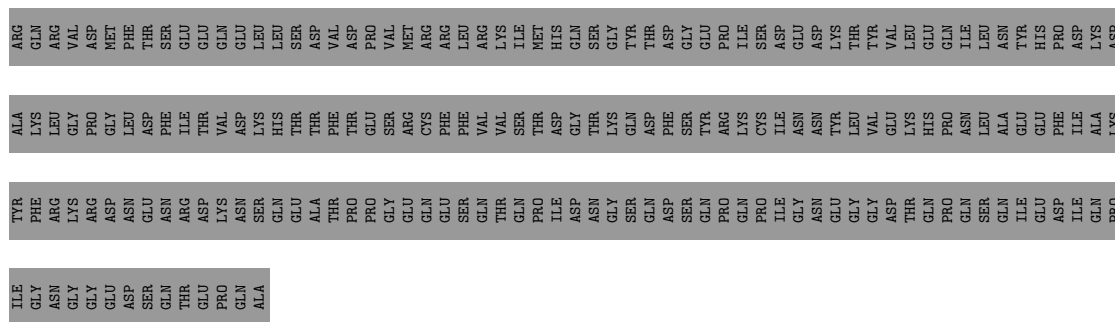
- Molecule 14 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

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

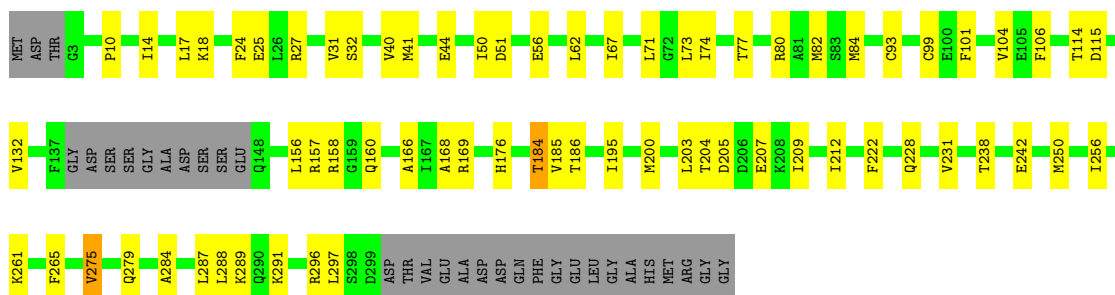
- Molecule 15 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
15	A	1	Total 1	Zn 1	0
15	C	1	Total 1	Zn 1	0
15	J	1	Total 1	Zn 1	0
15	L	1	Total 1	Zn 1	0
15	I	2	Total 2	Zn 2	0

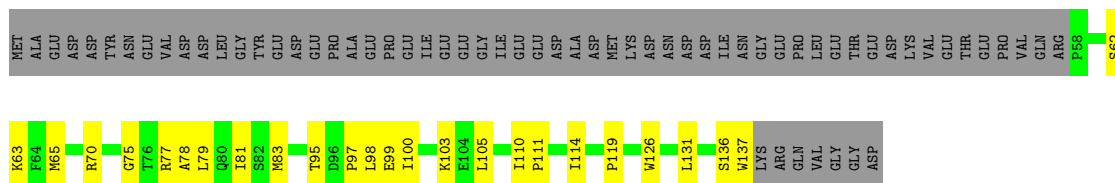
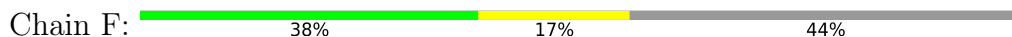




- Molecule 5: DNA-directed RNA polymerase RpoA/D/Rpb3-type domain-containing protein



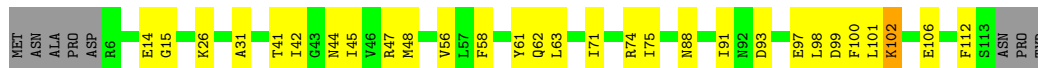
- Molecule 6: DNA-directed RNA polymerase RpoA/D/Rpb3-type domain-containing protein



- Molecule 7: DNA-directed RNA polymerase II, IV and V subunit 10

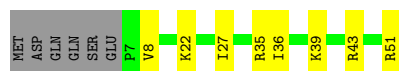


- Molecule 8: DNA-directed RNA polymerase RBP11-like dimerisation domain-containing protein



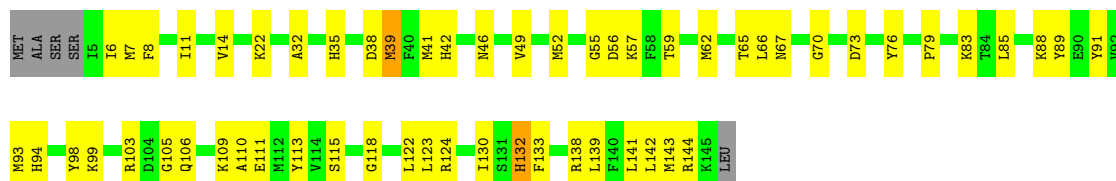
- Molecule 9: DNA-directed RNA polymerase II, IV and V subunit 12

Chain L:  73% 16% 12%



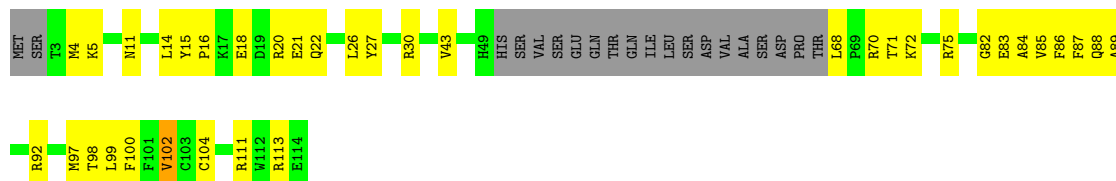
- Molecule 10: DNA-directed RNA polymerase II, IV and V subunit 8

Chain H:  58% 38% ..



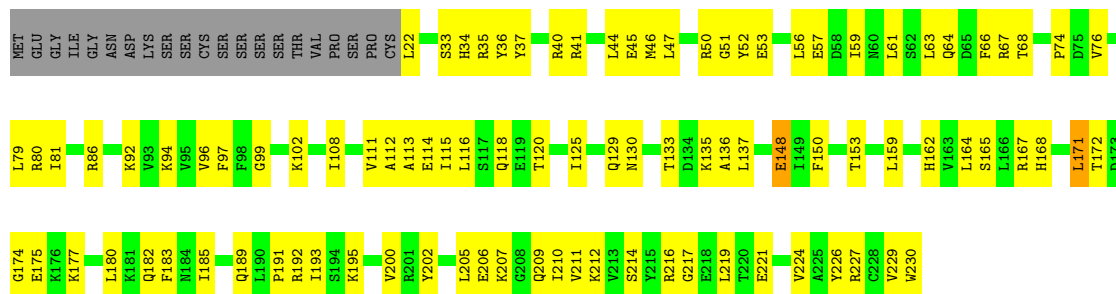
- Molecule 11: DNA-directed RNA polymerase subunit

Chain I:  51% 31% . 18%



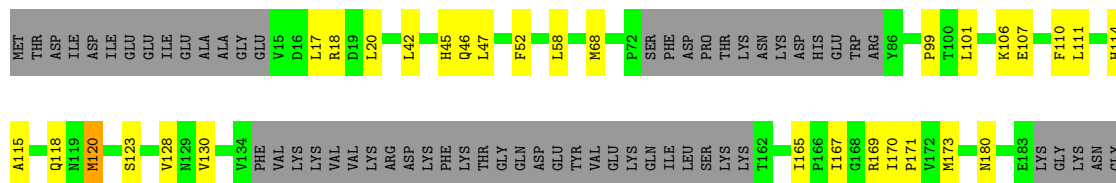
- Molecule 12: RNA polymerase subunit H/Rpb5 C-terminal domain-containing protein

Chain E:  50% 40% . 9%



- Molecule 13: DNA-directed RNA polymerase IV and V subunit 2

Chain B:  65% 17% 17%





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	28375	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: MG, ZN

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	T	0.35	0/295	0.57	1/450 (0.2%)
2	N	0.32	0/389	0.65	3/596 (0.5%)
3	P	0.09	0/167	0.20	0/258
4	A	0.23	0/6616	0.52	1/8931 (0.0%)
5	C	0.22	0/2286	0.47	0/3087
6	F	0.20	0/673	0.47	0/905
7	J	0.25	0/515	0.50	0/696
8	K	0.22	0/908	0.48	0/1224
9	L	0.22	0/369	0.50	0/493
10	H	0.20	0/1155	0.51	0/1557
11	I	0.18	0/778	0.44	0/1045
12	E	0.17	0/1732	0.44	0/2332
13	B	0.22	0/7794	0.46	4/10503 (0.0%)
All	All	0.22	0/23677	0.48	9/32077 (0.0%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	B	942	ILE	CA-C-N	8.13	132.03	120.49
13	B	942	ILE	C-N-CA	8.13	132.03	120.49
2	N	24	DT	P-O3'-C3'	-7.77	108.55	120.20
13	B	781	GLU	CA-CB-CG	6.35	126.81	114.10
2	N	26	DC	P-O3'-C3'	-5.93	111.31	120.20
13	B	877	GLY	N-CA-C	5.85	118.69	110.38
1	T	8	DA	P-O3'-C3'	-5.38	112.13	120.20
4	A	719	GLU	CA-CB-CG	5.32	124.74	114.10
2	N	25	DA	P-O3'-C3'	-5.17	112.44	120.20

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	T	265	0	148	17	0
2	N	349	0	194	17	0
3	P	150	0	77	7	0
4	A	6506	0	6559	213	0
5	C	2256	0	2269	49	0
6	F	660	0	669	25	0
7	J	507	0	512	12	0
8	K	890	0	883	29	0
9	L	365	0	364	12	0
10	H	1129	0	1128	50	0
11	I	763	0	714	28	0
12	E	1706	0	1759	79	0
13	B	7645	0	7580	156	0
14	A	1	0	0	0	0
15	A	1	0	0	0	0
15	C	1	0	0	0	0
15	I	2	0	0	0	0
15	J	1	0	0	0	0
15	L	1	0	0	0	0
All	All	23198	0	22856	600	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 (600) 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)
8:K:45:ILE:HA	8:K:48:MET:HE3	1.47	0.95
4:A:1096:LEU:HD22	12:E:35:ARG:HE	1.35	0.89
9:L:35:ARG:HH21	13:B:118:GLN:HB3	1.38	0.89
4:A:1096:LEU:HB2	12:E:35:ARG:HH21	1.37	0.88
4:A:529:VAL:HG22	10:H:93:MET:HE1	1.54	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:E:191:PRO:HB2	12:E:227:ARG:HD3	1.56	0.86
13:B:834:ARG:HB3	13:B:854:ASP:HA	1.56	0.85
5:C:32:SER:HB2	8:K:44:ASN:HD21	1.41	0.84
4:A:615:GLN:HE22	13:B:1024:ARG:HH22	1.28	0.81
12:E:92:LYS:HD2	12:E:120:THR:HG23	1.63	0.80
4:A:484:THR:HG23	4:A:486:GLN:H	1.47	0.79
13:B:872:LYS:HD2	13:B:873:HIS:H	1.46	0.79
12:E:171:LEU:HD11	12:E:210:ILE:HB	1.64	0.78
4:A:335:ASN:HB2	4:A:338:GLU:HG2	1.67	0.76
4:A:897:TYR:HE2	11:I:87:PHE:HA	1.52	0.75
13:B:101:LEU:HD21	13:B:120:MET:HE1	1.69	0.75
4:A:1093:ASP:HA	12:E:35:ARG:HH12	1.51	0.75
13:B:850:MET:HE3	13:B:850:MET:HA	1.67	0.74
4:A:897:TYR:HD2	11:I:88:GLN:HB2	1.52	0.74
1:T:6:DC:N4	2:N:29:DG:O6	2.20	0.74
10:H:111:GLU:HG2	10:H:124:ARG:HG2	1.70	0.73
13:B:748:LEU:HB3	13:B:965:ILE:HD11	1.70	0.73
10:H:7:MET:HE3	10:H:132:HIS:HB2	1.71	0.72
6:F:105:LEU:HA	6:F:110:ILE:HD11	1.72	0.71
4:A:568:LEU:HD12	10:H:115:SER:HB3	1.73	0.71
13:B:239:THR:HG22	13:B:241:ARG:H	1.54	0.70
12:E:41:ARG:HA	12:E:44:LEU:HD12	1.73	0.70
12:E:53:GLU:HB3	12:E:86:ARG:HD2	1.72	0.70
4:A:1108:ILE:HD11	4:A:1115:VAL:HG13	1.73	0.70
13:B:266:VAL:HG23	13:B:275:VAL:HG12	1.73	0.70
11:I:86:PHE:HB2	11:I:99:LEU:HD11	1.73	0.69
13:B:784:ILE:HG22	13:B:942:ILE:HG22	1.73	0.69
12:E:133:THR:HG22	12:E:135:LYS:H	1.59	0.68
4:A:415:PRO:HG3	4:A:456:HIS:CE1	2.29	0.68
4:A:1060:ARG:HH12	12:E:164:LEU:HG	1.58	0.67
4:A:592:LYS:H	6:F:137:TRP:HB2	1.60	0.67
13:B:68:MET:HE1	13:B:415:ARG:HB3	1.76	0.67
1:T:8:DA:H2''	1:T:9:DG:N7	2.10	0.67
13:B:229:SER:HB3	13:B:230:PRO:HD3	1.76	0.67
13:B:17:LEU:HD13	13:B:633:LEU:HD23	1.77	0.66
4:A:1042:ARG:HD3	4:A:1080:ASP:HB3	1.78	0.66
13:B:273:ILE:HD13	13:B:331:VAL:HG12	1.77	0.66
13:B:909:LYS:HG3	13:B:1037:LEU:HD13	1.76	0.66
4:A:941:LEU:HB2	4:A:1003:PRO:HB2	1.77	0.66
10:H:98:TYR:CZ	10:H:113:TYR:HB3	2.31	0.66
2:N:26:DC:H2'	2:N:27:DT:C2	2.32	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:751:PRO:HD2	13:B:670:TRP:HZ3	1.62	0.65
4:A:585:VAL:O	4:A:589:MET:HG3	1.96	0.65
4:A:663:ILE:O	4:A:667:LYS:HG2	1.97	0.64
4:A:411:PHE:CE1	4:A:458:PHE:HB2	2.32	0.64
12:E:195:LYS:HA	12:E:200:VAL:HG11	1.80	0.64
5:C:106:PHE:HB2	5:C:166:ALA:HB3	1.80	0.63
4:A:1123:CYS:SG	12:E:165:SER:HA	2.38	0.63
10:H:8:PHE:HB3	10:H:62:MET:HB3	1.81	0.63
4:A:715:LYS:O	4:A:719:GLU:OE1	2.17	0.63
4:A:596:GLU:H	6:F:137:TRP:HE1	1.46	0.63
4:A:667:LYS:HD2	4:A:696:VAL:HG11	1.80	0.62
13:B:835:VAL:HG13	13:B:838:LEU:HB2	1.82	0.62
4:A:480:ARG:HH21	4:A:589:MET:HE1	1.64	0.62
4:A:594:PRO:O	4:A:595:LYS:HD3	2.00	0.62
4:A:947:GLU:HB3	11:I:92:ARG:HD2	1.81	0.62
12:E:125:ILE:HG23	12:E:150:PHE:CE1	2.35	0.62
13:B:670:TRP:H	13:B:675:LEU:HD23	1.64	0.62
4:A:715:LYS:O	4:A:715:LYS:HD2	1.99	0.62
12:E:33:SER:HB3	12:E:74:PRO:HD3	1.81	0.61
11:I:21:GLU:HG2	11:I:22:GLN:HG3	1.81	0.61
4:A:646:VAL:HA	4:A:659:LEU:HD11	1.81	0.61
11:I:11:ASN:HD21	13:B:288:LYS:HG2	1.64	0.61
4:A:954:GLN:O	4:A:958:GLN:HG2	2.01	0.61
5:C:41:MET:HE3	5:C:185:VAL:HG11	1.83	0.61
12:E:76:VAL:HB	12:E:97:PHE:HB2	1.81	0.61
8:K:45:ILE:CA	8:K:48:MET:HE3	2.28	0.61
4:A:1043:ILE:HD11	4:A:1046:ALA:HB2	1.81	0.61
4:A:759:VAL:HG12	13:B:505:PRO:HD2	1.83	0.60
10:H:88:LYS:HB3	10:H:144:ARG:NH1	2.15	0.60
4:A:751:PRO:HD2	13:B:670:TRP:CZ3	2.36	0.60
12:E:63:LEU:HD21	12:E:67:ARG:HH21	1.67	0.60
13:B:307:VAL:O	13:B:311:ILE:HG13	2.02	0.60
4:A:888:LYS:HG3	4:A:891:CYS:HB3	1.84	0.59
13:B:215:ALA:HB3	13:B:489:THR:HA	1.84	0.59
1:T:19:DA:H2'	1:T:20:DG:H8	1.67	0.59
2:N:12:DG:H4'	13:B:464:MET:HE1	1.82	0.59
4:A:721:MET:HE1	4:A:755:MET:HE3	1.85	0.59
4:A:939:ILE:HG12	4:A:1029:TYR:HE2	1.67	0.59
13:B:772:VAL:HG12	13:B:942:ILE:HG13	1.84	0.59
13:B:414:ALA:O	13:B:418:MET:HG3	2.03	0.59
4:A:915:PHE:HB2	4:A:1029:TYR:CZ	2.38	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:H:93:MET:HE3	10:H:93:MET:HA	1.85	0.59
12:E:174:GLY:HA2	12:E:177:LYS:HD2	1.84	0.59
4:A:784:ALA:HA	4:A:787:ARG:HH12	1.67	0.59
5:C:17:LEU:HB3	8:K:112:PHE:HD1	1.68	0.58
4:A:877:VAL:HG11	4:A:1091:VAL:HG21	1.86	0.58
11:I:5:LYS:HG3	11:I:14:LEU:HD12	1.85	0.58
13:B:111:LEU:HB2	13:B:114:HIS:CE1	2.38	0.58
4:A:988:CYS:HB2	4:A:1001:ASP:HA	1.85	0.58
4:A:586:THR:HA	4:A:589:MET:SD	2.44	0.58
4:A:596:GLU:N	6:F:137:TRP:HE1	2.02	0.58
4:A:855:TRP:HE3	4:A:858:MET:HE3	1.68	0.58
12:E:172:THR:HG23	12:E:175:GLU:H	1.68	0.58
11:I:71:THR:HG22	11:I:84:ALA:H	1.69	0.58
13:B:973:LYS:HZ2	13:B:975:LYS:HB2	1.69	0.58
4:A:645:MET:HE3	4:A:659:LEU:HD23	1.85	0.57
10:H:93:MET:HB2	10:H:141:LEU:HB3	1.86	0.57
13:B:413:HIS:CE1	13:B:416:ARG:HH21	2.22	0.57
3:P:17:C:H2'	3:P:18:U:C6	2.39	0.57
4:A:593:GLY:HA2	6:F:136:SER:HB2	1.85	0.57
2:N:25:DA:H3'	2:N:26:DC:H6	1.68	0.57
4:A:877:VAL:HA	4:A:1109:PRO:HA	1.87	0.57
10:H:11:ILE:HG23	10:H:35:HIS:HB3	1.86	0.57
8:K:98:LEU:HD12	8:K:99:ASP:N	2.20	0.57
12:E:148:GLU:HB2	12:E:150:PHE:CE1	2.39	0.57
13:B:330:TYR:O	13:B:333:GLN:HG3	2.05	0.57
12:E:36:TYR:HD2	12:E:74:PRO:HG2	1.69	0.57
3:P:16:A:H2'	3:P:17:C:C6	2.40	0.57
4:A:323:SER:HB3	13:B:1048:ARG:HB2	1.85	0.57
11:I:16:PRO:HG3	11:I:27:TYR:HE1	1.68	0.57
11:I:88:GLN:HG2	11:I:97:MET:HB3	1.86	0.57
5:C:56:GLU:HG2	9:L:43:ARG:HD2	1.87	0.56
5:C:73:LEU:HB3	7:J:6:ARG:HE	1.69	0.56
10:H:38:ASP:O	10:H:39:MET:HE2	2.05	0.56
4:A:543:GLN:HA	4:A:546:GLN:HG2	1.88	0.56
9:L:35:ARG:HH22	13:B:120:MET:HG3	1.70	0.56
4:A:479:LEU:HD23	4:A:487:LEU:HD22	1.88	0.56
4:A:1089:ARG:O	4:A:1092:ILE:HG13	2.06	0.56
2:N:26:DC:H2'	2:N:27:DT:N3	2.20	0.56
4:A:715:LYS:HD2	4:A:718:VAL:HB	1.87	0.56
4:A:992:ARG:HD2	4:A:999:ASP:HA	1.88	0.55
4:A:1138:LYS:HD3	4:A:1138:LYS:N	2.22	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:H:130:ILE:HG23	10:H:133:PHE:HD2	1.71	0.55
13:B:20:LEU:HD21	13:B:637:LYS:HB3	1.89	0.55
4:A:949:TRP:HD1	4:A:951:ILE:HD11	1.71	0.55
4:A:1093:ASP:HA	12:E:35:ARG:NH1	2.21	0.55
13:B:414:ALA:HB2	13:B:443:ILE:HG21	1.89	0.55
4:A:978:PHE:HA	4:A:981:MET:SD	2.46	0.55
5:C:195:ILE:HG22	5:C:256:ILE:HG22	1.89	0.55
13:B:367:PHE:O	13:B:371:MET:HG3	2.07	0.55
1:T:20:DG:H2'	1:T:21:DT:C6	2.42	0.55
9:L:36:ILE:HD11	13:B:118:GLN:HE21	1.71	0.54
12:E:159:LEU:HD21	12:E:202:TYR:CD1	2.42	0.54
1:T:8:DA:H2''	1:T:9:DG:C8	2.42	0.54
4:A:537:PRO:HB2	4:A:539:TRP:HZ3	1.72	0.54
4:A:592:LYS:HB3	4:A:596:GLU:HG3	1.89	0.54
6:F:97:PRO:HA	6:F:100:ILE:HD12	1.90	0.54
11:I:85:VAL:HG13	11:I:102:VAL:HG13	1.89	0.54
1:T:9:DG:C8	1:T:10:DT:H72	2.42	0.54
4:A:514:GLN:OE1	8:K:58:PHE:HA	2.08	0.54
4:A:1116:GLN:HG3	4:A:1161:MET:HE1	1.90	0.54
4:A:1152:ALA:O	4:A:1156:THR:HG22	2.08	0.54
5:C:200:MET:HE1	5:C:228:GLN:HG2	1.90	0.54
1:T:7:DA:C8	1:T:7:DA:H5'	2.43	0.54
4:A:334:ARG:HG3	4:A:429:TYR:OH	2.08	0.54
12:E:47:LEU:HG	12:E:52:TYR:HB2	1.90	0.54
4:A:725:TYR:HB2	4:A:752:TYR:CZ	2.43	0.53
13:B:938:PRO:HG3	13:B:1029:MET:HE3	1.90	0.53
6:F:114:ILE:HG13	6:F:126:TRP:HB3	1.90	0.53
3:P:17:C:H2'	3:P:18:U:H6	1.74	0.53
4:A:1111:SER:HB3	4:A:1114:GLN:OE1	2.08	0.53
10:H:7:MET:HE2	10:H:133:PHE:CD1	2.43	0.53
13:B:557:MET:HE2	13:B:557:MET:HA	1.90	0.53
4:A:463:LEU:HD23	4:A:463:LEU:H	1.73	0.53
5:C:93:CYS:HB3	5:C:99:CYS:SG	2.48	0.53
5:C:104:VAL:HG21	5:C:132:VAL:HG21	1.91	0.53
5:C:212:ILE:HD12	5:C:222:PHE:HB2	1.91	0.53
13:B:244:PHE:CD2	13:B:371:MET:HE1	2.44	0.53
12:E:115:ILE:HD12	12:E:118:GLN:HG3	1.90	0.53
4:A:588:ILE:HG13	4:A:592:LYS:HG3	1.90	0.53
4:A:1030:PRO:HG3	13:B:259:ARG:HD2	1.90	0.53
6:F:99:GLU:C	6:F:103:LYS:HZ3	2.17	0.53
5:C:32:SER:HB2	8:K:44:ASN:ND2	2.18	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:B:106:LYS:HD2	13:B:107:GLU:H	1.74	0.53
13:B:827:LYS:HA	13:B:838:LEU:HD23	1.90	0.53
12:E:37:TYR:HB2	12:E:66:PHE:CE2	2.43	0.52
4:A:903:LEU:HD12	4:A:1043:ILE:HD12	1.90	0.52
4:A:1170:LYS:HA	4:A:1173:THR:HG22	1.91	0.52
5:C:14:ILE:HG12	5:C:24:PHE:HB3	1.91	0.52
11:I:75:ARG:HA	11:I:82:GLY:HA2	1.90	0.52
5:C:296:ARG:HG2	8:K:91:ILE:HG21	1.91	0.52
12:E:182:GLN:HB2	12:E:183:PHE:CD2	2.45	0.52
4:A:414:ARG:HG3	4:A:415:PRO:HD2	1.91	0.52
12:E:214:SER:HB2	12:E:224:VAL:HG12	1.90	0.52
13:B:225:TRP:CG	13:B:236:ARG:HH12	2.28	0.52
13:B:244:PHE:HD2	13:B:371:MET:HE1	1.74	0.52
11:I:15:TYR:CE1	11:I:30:ARG:HG3	2.44	0.52
11:I:11:ASN:ND2	13:B:288:LYS:HG2	2.24	0.52
12:E:94:LYS:O	12:E:125:ILE:HD12	2.09	0.52
12:E:47:LEU:O	12:E:50:ARG:HG2	2.10	0.52
1:T:23:DG:H2'	1:T:24:DC:C6	2.44	0.52
12:E:193:ILE:HG23	12:E:227:ARG:HB3	1.92	0.52
13:B:18:ARG:HH22	13:B:678:GLN:HA	1.75	0.52
4:A:917:VAL:HG11	4:A:1021:LEU:HD11	1.91	0.51
4:A:959:ARG:HE	4:A:1037:ILE:C	2.19	0.51
13:B:718:HIS:CE1	13:B:915:GLY:HA2	2.45	0.51
4:A:512:SER:O	4:A:516:LEU:HG	2.10	0.51
4:A:638:ILE:HD11	4:A:701:PHE:CG	2.45	0.51
13:B:165:ILE:HG13	13:B:436:GLU:HG2	1.91	0.51
4:A:1087:ALA:O	4:A:1091:VAL:HG22	2.11	0.51
11:I:68:LEU:HD21	11:I:87:PHE:HB3	1.93	0.51
6:F:100:ILE:HA	6:F:103:LYS:HE2	1.92	0.51
12:E:113:ALA:HA	12:E:116:LEU:HD23	1.91	0.51
4:A:906:VAL:HG22	4:A:1038:LYS:HB2	1.92	0.51
12:E:112:ALA:HA	12:E:115:ILE:HG22	1.93	0.51
4:A:527:PRO:HG3	4:A:539:TRP:CH2	2.46	0.51
4:A:544:ILE:HD12	4:A:544:ILE:H	1.76	0.51
12:E:206:GLU:O	12:E:209:GLN:HG3	2.10	0.51
13:B:475:GLY:HA3	13:B:481:GLN:HE21	1.76	0.51
4:A:537:PRO:HB2	4:A:539:TRP:CZ3	2.45	0.51
4:A:680:MET:HE1	13:B:948:PRO:HB3	1.92	0.50
13:B:872:LYS:CD	13:B:873:HIS:H	2.19	0.50
5:C:204:THR:HG23	5:C:207:GLU:H	1.76	0.50
12:E:45:GLU:HG3	12:E:59:ILE:HG21	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:518:MET:HG2	8:K:62:GLN:HB3	1.93	0.50
10:H:14:VAL:HA	10:H:32:ALA:HB2	1.93	0.50
12:E:40:ARG:O	12:E:44:LEU:HG	2.11	0.50
1:T:6:DC:H2''	1:T:7:DA:C8	2.47	0.50
4:A:1096:LEU:HD22	12:E:35:ARG:NE	2.16	0.50
11:I:18:GLU:HA	11:I:26:LEU:H	1.76	0.50
13:B:779:ASN:O	13:B:943:ASN:HB2	2.10	0.50
13:B:970:GLN:HE22	13:B:972:LYS:HA	1.76	0.50
13:B:972:LYS:NZ	13:B:1003:ARG:HA	2.27	0.50
10:H:14:VAL:HG13	10:H:55:GLY:H	1.77	0.50
4:A:754:GLU:OE2	13:B:515:PHE:HE1	1.95	0.50
4:A:896:ALA:HB1	4:A:1048:ILE:HD13	1.92	0.50
4:A:940:HIS:HE1	4:A:989:CYS:SG	2.26	0.50
4:A:1084:SER:HB3	4:A:1117:GLU:OE1	2.12	0.50
4:A:817:GLU:HA	6:F:63:LYS:HE3	1.94	0.50
10:H:66:LEU:HD12	10:H:85:LEU:HD13	1.93	0.50
1:T:6:DC:C4	1:T:7:DA:N6	2.80	0.50
4:A:935:LEU:HD13	4:A:1021:LEU:HD13	1.94	0.50
4:A:969:GLN:HA	4:A:972:LYS:HE2	1.93	0.50
11:I:83:GLU:HG2	11:I:104:CYS:SG	2.52	0.49
13:B:549:PHE:HA	13:B:553:MET:HB3	1.92	0.49
4:A:322:PHE:HB2	4:A:459:TYR:CD1	2.47	0.49
4:A:943:LYS:O	4:A:947:GLU:HG2	2.12	0.49
13:B:273:ILE:CG1	13:B:334:GLN:HG2	2.42	0.49
4:A:593:GLY:H	6:F:137:TRP:H	1.60	0.49
4:A:864:CYS:O	4:A:1163:GLY:HA3	2.13	0.49
2:N:25:DA:H3'	2:N:26:DC:C6	2.46	0.49
4:A:728:LYS:HE3	13:B:670:TRP:HE1	1.78	0.49
13:B:362:THR:HG23	13:B:560:THR:HG22	1.94	0.49
5:C:176:HIS:CD2	9:L:51:ARG:HG3	2.47	0.49
13:B:741:LEU:HD13	13:B:766:GLN:HE21	1.77	0.49
4:A:606:PRO:O	4:A:610:GLU:HG2	2.13	0.49
4:A:855:TRP:HA	4:A:858:MET:HE2	1.94	0.49
13:B:245:ILE:HB	13:B:267:TYR:HB2	1.95	0.49
5:C:40:VAL:HG13	5:C:44:GLU:HB2	1.95	0.49
5:C:71:LEU:HA	5:C:74:ILE:HD12	1.93	0.49
8:K:41:THR:O	8:K:45:ILE:HG12	2.12	0.49
12:E:79:LEU:HD22	12:E:96:VAL:HA	1.95	0.49
4:A:1050:TRP:NE1	11:I:72:LYS:HD3	2.28	0.49
11:I:4:MET:HE3	13:B:308:VAL:HG12	1.93	0.49
13:B:284:VAL:HG21	13:B:290:ALA:HB2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:855:TRP:O	4:A:859:LYS:HG3	2.13	0.48
4:A:1048:ILE:HG12	4:A:1072:LEU:HG	1.95	0.48
6:F:75:GLY:O	6:F:79:LEU:HG	2.12	0.48
13:B:827:LYS:HG3	13:B:838:LEU:HB3	1.95	0.48
4:A:586:THR:O	4:A:590:VAL:HG23	2.13	0.48
4:A:591:GLU:O	4:A:592:LYS:HD3	2.13	0.48
4:A:1145:LYS:HE3	12:E:219:LEU:HD12	1.94	0.48
5:C:62:LEU:HD11	7:J:2:ILE:HD11	1.95	0.48
5:C:207:GLU:HG2	5:C:250:MET:HE2	1.95	0.48
5:C:275:VAL:HG13	5:C:279:GLN:HB3	1.94	0.48
13:B:128:VAL:HG12	13:B:167:ILE:HD11	1.93	0.48
13:B:463:LYS:HB3	13:B:464:MET:SD	2.53	0.48
13:B:859:ARG:HB3	13:B:867:HIS:O	2.13	0.48
4:A:441:LEU:C	4:A:442:MET:HE2	2.38	0.48
4:A:594:PRO:C	4:A:595:LYS:HD3	2.38	0.48
10:H:46:ASN:HB3	10:H:49:VAL:HG22	1.94	0.48
12:E:46:MET:HB2	12:E:202:TYR:CE1	2.49	0.48
4:A:1100:HIS:ND1	4:A:1101:LEU:HG	2.29	0.48
6:F:79:LEU:O	6:F:83:MET:HG3	2.13	0.48
7:J:3:ILE:HD12	7:J:4:PRO:HD2	1.95	0.48
7:J:4:PRO:HG2	7:J:48:MET:HE1	1.96	0.48
4:A:989:CYS:HB3	4:A:1004:CYS:SG	2.52	0.48
10:H:65:THR:HG23	10:H:73:ASP:HB2	1.94	0.48
12:E:209:GLN:O	12:E:229:VAL:HG12	2.13	0.48
13:B:594:ARG:HA	13:B:599:LEU:HB2	1.95	0.48
4:A:1027:THR:C	4:A:1030:PRO:HD2	2.38	0.48
4:A:1156:THR:HG23	12:E:227:ARG:HH22	1.78	0.48
10:H:103:ARG:HG3	10:H:110:ALA:HA	1.95	0.48
1:T:20:DG:H2'	1:T:21:DT:H6	1.78	0.48
4:A:336:VAL:HG12	4:A:442:MET:HE3	1.95	0.48
10:H:32:ALA:HB3	10:H:41:MET:SD	2.53	0.48
4:A:1085:GLY:O	4:A:1089:ARG:HG3	2.14	0.47
5:C:77:THR:O	5:C:132:VAL:HG12	2.14	0.47
5:C:288:LEU:HA	5:C:291:LYS:HG2	1.96	0.47
1:T:6:DC:H5''	1:T:6:DC:H6	1.80	0.47
4:A:585:VAL:HA	4:A:588:ILE:HG22	1.96	0.47
13:B:924:GLU:HB3	13:B:929:PHE:CE2	2.49	0.47
5:C:10:PRO:HD2	8:K:100:PHE:HD2	1.80	0.47
9:L:35:ARG:CZ	13:B:887:ASN:HA	2.44	0.47
12:E:102:LYS:HG2	12:E:130:ASN:HD21	1.80	0.47
12:E:167:ARG:HH12	12:E:216:ARG:HH12	1.61	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:B:396:ILE:HD12	13:B:623:LEU:HD21	1.95	0.47
2:N:10:DG:H2"	13:B:416:ARG:NH1	2.29	0.47
4:A:542:PHE:CD2	10:H:118:GLY:HA3	2.49	0.47
5:C:289:LYS:HE3	5:C:289:LYS:HB3	1.76	0.47
6:F:99:GLU:O	6:F:103:LYS:HG3	2.14	0.47
12:E:41:ARG:NH2	12:E:61:LEU:HD11	2.30	0.47
4:A:594:PRO:HB2	4:A:595:LYS:HE2	1.96	0.47
4:A:879:LEU:HD22	4:A:1074:VAL:HG21	1.96	0.47
10:H:62:MET:HE1	10:H:139:LEU:HB3	1.95	0.47
13:B:315:ASP:HA	13:B:321:PHE:HE1	1.80	0.47
13:B:318:CYS:HB2	13:B:321:PHE:HD1	1.79	0.47
4:A:437:LYS:O	4:A:438:ILE:HD13	2.14	0.47
4:A:1137:ARG:HD2	4:A:1137:ARG:HA	1.61	0.47
8:K:56:VAL:HG12	8:K:75:ILE:HD11	1.96	0.47
10:H:94:HIS:HE1	10:H:138:ARG:HB3	1.78	0.47
4:A:763:GLU:HG3	4:A:764:VAL:N	2.30	0.47
12:E:217:GLY:O	12:E:221:GLU:HG3	2.15	0.47
2:N:14:DC:H5	13:B:340:PHE:HB2	1.79	0.47
4:A:885:ARG:HE	12:E:22:LEU:HB2	1.79	0.47
10:H:103:ARG:HD2	10:H:111:GLU:HG3	1.97	0.47
13:B:42:LEU:HD11	13:B:757:LEU:HD11	1.96	0.47
13:B:304:THR:HA	13:B:307:VAL:HG12	1.97	0.47
13:B:604:GLU:OE1	13:B:622:ARG:HD2	2.15	0.47
10:H:123:LEU:HG	10:H:124:ARG:O	2.14	0.46
4:A:414:ARG:NH1	4:A:453:ASP:HB3	2.30	0.46
4:A:1048:ILE:HG22	4:A:1070:TRP:HE3	1.79	0.46
4:A:613:ASP:OD1	13:B:776:LEU:HD12	2.15	0.46
13:B:776:LEU:HB3	13:B:778:PHE:HD2	1.80	0.46
5:C:80:ARG:O	5:C:84:MET:HG3	2.16	0.46
12:E:102:LYS:HG2	12:E:130:ASN:ND2	2.30	0.46
13:B:52:PHE:CZ	13:B:539:GLN:HB3	2.51	0.46
4:A:474:SER:HB3	4:A:477:LYS:HG3	1.98	0.46
4:A:698:GLN:CD	13:B:951:GLN:HA	2.41	0.46
4:A:1125:PHE:HD2	4:A:1126:GLU:OE1	1.98	0.46
11:I:98:THR:HG21	11:I:113:ARG:CZ	2.46	0.46
12:E:64:GLN:O	12:E:68:THR:HG23	2.16	0.46
12:E:81:ILE:HG23	12:E:94:LYS:HG2	1.98	0.46
13:B:315:ASP:HA	13:B:321:PHE:CE1	2.51	0.46
5:C:84:MET:HB3	5:C:101:PHE:O	2.16	0.46
13:B:362:THR:HG21	13:B:558:ASP:HA	1.97	0.46
4:A:1159:GLY:HA2	12:E:192:ARG:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:J:9:THR:HG21	13:B:936:ILE:HG23	1.98	0.46
8:K:42:ILE:O	8:K:45:ILE:HG13	2.16	0.46
9:L:27:ILE:HB	13:B:886:SER:HB3	1.98	0.46
13:B:663:GLU:HA	13:B:666:CYS:SG	2.56	0.46
3:P:15:G:H2'	3:P:16:A:H8	1.80	0.46
4:A:920:ARG:HB2	4:A:936:HIS:NE2	2.31	0.46
8:K:102:LYS:O	8:K:106:GLU:HG2	2.16	0.46
12:E:81:ILE:HG23	12:E:94:LYS:HE3	1.97	0.46
4:A:784:ALA:HA	4:A:787:ARG:NH1	2.31	0.46
13:B:216:GLN:HE22	13:B:470:VAL:HA	1.81	0.46
3:P:15:G:H2'	3:P:16:A:C8	2.51	0.45
4:A:761:ALA:O	4:A:765:ILE:HG22	2.14	0.45
9:L:35:ARG:HE	13:B:118:GLN:HG2	1.81	0.45
12:E:111:VAL:O	12:E:114:GLU:HG3	2.16	0.45
13:B:279:PHE:O	13:B:284:VAL:HG12	2.16	0.45
4:A:1040:ASP:HB3	4:A:1043:ILE:HG22	1.98	0.45
10:H:6:ILE:C	10:H:6:ILE:HD12	2.42	0.45
4:A:875:ARG:HD2	4:A:1076:VAL:HB	1.98	0.45
4:A:906:VAL:HG23	4:A:1037:ILE:HG13	1.97	0.45
13:B:1046:LYS:HB3	13:B:1046:LYS:HE2	1.67	0.45
4:A:792:THR:HG21	6:F:119:PRO:HG3	1.99	0.45
4:A:885:ARG:NH1	4:A:886:CYS:HB2	2.31	0.45
4:A:953:MET:HA	4:A:956:ILE:HG12	1.99	0.45
5:C:51:ASP:OD1	5:C:169:ARG:HD2	2.16	0.45
5:C:242:GLU:OE1	13:B:1007:SER:HA	2.17	0.45
4:A:770:ARG:NE	4:A:770:ARG:HA	2.32	0.45
4:A:1231:TRP:CZ3	6:F:111:PRO:HB2	2.51	0.45
8:K:26:LYS:N	8:K:26:LYS:HD3	2.32	0.45
4:A:769:SER:HB2	4:A:770:ARG:NH2	2.32	0.45
12:E:56:LEU:O	12:E:57:GLU:HG3	2.17	0.45
12:E:168:HIS:HB3	12:E:211:VAL:HG21	1.99	0.45
13:B:252:GLN:HB3	13:B:260:LYS:HE3	1.99	0.45
1:T:6:DC:H5''	1:T:6:DC:C6	2.52	0.45
4:A:905:LYS:HG3	4:A:1036:VAL:CG2	2.46	0.45
12:E:207:LYS:HE2	12:E:230:TRP:HA	1.98	0.45
13:B:165:ILE:HD12	13:B:435:ILE:HG23	1.97	0.45
13:B:785:VAL:HG22	13:B:922:TYR:HB3	1.97	0.45
4:A:859:LYS:HB3	4:A:859:LYS:HE2	1.68	0.45
4:A:987:GLU:O	4:A:1003:PRO:HA	2.17	0.45
8:K:63:LEU:HG	8:K:71:ILE:HG22	1.98	0.45
12:E:86:ARG:HD2	12:E:86:ARG:HA	1.84	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:B:347:ASP:O	13:B:350:LEU:HG	2.16	0.45
13:B:360:SER:O	13:B:364:LYS:HG3	2.17	0.45
2:N:29:DG:H2''	2:N:30:DA:C8	2.51	0.45
4:A:1023:VAL:HG13	4:A:1024:LEU:HD12	1.99	0.44
11:I:100:PHE:CE1	11:I:113:ARG:HB2	2.52	0.44
13:B:770:VAL:HG22	13:B:940:ILE:HG22	1.99	0.44
4:A:534:LYS:HD3	10:H:49:VAL:HA	1.99	0.44
4:A:572:PHE:CE2	10:H:22:LYS:HD2	2.52	0.44
4:A:698:GLN:HG3	13:B:951:GLN:HG2	1.99	0.44
5:C:291:LYS:HB3	5:C:291:LYS:HE2	1.78	0.44
7:J:46:ARG:NH1	13:B:968:PRO:HB3	2.32	0.44
13:B:290:ALA:O	13:B:294:ILE:HG12	2.17	0.44
13:B:419:THR:HA	13:B:422:MET:SD	2.57	0.44
3:P:12:A:H2'	3:P:13:G:C8	2.52	0.44
4:A:341:ILE:HD11	4:A:346:ALA:HB2	1.99	0.44
4:A:542:PHE:HE1	4:A:570:PHE:HB3	1.81	0.44
4:A:542:PHE:HB3	4:A:567:LEU:HD23	1.98	0.44
4:A:670:ALA:O	4:A:674:MET:HG2	2.18	0.44
12:E:46:MET:HA	12:E:202:TYR:CZ	2.53	0.44
13:B:277:VAL:HG11	13:B:330:TYR:CD2	2.52	0.44
13:B:570:VAL:HG22	13:B:578:GLY:O	2.17	0.44
5:C:51:ASP:OD2	5:C:51:ASP:C	2.61	0.44
10:H:130:ILE:HG23	10:H:133:PHE:CD2	2.53	0.44
12:E:159:LEU:HD23	12:E:159:LEU:H	1.83	0.44
13:B:111:LEU:HB2	13:B:114:HIS:ND1	2.33	0.44
3:P:16:A:H2'	3:P:17:C:H6	1.80	0.44
4:A:349:ILE:HG21	4:A:459:TYR:CZ	2.52	0.44
4:A:582:ASN:HA	4:A:585:VAL:HG12	2.00	0.44
2:N:24:DT:P	2:N:24:DT:H6	2.41	0.44
4:A:588:ILE:HD11	4:A:596:GLU:HB3	2.00	0.44
4:A:592:LYS:HD3	4:A:592:LYS:HA	1.74	0.44
4:A:808:PHE:CE2	12:E:226:TYR:HB2	2.51	0.44
4:A:904:LYS:NZ	4:A:1045:SER:HA	2.33	0.44
4:A:1093:ASP:HA	12:E:35:ARG:HH22	1.81	0.44
6:F:65:MET:HE2	6:F:70:ARG:HG3	1.99	0.44
8:K:47:ARG:HD3	8:K:61:TYR:HD2	1.81	0.44
13:B:99:PRO:HG2	13:B:180:ASN:ND2	2.33	0.44
4:A:583:GLY:O	4:A:586:THR:HG22	2.17	0.44
4:A:1086:ASP:OD1	4:A:1089:ARG:HD2	2.18	0.44
11:I:20:ARG:H	11:I:20:ARG:HG3	1.58	0.44
13:B:225:TRP:HH2	13:B:388:ARG:HD2	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:B:308:VAL:HA	13:B:311:ILE:HD12	2.00	0.44
1:T:19:DA:H2'	1:T:20:DG:C8	2.50	0.44
4:A:662:SER:O	4:A:666:VAL:HG23	2.18	0.44
5:C:205:ASP:O	5:C:209:ILE:HG12	2.18	0.44
8:K:14:GLU:CD	8:K:15:GLY:H	2.26	0.44
12:E:37:TYR:HB2	12:E:66:PHE:CD2	2.53	0.44
13:B:47:LEU:HD23	13:B:173:MET:SD	2.58	0.44
13:B:479:PRO:HG2	13:B:761:VAL:HB	2.00	0.44
2:N:18:DC:C2	13:B:388:ARG:NH2	2.86	0.44
4:A:585:VAL:O	4:A:588:ILE:HG22	2.18	0.44
4:A:897:TYR:CD2	11:I:88:GLN:HB2	2.41	0.44
4:A:1156:THR:HB	4:A:1161:MET:HG3	1.99	0.44
5:C:261:LYS:HE3	5:C:261:LYS:HB2	1.74	0.44
13:B:58:LEU:HD12	13:B:58:LEU:HA	1.86	0.44
13:B:640:LYS:HA	13:B:640:LYS:HD3	1.67	0.44
13:B:741:LEU:HB2	13:B:744:PRO:HG3	1.99	0.44
13:B:750:LYS:HD2	13:B:750:LYS:HA	1.71	0.44
13:B:791:LEU:HD21	13:B:903:SER:HB2	1.99	0.44
4:A:725:TYR:HB2	4:A:752:TYR:OH	2.18	0.43
12:E:99:GLY:O	12:E:129:GLN:HG3	2.18	0.43
4:A:839:PRO:O	4:A:1139:VAL:HG11	2.17	0.43
10:H:67:ASN:HB2	10:H:70:GLY:O	2.18	0.43
12:E:40:ARG:HD3	12:E:80:ARG:HD3	2.00	0.43
4:A:589:MET:C	6:F:137:TRP:HB3	2.44	0.43
4:A:816:ASN:OD1	6:F:62:SER:HA	2.18	0.43
4:A:939:ILE:HG12	4:A:1029:TYR:CE2	2.51	0.43
10:H:89:TYR:HD2	10:H:143:MET:C	2.26	0.43
12:E:135:LYS:HE2	12:E:135:LYS:HB3	1.89	0.43
13:B:909:LYS:HZ1	13:B:917:LYS:HD3	1.84	0.43
9:L:22:LYS:HA	9:L:22:LYS:HD3	1.83	0.43
9:L:35:ARG:NH2	13:B:120:MET:HG3	2.33	0.43
9:L:43:ARG:HA	9:L:43:ARG:HD3	1.67	0.43
10:H:79:PRO:HB3	10:H:83:LYS:HZ3	1.83	0.43
12:E:180:LEU:HG	12:E:185:ILE:HG23	1.99	0.43
4:A:855:TRP:CZ2	4:A:859:LYS:HD2	2.53	0.43
4:A:1057:THR:HB	4:A:1060:ARG:HB3	2.01	0.43
10:H:91:TYR:HB3	10:H:143:MET:HG3	2.00	0.43
10:H:103:ARG:C	10:H:105:GLY:H	2.27	0.43
12:E:51:GLY:O	12:E:86:ARG:HB2	2.18	0.43
13:B:861:THR:H	13:B:866:ASP:HA	1.82	0.43
13:B:872:LYS:HD2	13:B:873:HIS:N	2.23	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:K:93:ASP:O	8:K:97:GLU:HG2	2.19	0.43
10:H:79:PRO:HB3	10:H:83:LYS:NZ	2.33	0.43
13:B:277:VAL:HG11	13:B:330:TYR:HD2	1.84	0.43
13:B:557:MET:SD	13:B:558:ASP:N	2.92	0.43
2:N:26:DC:C6	2:N:26:DC:H5''	2.54	0.43
4:A:502:MET:SD	4:A:541:PHE:HB2	2.59	0.43
10:H:89:TYR:CD1	10:H:142:LEU:HD23	2.53	0.43
13:B:770:VAL:HG13	13:B:940:ILE:HG22	2.00	0.43
5:C:156:LEU:HD13	5:C:160:GLN:O	2.18	0.43
10:H:14:VAL:HG12	10:H:56:ASP:H	1.84	0.43
4:A:1038:LYS:HA	4:A:1038:LYS:HD3	1.86	0.43
13:B:331:VAL:O	13:B:335:ILE:HG22	2.19	0.43
4:A:1032:LEU:HD23	4:A:1032:LEU:HA	1.84	0.42
10:H:99:LYS:HB3	10:H:113:TYR:HB2	2.00	0.42
11:I:89:ALA:HB3	11:I:100:PHE:CD2	2.53	0.42
2:N:24:DT:H2''	2:N:25:DA:C8	2.55	0.42
7:J:24:LEU:O	7:J:29:TYR:HB2	2.19	0.42
13:B:323:HIS:HB2	13:B:326:ASN:ND2	2.34	0.42
2:N:10:DG:H22	13:B:463:LYS:HD3	1.84	0.42
4:A:591:GLU:O	4:A:591:GLU:HG2	2.19	0.42
12:E:137:LEU:H	12:E:137:LEU:HD23	1.84	0.42
13:B:912:SER:HB3	13:B:1034:TYR:CE1	2.54	0.42
4:A:553:LEU:HA	4:A:592:LYS:NZ	2.34	0.42
4:A:885:ARG:O	4:A:888:LYS:HG2	2.20	0.42
4:A:959:ARG:NH2	4:A:1036:VAL:HG22	2.35	0.42
5:C:82:MET:HE1	5:C:287:LEU:CD2	2.50	0.42
13:B:772:VAL:HA	13:B:942:ILE:O	2.19	0.42
4:A:1088:TRP:HA	4:A:1091:VAL:HG22	2.00	0.42
4:A:1089:ARG:HD3	12:E:153:THR:HG23	2.01	0.42
4:A:1119:LEU:HD23	4:A:1119:LEU:HA	1.86	0.42
6:F:65:MET:HB2	6:F:131:LEU:CB	2.50	0.42
8:K:31:ALA:O	8:K:74:ARG:HD3	2.20	0.42
13:B:123:SER:HA	13:B:171:PRO:HA	2.01	0.42
13:B:626:PRO:HA	13:B:656:GLU:O	2.20	0.42
10:H:103:ARG:NH1	10:H:124:ARG:HD3	2.35	0.42
13:B:741:LEU:HD13	13:B:766:GLN:NE2	2.33	0.42
2:N:25:DA:C6	2:N:26:DC:H1'	2.55	0.42
4:A:1137:ARG:HH21	4:A:1142:GLY:H	1.67	0.42
5:C:17:LEU:HB3	8:K:112:PHE:CD1	2.51	0.42
10:H:42:HIS:NE2	10:H:122:LEU:HB3	2.35	0.42
13:B:475:GLY:HA3	13:B:481:GLN:NE2	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1058:TRP:CE3	4:A:1059:ILE:HG23	2.55	0.42
6:F:78:ALA:HB2	6:F:98:LEU:HD13	2.02	0.42
7:J:25:LEU:HD23	7:J:25:LEU:HA	1.85	0.42
8:K:42:ILE:HD13	8:K:45:ILE:HD11	2.01	0.42
13:B:406:GLU:HB2	13:B:457:TRP:NE1	2.35	0.42
13:B:780:GLN:O	13:B:781:GLU:C	2.63	0.42
13:B:786:MET:HG2	13:B:940:ILE:HD12	2.02	0.42
4:A:1049:ILE:HG22	4:A:1051:ASN:H	1.85	0.42
5:C:10:PRO:HD2	8:K:100:PHE:CD2	2.55	0.42
12:E:217:GLY:H	12:E:221:GLU:HG3	1.84	0.42
4:A:832:ALA:HA	4:A:1147:HIS:HB3	2.02	0.42
4:A:964:ILE:HG13	4:A:965:ASN:N	2.35	0.42
5:C:17:LEU:O	5:C:18:LYS:HG3	2.20	0.42
4:A:562:VAL:HG23	4:A:566:ASP:O	2.19	0.41
4:A:626:MET:HE2	4:A:674:MET:HE1	2.02	0.41
5:C:291:LYS:HD3	8:K:42:ILE:HD11	2.02	0.41
6:F:110:ILE:HD12	6:F:110:ILE:H	1.84	0.41
8:K:47:ARG:HD3	8:K:61:TYR:CD2	2.55	0.41
11:I:102:VAL:HB	11:I:111:ARG:HG3	2.01	0.41
12:E:205:LEU:HD22	12:E:209:GLN:NE2	2.35	0.41
1:T:9:DG:H1	2:N:26:DC:H42	1.67	0.41
1:T:9:DG:H1'	1:T:10:DT:H5'	2.01	0.41
4:A:751:PRO:HA	4:A:754:GLU:HG3	2.01	0.41
4:A:1063:HIS:CG	4:A:1064:ALA:N	2.88	0.41
7:J:35:LEU:HA	7:J:38:ILE:HG22	2.02	0.41
10:H:11:ILE:HD12	10:H:59:THR:HB	2.01	0.41
13:B:512:ARG:HD3	13:B:623:LEU:HB2	2.02	0.41
13:B:784:ILE:HG13	13:B:920:LEU:HA	2.03	0.41
4:A:491:LEU:HD23	4:A:491:LEU:HA	1.81	0.41
11:I:70:ARG:HD2	11:I:104:CYS:SG	2.60	0.41
11:I:70:ARG:HG3	11:I:85:VAL:HB	2.01	0.41
4:A:885:ARG:HE	12:E:22:LEU:N	2.18	0.41
4:A:1096:LEU:HD21	12:E:34:HIS:HB3	2.02	0.41
5:C:31:VAL:HG12	5:C:265:PHE:CE1	2.55	0.41
8:K:14:GLU:CG	8:K:15:GLY:H	2.34	0.41
4:A:542:PHE:HD1	4:A:567:LEU:HD21	1.84	0.41
4:A:875:ARG:CG	4:A:1076:VAL:H	2.33	0.41
12:E:37:TYR:HA	12:E:41:ARG:NH1	2.36	0.41
13:B:571:LEU:HA	13:B:575:ASP:O	2.20	0.41
13:B:961:LEU:O	13:B:965:ILE:HG23	2.19	0.41
4:A:1050:TRP:HE1	11:I:72:LYS:HD3	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:J:35:LEU:HA	7:J:35:LEU:HD23	1.81	0.41
10:H:57:LYS:HD2	10:H:57:LYS:O	2.20	0.41
13:B:123:SER:OG	13:B:169:ARG:HD3	2.21	0.41
13:B:328:LEU:HA	13:B:328:LEU:HD12	1.84	0.41
1:T:21:DT:H2'	1:T:22:DC:C6	2.55	0.41
4:A:539:TRP:HZ2	10:H:76:TYR:HE2	1.68	0.41
4:A:1132:LEU:HD12	4:A:1132:LEU:HA	1.84	0.41
5:C:10:PRO:HG2	8:K:101:LEU:HB2	2.03	0.41
10:H:52:MET:HB2	10:H:56:ASP:OD2	2.21	0.41
10:H:111:GLU:HB3	10:H:122:LEU:HD11	2.02	0.41
13:B:45:HIS:CD2	13:B:46:GLN:HG2	2.56	0.41
13:B:110:PHE:CZ	13:B:115:ALA:HB2	2.56	0.41
4:A:916:LEU:O	4:A:938:HIS:HB2	2.20	0.41
5:C:157:ARG:HG3	5:C:158:ARG:H	1.86	0.41
5:C:184:THR:HG21	7:J:42:ARG:HH12	1.86	0.41
8:K:58:PHE:O	8:K:75:ILE:HA	2.21	0.41
13:B:336:LYS:HA	13:B:336:LYS:HD2	1.91	0.41
4:A:470:LEU:O	4:A:474:SER:HB2	2.20	0.41
4:A:539:TRP:CZ2	10:H:76:TYR:HE2	2.38	0.41
4:A:767:ARG:HH22	4:A:844:VAL:HA	1.85	0.41
4:A:836:MET:O	4:A:839:PRO:HD2	2.21	0.41
4:A:883:GLU:HG3	4:A:884:CYS:N	2.35	0.41
4:A:1096:LEU:HD12	4:A:1099:LEU:HD13	2.02	0.41
4:A:1145:LYS:HE3	12:E:219:LEU:CD1	2.50	0.41
5:C:114:THR:HG22	5:C:115:ASP:H	1.86	0.41
6:F:81:ILE:CG2	6:F:97:PRO:HB3	2.50	0.41
10:H:109:LYS:HA	10:H:109:LYS:HD3	1.91	0.41
12:E:108:ILE:HA	12:E:111:VAL:HG12	2.02	0.41
12:E:133:THR:HB	12:E:136:ALA:HB2	2.03	0.41
13:B:709:ARG:HA	13:B:709:ARG:HD2	1.93	0.41
13:B:905:CYS:O	13:B:920:LEU:HD23	2.20	0.41
4:A:605:GLN:HB3	4:A:606:PRO:HD3	2.02	0.41
6:F:77:ARG:HA	6:F:77:ARG:HD2	1.80	0.41
4:A:360:ILE:O	4:A:364:GLN:HB2	2.20	0.40
4:A:677:SER:OG	4:A:680:MET:HB2	2.21	0.40
4:A:1165:ASN:O	4:A:1169:TYR:HB3	2.21	0.40
5:C:50:ILE:HA	5:C:168:ALA:HA	2.03	0.40
10:H:93:MET:HB2	10:H:141:LEU:CB	2.51	0.40
10:H:106:GLN:O	10:H:106:GLN:CG	2.69	0.40
12:E:115:ILE:HD12	12:E:115:ILE:HA	1.92	0.40
13:B:480:LEU:HD13	13:B:762:LEU:HD22	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:326:SER:OG	13:B:1045:VAL:HG22	2.21	0.40
4:A:355:VAL:HG12	4:A:398:GLN:O	2.21	0.40
10:H:88:LYS:O	10:H:144:ARG:HD3	2.21	0.40
4:A:804:SER:HA	12:E:189:GLN:HB3	2.03	0.40
5:C:203:LEU:HD23	5:C:207:GLU:HG3	2.01	0.40
13:B:20:LEU:HD23	13:B:20:LEU:HA	1.92	0.40
13:B:354:LEU:HG	13:B:355:PHE:CD2	2.57	0.40
13:B:362:THR:HG21	13:B:559:ASP:N	2.36	0.40
4:A:328:ILE:HD13	4:A:414:ARG:HH22	1.87	0.40
4:A:358:HIS:O	6:F:95:THR:HG23	2.22	0.40
4:A:767:ARG:NH2	4:A:844:VAL:HA	2.36	0.40
5:C:41:MET:HG3	5:C:284:ALA:HB2	2.04	0.40
7:J:32:GLY:HA3	13:B:979:TYR:CE1	2.56	0.40
9:L:8:VAL:HG13	9:L:39:LYS:HE2	2.04	0.40
12:E:212:LYS:HE3	12:E:212:LYS:HB2	1.82	0.40
13:B:217:GLU:HB3	13:B:394:LYS:HE3	2.04	0.40
13:B:422:MET:HE2	13:B:422:MET:C	2.46	0.40
2:N:13:DC:P	13:B:463:LYS:HD2	2.61	0.40
5:C:25:GLU:HG3	5:C:27:ARG:HH21	1.87	0.40
5:C:297:LEU:HD11	8:K:88:ASN:HD21	1.85	0.40
13:B:880:GLN:OE1	13:B:899:ARG:HD3	2.21	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	
4	A	818/2032 (40%)	771 (94%)	47 (6%)	0	100	100
5	C	283/319 (89%)	269 (95%)	14 (5%)	0	100	100
6	F	78/144 (54%)	69 (88%)	9 (12%)	0	100	100
7	J	61/71 (86%)	57 (93%)	4 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	K	106/116 (91%)	97 (92%)	9 (8%)	0	100	100
9	L	43/51 (84%)	39 (91%)	4 (9%)	0	100	100
10	H	139/146 (95%)	119 (86%)	20 (14%)	0	100	100
11	I	90/114 (79%)	82 (91%)	8 (9%)	0	100	100
12	E	207/230 (90%)	194 (94%)	13 (6%)	0	100	100
13	B	951/1169 (81%)	896 (94%)	54 (6%)	1 (0%)	48	79
All	All	2776/4392 (63%)	2593 (93%)	182 (7%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
13	B	781	GLU

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	
4	A	737/1709 (43%)	725 (98%)	12 (2%)	55	68
5	C	253/276 (92%)	247 (98%)	6 (2%)	43	62
6	F	72/128 (56%)	72 (100%)	0	100	100
7	J	56/63 (89%)	55 (98%)	1 (2%)	51	67
8	K	98/105 (93%)	97 (99%)	1 (1%)	68	74
9	L	40/46 (87%)	40 (100%)	0	100	100
10	H	123/127 (97%)	121 (98%)	2 (2%)	55	68
11	I	82/101 (81%)	80 (98%)	2 (2%)	43	62
12	E	190/209 (91%)	187 (98%)	3 (2%)	55	68
13	B	844/1026 (82%)	836 (99%)	8 (1%)	70	74
All	All	2495/3790 (66%)	2460 (99%)	35 (1%)	57	70

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	A	558	ASP
4	A	626	MET
4	A	631	MET
4	A	712	LEU
4	A	716	THR
4	A	741	VAL
4	A	1043	ILE
4	A	1049	ILE
4	A	1076	VAL
4	A	1077	GLU
4	A	1129	VAL
4	A	1169	TYR
5	C	67	ILE
5	C	184	THR
5	C	186	THR
5	C	231	VAL
5	C	238	THR
5	C	275	VAL
7	J	20	THR
8	K	102	LYS
10	H	39	MET
10	H	132	HIS
11	I	43	VAL
11	I	102	VAL
12	E	148	GLU
12	E	162	HIS
12	E	171	LEU
13	B	120	MET
13	B	130	VAL
13	B	170	ILE
13	B	393	ASN
13	B	518	THR
13	B	752	MET
13	B	781	GLU
13	B	940	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
4	A	582	ASN
4	A	615	GLN
4	A	936	HIS
4	A	1127	GLN

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Mol	Chain	Res	Type
5	C	148	GLN
8	K	44	ASN
13	B	216	GLN
13	B	334	GLN
13	B	390	ASN
13	B	413	HIS
13	B	423	GLN
13	B	473	ASN
13	B	492	GLN
13	B	539	GLN
13	B	602	GLN
13	B	720	GLN
13	B	780	GLN
13	B	824	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	P	6/20 (30%)	2 (33%)	0

All (2) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	P	13	G
3	P	14	C

There are no RNA pucker outliers to report.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 7 ligands modelled in this entry, 7 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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.