



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 23, 2026 – 03:17 AM EDT

PDB ID : 8UKT / pdb_00008ukt
Title : RNA polymerase II elongation complex with Fapy-dG lesion with AMP added
Authors : Hou, P.; Oh, J.; Wang, D.
Deposited on : 2023-10-15
Resolution : 3.60 Å(reported)

This is a Full wwPDB X-ray Structure 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/XrayValidationReportHelp>

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:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

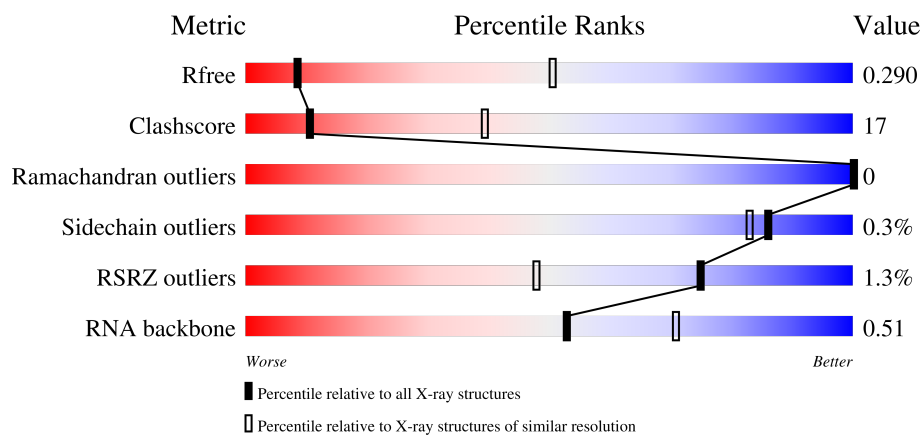
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.60 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1747 (3.70-3.50)
Clashscore	190562	1827 (3.70-3.50)
Ramachandran outliers	187476	1773 (3.70-3.50)
Sidechain outliers	187428	1772 (3.70-3.50)
RSRZ outliers	180081	1745 (3.70-3.50)
RNA backbone	3983	1014 (4.14-3.06)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	R	10	
2	T	29	
3	N	18	
4	A	1733	

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Mol	Chain	Length	Quality of chain
5	B	1224	
6	C	318	
7	E	215	
8	F	155	
9	H	146	
10	I	122	
11	J	70	
12	K	120	
13	L	70	

2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 29013 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 RNA chain called RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	R	10	Total	C	N	O	P	0	0	0
			217	98	45	65	9			

- Molecule 2 is a DNA chain called tsDNA with Fapy-dG lesion.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	T	24	Total	C	N	O	P	0	0	0
			481	230	76	151	24			

- Molecule 3 is a DNA chain called ntsDNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	N	13	Total	C	N	O	P	0	0	0
			275	128	61	73	13			

- Molecule 4 is a protein called DNA-directed RNA polymerase II subunit RPB1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	A	1384	Total	C	N	O	S	0	0	0
			10828	6831	1896	2041	60			

- Molecule 5 is a protein called DNA-directed RNA polymerase II subunit RPB2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	B	1126	Total	C	N	O	S	0	0	0
			8878	5618	1555	1652	53			

- Molecule 6 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	C	267	Total	C	N	O	S	0	0	0
			2101	1320	349	419	13			

- Molecule 7 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	E	212	Total	C	N	O	S	0	0	0
			1731	1100	305	315	11			

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	F	86	Total	C	N	O	S	0	0	0
			684	437	115	129	3			

- Molecule 9 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	H	133	Total	C	N	O	S	0	0	0
			1064	670	179	211	4			

- Molecule 10 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	I	118	Total	C	N	O	S	0	0	0
			948	582	172	184	10			

- Molecule 11 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	J	65	Total	C	N	O	S	0	0	0
			532	339	93	94	6			

- Molecule 12 is a protein called DNA-directed RNA polymerase II subunit RPB11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	K	114	Total	C	N	O	S	0	0	0
			919	590	156	171	2			

- Molecule 13 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	L	43	Total	C	N	O	S	0	0	0
			337	208	66	59	4			

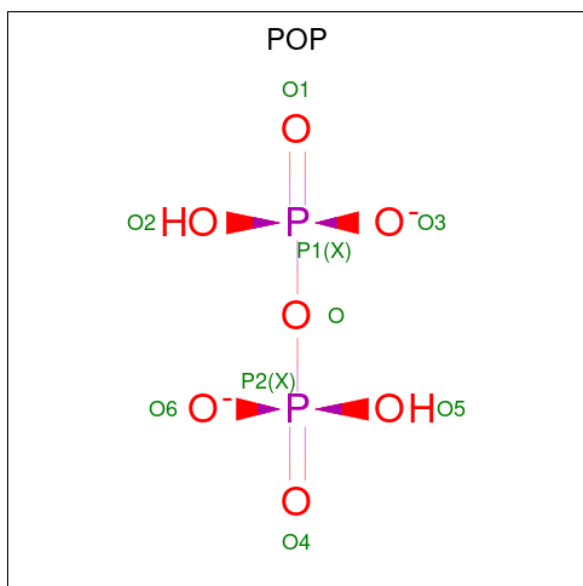
- Molecule 14 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	R	1	Total Mg 1 1	0	0

- Molecule 15 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 16 is PYROPHOSPHATE 2- (CCD ID: POP) (formula: $\text{H}_2\text{O}_7\text{P}_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	B	1	Total O P 9 7 2	0	0

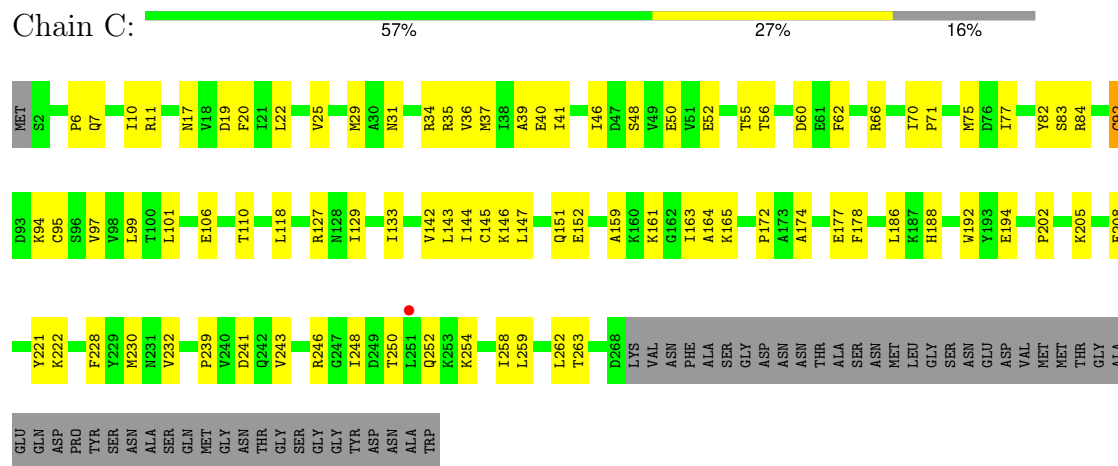


Chain B: 59% 33% 8%

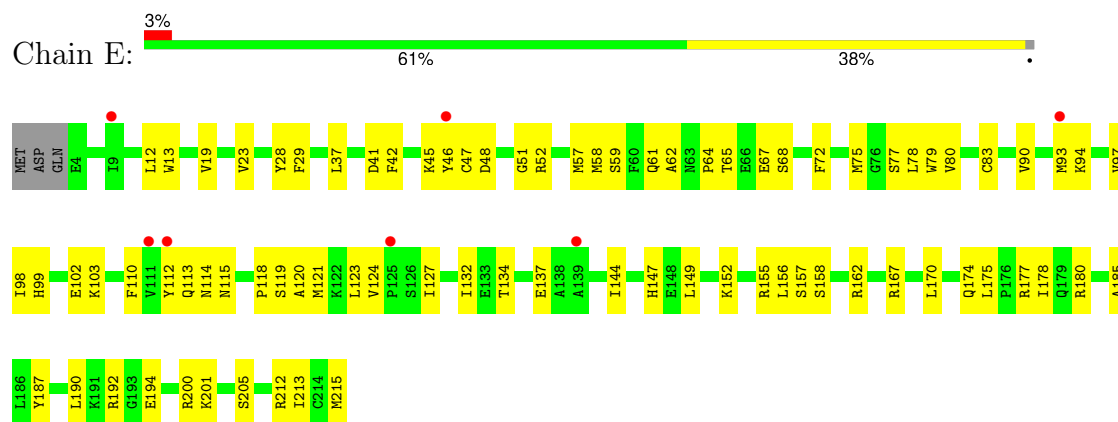


ASP
PHE

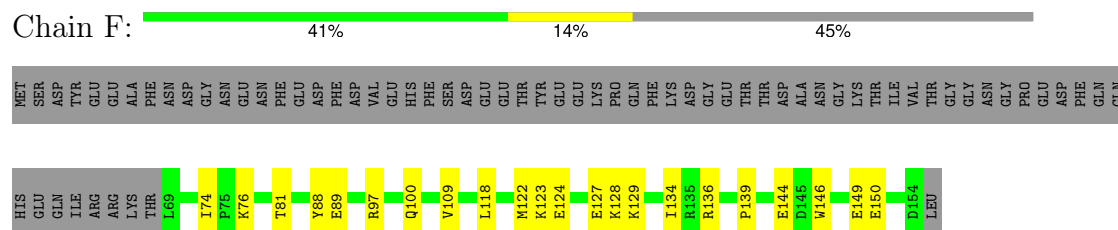
• Molecule 6: DNA-directed RNA polymerase II subunit RPB3



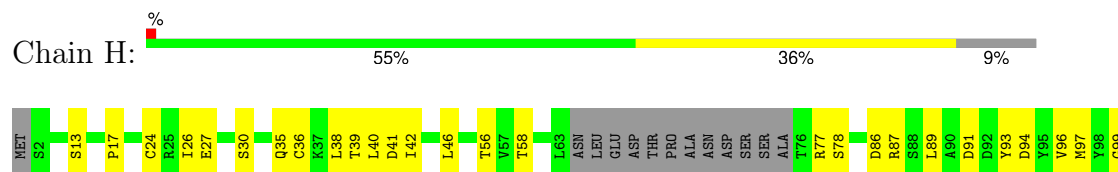
• Molecule 7: DNA-directed RNA polymerases I, II, and III subunit RPABC1



• Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC2

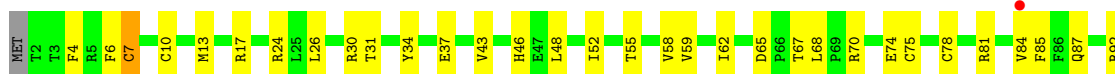


• Molecule 9: DNA-directed RNA polymerases I, II, and III subunit RPABC3





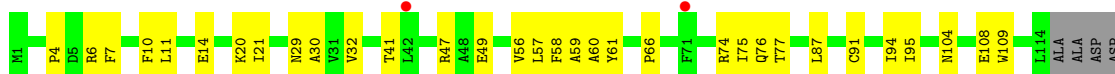
- Molecule 10: DNA-directed RNA polymerase II subunit RPB9



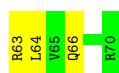
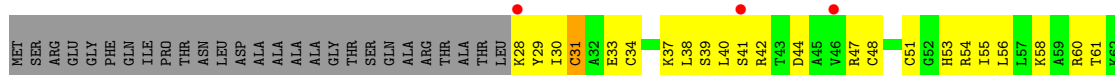
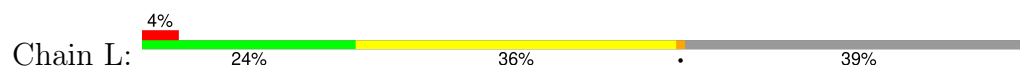
- Molecule 11: DNA-directed RNA polymerases I, II, and III subunit RPABC5



- Molecule 12: DNA-directed RNA polymerase II subunit RPB11



- Molecule 13: DNA-directed RNA polymerases I, II, and III subunit RPABC4



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	156.68Å 221.39Å 190.54Å 90.00° 97.67° 90.00°	Depositor
Resolution (Å)	47.75 – 3.60 47.75 – 3.60	Depositor EDS
% Data completeness (in resolution range)	99.8 (47.75-3.60) 99.7 (47.75-3.60)	Depositor EDS
R_{merge}	0.58	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.14 (at 3.57Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.251 , 0.289 0.252 , 0.290	Depositor DCC
R_{free} test set	2000 reflections (2.64%)	wwPDB-VP
Wilson B-factor (Å ²)	98.4	Xtriage
Anisotropy	0.506	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 124.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	29013	wwPDB-VP
Average B, all atoms (Å ²)	127.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.58% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	R	0.15	0/244	0.33	0/380
2	T	0.22	0/507	0.49	0/775
3	N	0.21	0/311	0.44	0/479
4	A	0.15	0/11020	0.40	3/14907 (0.0%)
5	B	0.14	0/9050	0.36	0/12215
6	C	0.12	0/2139	0.31	0/2899
7	E	0.14	0/1767	0.34	0/2378
8	F	0.12	0/696	0.32	0/943
9	H	0.17	0/1082	0.45	0/1466
10	I	0.14	0/966	0.41	0/1304
11	J	0.17	0/541	0.37	0/727
12	K	0.14	0/937	0.39	0/1265
13	L	0.20	0/339	0.49	0/450
All	All	0.15	0/29599	0.38	3/40188 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	311	GLN	CA-CB-CG	5.30	124.71	114.10
4	A	1097	GLY	CA-C-N	5.11	124.42	120.33
4	A	1097	GLY	C-N-CA	5.11	124.42	120.33

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	R	217	0	111	9	0
2	T	481	0	262	18	0
3	N	275	0	144	9	0
4	A	10828	0	10876	424	0
5	B	8878	0	8827	318	0
6	C	2101	0	2057	73	0
7	E	1731	0	1758	59	0
8	F	684	0	692	16	0
9	H	1064	0	1029	44	0
10	I	948	0	886	35	0
11	J	532	0	542	29	0
12	K	919	0	929	27	0
13	L	337	0	352	34	1
14	R	1	0	0	0	0
15	A	2	0	0	0	0
15	B	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
16	B	9	0	0	2	0
All	All	29013	0	28465	965	1

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 17.

All (965) 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)
4:A:108:MET:HE3	4:A:210:ILE:HD13	1.52	0.90
9:H:36:CYS:HA	9:H:126:GLU:O	1.72	0.89
11:J:21:TYR:HB2	11:J:39:LEU:HD11	1.56	0.85
5:B:942:ARG:HB2	5:B:945:GLU:HG3	1.60	0.84
10:I:24:ARG:HH11	10:I:26:LEU:HD11	1.40	0.83
4:A:919:ILE:HG12	4:A:983:ILE:HD12	1.63	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:703:ILE:HG22	5:B:740:HIS:HB2	1.62	0.79
4:A:587:HIS:HA	4:A:607:ILE:O	1.82	0.79
6:C:39:ALA:HA	6:C:164:ALA:HB3	1.64	0.78
4:A:1224:LEU:HD21	4:A:1240:CYS:HB3	1.64	0.78
13:L:29:TYR:O	13:L:38:LEU:HB2	1.84	0.78
4:A:114:LEU:HD22	4:A:148:CYS:HB2	1.66	0.77
9:H:96:VAL:HA	9:H:142:LEU:O	1.84	0.77
5:B:102:VAL:HG22	5:B:112:LEU:HB2	1.65	0.76
5:B:519:TRP:CD1	5:B:635:ARG:HH12	2.04	0.76
5:B:373:ARG:H	5:B:373:ARG:HD2	1.50	0.76
5:B:642:ASP:HA	5:B:649:LYS:HA	1.68	0.75
4:A:224:PHE:HB3	4:A:229:SER:HB3	1.67	0.75
4:A:973:ILE:HG22	4:A:975:HIS:H	1.51	0.74
5:B:365:THR:HG22	5:B:367:LEU:H	1.53	0.73
4:A:702:LEU:HG	4:A:710:LEU:HD12	1.71	0.73
4:A:67:CYS:HB3	4:A:70:CYS:HB2	1.70	0.73
5:B:364:ILE:HG12	5:B:585:VAL:HG13	1.71	0.73
4:A:170:THR:HG23	4:A:185:TRP:HE1	1.52	0.73
4:A:526:ASP:HB2	5:B:835:GLN:HE21	1.54	0.72
4:A:447:GLN:OE1	4:A:488:ASN:ND2	2.23	0.72
5:B:1174:LYS:HB2	5:B:1177:HIS:HB2	1.71	0.72
7:E:72:PHE:HB2	7:E:75:MET:HG2	1.71	0.72
4:A:540:PHE:HB3	4:A:571:LEU:HD12	1.72	0.72
4:A:1278:ASN:HB2	4:A:1312:ASN:HB2	1.72	0.71
4:A:606:LEU:HG	4:A:613:ILE:HD13	1.73	0.71
4:A:434:ARG:NH2	4:A:440:ASP:OD2	2.24	0.71
4:A:885:THR:HG23	4:A:1024:SER:HB3	1.71	0.71
4:A:998:LEU:HB2	4:A:1001:ARG:HH21	1.54	0.71
6:C:22:LEU:HB3	6:C:25:VAL:HG21	1.72	0.71
7:E:62:ALA:HB3	7:E:78:LEU:HB3	1.71	0.71
11:J:2:ILE:HD13	11:J:57:ILE:HD13	1.71	0.71
4:A:830:LYS:O	4:A:834:THR:HG23	1.91	0.70
4:A:881:GLN:HG2	4:A:959:ASN:HD22	1.55	0.70
4:A:444:PHE:HE2	4:A:470:LEU:HD23	1.57	0.70
6:C:71:PRO:HB2	6:C:133:ILE:HD12	1.74	0.70
11:J:13:VAL:O	11:J:17:LYS:NZ	2.23	0.70
4:A:446:ARG:HG3	4:A:448:PRO:HD2	1.74	0.70
4:A:1004:ASN:HD22	4:A:1007:ILE:HG12	1.57	0.70
6:C:36:VAL:HG13	6:C:40:GLU:HB2	1.73	0.70
13:L:47:ARG:HB2	13:L:54:ARG:HA	1.75	0.69
5:B:69:LEU:HD21	5:B:429:PHE:HB2	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:325:ILE:HA	4:A:328:ARG:HD2	1.74	0.69
11:J:17:LYS:HB3	11:J:39:LEU:HD13	1.73	0.69
5:B:1210:MET:O	5:B:1211:ASN:ND2	2.26	0.69
4:A:1192:LEU:HD22	4:A:1239:ARG:HH21	1.59	0.68
4:A:605:MET:HE3	4:A:621:THR:HG21	1.74	0.68
5:B:519:TRP:HD1	5:B:635:ARG:HH12	1.41	0.68
5:B:1056:SER:HB3	5:B:1066:SER:HB2	1.74	0.68
5:B:955:THR:HB	13:L:55:ILE:HA	1.75	0.67
10:I:78:CYS:HB2	10:I:105:SER:HB2	1.76	0.67
13:L:28:LYS:N	13:L:40:LEU:HA	2.10	0.67
5:B:882:THR:HG22	5:B:934:LYS:HB2	1.77	0.67
12:K:30:ALA:HA	12:K:75:ILE:O	1.95	0.67
4:A:672:ASP:H	4:A:736:ASN:HD21	1.42	0.67
4:A:960:ILE:HG21	4:A:1025:ARG:HB3	1.77	0.67
4:A:464:PRO:HB2	12:K:4:PRO:HD3	1.77	0.66
10:I:17:ARG:HH22	10:I:30:ARG:HH21	1.42	0.66
6:C:6:PRO:O	12:K:104:ASN:ND2	2.29	0.66
6:C:56:THR:HG22	6:C:147:LEU:HD21	1.75	0.66
4:A:243:PRO:HB2	4:A:245:PRO:HD2	1.77	0.66
5:B:651:LEU:HD12	5:B:653:VAL:O	1.96	0.66
9:H:38:LEU:HB2	9:H:125:LEU:HD13	1.76	0.66
5:B:892:LYS:HD2	5:B:909:ASP:HB3	1.78	0.65
4:A:332:LYS:HA	4:A:337:ARG:HD3	1.76	0.65
5:B:780:VAL:HG22	5:B:795:ILE:HG23	1.78	0.65
3:N:7:DA:H2'	3:N:8:DG:C8	2.31	0.65
7:E:170:LEU:HD21	7:E:175:LEU:HB2	1.78	0.65
5:B:24:PRO:HA	5:B:654:ARG:HD3	1.78	0.65
5:B:384:ARG:NH1	5:B:623:GLU:OE2	2.28	0.65
5:B:90:ILE:HD11	5:B:432:MET:HE1	1.78	0.65
5:B:121:ASN:HA	5:B:207:GLY:HA3	1.78	0.65
4:A:18:GLN:NE2	4:A:19:PHE:O	2.30	0.65
5:B:428:ILE:HG12	5:B:448:ILE:HG22	1.78	0.65
4:A:890:ASP:HA	4:A:940:ARG:HH12	1.60	0.65
4:A:1341:ILE:HG13	4:A:1376:THR:HG23	1.78	0.64
5:B:996:ARG:HG3	5:B:1007:VAL:HG21	1.79	0.64
8:F:127:GLU:HB3	8:F:129:LYS:HG2	1.78	0.64
6:C:31:ASN:OD1	6:C:34:ARG:NH1	2.30	0.64
6:C:99:LEU:HD12	6:C:118:LEU:HB3	1.79	0.64
8:F:128:LYS:HD2	8:F:149:GLU:HA	1.78	0.64
5:B:1196:ILE:HD11	5:B:1201:LYS:HB2	1.79	0.64
8:F:76:LYS:NZ	8:F:150:GLU:OE2	2.26	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:H:125:LEU:HG	9:H:130:ARG:HH12	1.63	0.64
6:C:147:LEU:HD22	6:C:151:GLN:HB3	1.80	0.63
4:A:507:VAL:HG13	4:A:521:MET:HE1	1.80	0.63
4:A:586:ILE:HD13	4:A:633:VAL:HG22	1.79	0.63
4:A:868:TYR:CE1	4:A:1064:VAL:HG11	2.34	0.63
5:B:639:ILE:HD11	5:B:691:GLU:HB2	1.80	0.63
9:H:110:ASP:OD1	9:H:128:ASN:ND2	2.32	0.63
4:A:1348:LEU:HD23	4:A:1372:VAL:HG13	1.81	0.63
5:B:953:LEU:O	5:B:964:VAL:HA	1.98	0.63
7:E:47:CYS:HB3	7:E:51:GLY:HA2	1.81	0.63
1:R:8:G:H5'	5:B:776:GLN:HE22	1.63	0.63
4:A:71:GLN:HE22	5:B:1176:ASN:HB3	1.64	0.63
5:B:751:VAL:HG23	5:B:812:LEU:HD13	1.81	0.63
12:K:32:VAL:HG12	12:K:74:ARG:HG3	1.81	0.62
9:H:93:TYR:HA	9:H:145:ARG:HD3	1.81	0.62
4:A:443:LEU:HD21	4:A:455:MET:HB3	1.82	0.62
5:B:862:GLN:HB3	5:B:963:PHE:HB3	1.82	0.62
4:A:560:ILE:H	9:H:78:SER:HB2	1.65	0.62
4:A:1364:ASN:OD1	4:A:1366:ARG:NH1	2.33	0.62
4:A:1425:SER:O	4:A:1429:ILE:HD12	2.00	0.62
4:A:169:ASN:O	4:A:171:GLN:NE2	2.33	0.62
7:E:175:LEU:HD23	7:E:213:ILE:HB	1.81	0.62
4:A:1421:CYS:O	4:A:1427:ASN:ND2	2.32	0.61
5:B:118:ARG:NH2	5:B:202:TYR:OH	2.32	0.61
9:H:101:ALA:HA	9:H:116:TYR:HA	1.83	0.61
9:H:135:LEU:HB3	9:H:137:GLN:HG2	1.80	0.61
7:E:177:ARG:HD3	7:E:215:MET:HE2	1.83	0.61
5:B:845:SER:HB3	11:J:8:PHE:HB3	1.83	0.61
2:T:17:DG:H4'	4:A:1403:GLU:HG2	1.83	0.61
4:A:326:ARG:HG3	4:A:1406:VAL:HG11	1.82	0.61
4:A:1219:THR:HG21	4:A:1271:ILE:HG23	1.83	0.61
6:C:146:LYS:NZ	11:J:58:GLU:OE2	2.31	0.61
10:I:78:CYS:HB3	10:I:106:CYS:HB3	1.83	0.61
2:T:12:DT:H2'	2:T:13:DC:C6	2.35	0.61
5:B:521:LEU:HD22	5:B:633:VAL:HG12	1.83	0.60
5:B:862:GLN:O	5:B:914:LYS:NZ	2.35	0.60
5:B:778:MET:HE2	5:B:1094:ARG:HB3	1.83	0.60
4:A:451:HIS:HD2	4:A:1070:GLN:HB3	1.66	0.60
4:A:1188:GLN:N	4:A:1188:GLN:OE1	2.34	0.60
4:A:1128:GLN:HG3	4:A:1304:TRP:HE1	1.65	0.60
4:A:1193:LEU:HB2	4:A:1260:LEU:HD11	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:I:92:ARG:HG3	10:I:94:ASP:H	1.67	0.60
5:B:950:ASP:HB3	5:B:967:ARG:HG2	1.84	0.60
10:I:55:THR:HG21	10:I:109:ILE:HG21	1.84	0.60
4:A:14:VAL:HA	5:B:1218:THR:HA	1.84	0.60
5:B:877:PRO:HB2	5:B:885:MET:HE2	1.83	0.60
5:B:953:LEU:HD11	13:L:55:ILE:HB	1.84	0.60
5:B:120:ARG:HH22	13:L:54:ARG:HD3	1.67	0.59
5:B:259:TYR:OH	5:B:279:ASP:OD2	2.20	0.59
7:E:124:VAL:HG13	7:E:132:ILE:HB	1.83	0.59
4:A:457:ALA:HB3	4:A:506:ALA:HA	1.84	0.59
4:A:1169:ILE:HA	4:A:1172:LEU:HD12	1.84	0.59
4:A:1345:ARG:HG3	4:A:1372:VAL:HG12	1.85	0.59
6:C:55:THR:OG1	6:C:152:GLU:N	2.33	0.59
4:A:106:VAL:HG11	4:A:214:ILE:HG12	1.84	0.59
8:F:118:LEU:O	8:F:122:MET:HG3	2.02	0.59
5:B:1054:GLY:HA2	5:B:1057:LYS:HD2	1.83	0.59
4:A:565:ILE:HG21	9:H:46:LEU:HD13	1.83	0.59
4:A:666:ILE:HD11	5:B:1067:ARG:HA	1.84	0.59
4:A:228:PHE:HE1	5:B:1215:ARG:HD3	1.66	0.59
5:B:496:ARG:NH1	5:B:540:SER:O	2.36	0.59
6:C:177:GLU:O	6:C:230:MET:HA	2.02	0.58
5:B:800:GLN:NE2	11:J:49:MET:SD	2.76	0.58
4:A:22:PHE:HE2	5:B:1208:MET:HA	1.68	0.58
4:A:583:PRO:HD3	4:A:645:LEU:HD13	1.86	0.58
5:B:847:ASP:OD2	12:K:6:ARG:NH2	2.37	0.58
5:B:605:ARG:NH1	5:B:691:GLU:OE2	2.36	0.58
4:A:344:ARG:HA	5:B:1129:ARG:HA	1.85	0.58
4:A:391:LEU:HD22	4:A:400:PRO:HB2	1.84	0.58
4:A:830:LYS:HD3	4:A:1080:THR:HA	1.86	0.58
7:E:13:TRP:NE1	7:E:37:LEU:O	2.37	0.58
4:A:908:LEU:HD21	4:A:983:ILE:HD11	1.86	0.58
4:A:944:ARG:NH2	4:A:1296:GLY:O	2.37	0.58
5:B:39:ARG:NH2	5:B:668:ASP:OD2	2.37	0.58
4:A:946:VAL:HG22	7:E:201:LYS:HG2	1.86	0.58
5:B:724:ASP:HB2	5:B:727:LYS:HZ2	1.69	0.58
4:A:42:ASP:HB2	4:A:49:LYS:H	1.69	0.57
4:A:592:ASP:N	4:A:595:THR:OG1	2.35	0.57
4:A:1095:THR:H	4:A:1113:THR:HG21	1.69	0.57
5:B:915:THR:HB	5:B:934:LYS:HB3	1.86	0.57
9:H:125:LEU:HG	9:H:130:ARG:HH22	1.68	0.57
4:A:665:GLY:HA2	5:B:1086:PHE:CD2	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:752:LYS:NZ	16:B:1302:POP:O5	2.37	0.57
5:B:750:GLY:O	5:B:754:SER:OG	2.20	0.57
1:R:2:U:H2'	1:R:3:C:C6	2.40	0.57
10:I:24:ARG:NH1	10:I:26:LEU:HD11	2.14	0.57
7:E:180:ARG:HH11	7:E:192:ARG:HG2	1.70	0.57
4:A:37:PHE:H	4:A:52:GLY:HA3	1.69	0.57
5:B:470:LYS:HG3	5:B:473:MET:H	1.70	0.57
5:B:622:LYS:HD3	10:I:59:VAL:HG21	1.87	0.57
6:C:83:SER:HA	6:C:95:CYS:SG	2.45	0.57
4:A:1363:VAL:HB	4:A:1368:MET:HE3	1.87	0.57
4:A:694:THR:HG22	4:A:698:GLN:HE21	1.69	0.57
4:A:466:SER:HB2	5:B:1103:ILE:HD11	1.87	0.57
6:C:94:LYS:HA	6:C:127:ARG:HH22	1.69	0.57
13:L:47:ARG:NH1	13:L:54:ARG:HE	2.03	0.57
13:L:30:ILE:HG13	13:L:37:LYS:HA	1.85	0.56
4:A:269:ILE:HG13	4:A:299:HIS:HB3	1.86	0.56
4:A:859:SER:O	4:A:1422:ARG:NH1	2.38	0.56
4:A:567:LYS:HB2	9:H:96:VAL:HB	1.87	0.56
4:A:813:PHE:HE2	5:B:749:LEU:HD21	1.70	0.56
4:A:849:MET:HE2	4:A:1061:GLY:HA2	1.86	0.56
4:A:121:LEU:HD23	4:A:141:LEU:HD22	1.87	0.56
5:B:977:GLY:HA2	5:B:989:THR:HG22	1.86	0.56
5:B:1135:ARG:O	5:B:1139:ILE:HG12	2.04	0.56
5:B:29:ASP:HB3	5:B:658:ILE:HG21	1.86	0.56
5:B:461:LEU:HD13	5:B:466:TRP:HH2	1.70	0.56
4:A:138:ILE:O	4:A:142:CYS:HB2	2.06	0.56
5:B:834:ASN:OD1	5:B:1013:ASN:ND2	2.39	0.56
9:H:26:ILE:O	9:H:39:THR:HA	2.06	0.56
10:I:65:ASP:HB3	10:I:68:LEU:HD12	1.88	0.56
12:K:56:VAL:HG22	12:K:77:THR:HG22	1.87	0.56
4:A:308:ILE:HG13	4:A:312:PRO:HD2	1.88	0.56
6:C:241:ASP:HB3	12:K:109:TRP:CD1	2.41	0.56
4:A:761:MET:HA	4:A:804:TYR:HB2	1.87	0.56
4:A:861:GLY:HA3	7:E:174:GLN:HE21	1.69	0.56
8:F:74:ILE:HG13	8:F:144:GLU:HG2	1.88	0.56
4:A:727:ASP:O	4:A:731:ARG:HG2	2.05	0.56
5:B:493:SER:OG	5:B:526:GLU:OE2	2.20	0.56
5:B:473:MET:O	5:B:476:ARG:NH2	2.39	0.56
5:B:1114:LEU:HG	5:B:1202:LEU:HD11	1.88	0.56
9:H:40:LEU:HD12	9:H:123:MET:HG3	1.86	0.56
4:A:1262:LYS:HA	4:A:1265:ASN:OD1	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:464:GLY:HA2	5:B:480:SER:HB3	1.87	0.55
4:A:336:ILE:HD11	5:B:1203:LEU:HD13	1.87	0.55
4:A:1325:THR:HA	7:E:147:HIS:HA	1.87	0.55
4:A:932:GLU:O	4:A:936:LEU:HG	2.07	0.55
4:A:528:LEU:O	4:A:531:ILE:HG22	2.06	0.55
4:A:1012:ARG:O	4:A:1016:THR:OG1	2.21	0.55
9:H:58:THR:HB	9:H:143:LEU:HB2	1.89	0.55
4:A:387:ARG:O	4:A:391:LEU:HG	2.06	0.55
4:A:1191:TRP:HZ3	10:I:43:VAL:HG21	1.72	0.55
5:B:980:PHE:CE1	5:B:990:ILE:HD11	2.41	0.55
9:H:30:SER:HB2	9:H:36:CYS:HB2	1.88	0.55
2:T:27:DA:H2'	2:T:28:DT:C6	2.42	0.55
11:J:2:ILE:HG13	11:J:3:VAL:H	1.71	0.55
4:A:1336:MET:HG3	4:A:1341:ILE:HA	1.89	0.55
11:J:1:MET:HE2	11:J:60:PHE:CE2	2.42	0.55
4:A:1075:PRO:O	4:A:1079:MET:N	2.39	0.55
5:B:612:GLU:O	5:B:632:ARG:NH1	2.37	0.55
5:B:350:GLN:HA	5:B:353:LYS:HD3	1.88	0.54
7:E:170:LEU:HG	7:E:174:GLN:HB2	1.88	0.54
4:A:993:LEU:HD22	4:A:1046:LEU:HG	1.89	0.54
10:I:92:ARG:HB3	10:I:95:THR:HG23	1.88	0.54
4:A:1261:LYS:O	4:A:1265:ASN:OD1	2.24	0.54
5:B:839:MET:HB3	5:B:1010:LEU:HD21	1.89	0.54
5:B:899:ILE:HG12	5:B:903:VAL:HG11	1.88	0.54
5:B:1168:LEU:HD23	5:B:1208:MET:HE2	1.88	0.54
4:A:260:ASP:OD2	4:A:328:ARG:NH2	2.41	0.54
7:E:119:SER:O	7:E:123:LEU:HG	2.07	0.54
5:B:766:ARG:HD2	5:B:1020:ARG:HB3	1.88	0.54
4:A:378:GLU:HG2	4:A:388:LEU:HD11	1.89	0.54
4:A:1383:SER:OG	4:A:1387:HIS:O	2.23	0.54
4:A:633:VAL:HG21	4:A:645:LEU:HD22	1.88	0.54
5:B:373:ARG:H	5:B:373:ARG:CD	2.19	0.54
4:A:185:TRP:HB3	4:A:199:LEU:HD12	1.89	0.54
4:A:298:PHE:HE1	4:A:312:PRO:HB2	1.73	0.54
5:B:101:MET:HA	5:B:112:LEU:H	1.73	0.54
5:B:570:VAL:HG23	5:B:573:GLN:HB2	1.90	0.54
6:C:7:GLN:HA	12:K:104:ASN:HD22	1.72	0.54
11:J:7:CYS:HA	11:J:49:MET:HE3	1.89	0.54
12:K:47:ARG:HD3	12:K:61:TYR:HB2	1.90	0.54
5:B:219:ALA:HB2	5:B:405:ARG:HG2	1.89	0.54
7:E:57:MET:HE1	7:E:58:MET:HE2	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:986:ILE:HD12	4:A:1028:THR:HG23	1.90	0.54
4:A:888:GLY:O	4:A:940:ARG:NH2	2.41	0.53
4:A:1288:ASP:HA	4:A:1302:PRO:HA	1.88	0.53
5:B:840:ILE:HB	5:B:1011:ILE:HB	1.90	0.53
4:A:886:ILE:HD12	4:A:943:LEU:HB3	1.90	0.53
6:C:41:ILE:HB	6:C:172:PRO:HG2	1.90	0.53
12:K:59:ALA:HA	12:K:74:ARG:O	2.09	0.53
4:A:1303:GLU:OE1	4:A:1326:ARG:NH2	2.35	0.53
5:B:796:LEU:HB3	5:B:799:PRO:HG3	1.89	0.53
13:L:33:GLU:HG2	13:L:53:HIS:CD2	2.43	0.53
4:A:806:ARG:NH1	5:B:727:LYS:O	2.40	0.53
4:A:881:GLN:O	4:A:953:ASN:HA	2.09	0.53
4:A:1209:MET:HE3	4:A:1236:LEU:HD13	1.91	0.53
5:B:878:GLN:HB2	5:B:881:ASN:HB2	1.90	0.53
4:A:578:LEU:O	4:A:582:ILE:HG13	2.09	0.53
5:B:213:ILE:HG23	5:B:497:ARG:HG2	1.91	0.53
5:B:369:GLY:O	5:B:373:ARG:NH1	2.42	0.53
5:B:1076:HIS:O	6:C:31:ASN:ND2	2.42	0.53
5:B:1147:LEU:O	5:B:1151:LEU:HB2	2.09	0.53
7:E:185:ALA:HA	7:E:190:LEU:HD23	1.91	0.53
4:A:636:GLU:OE1	4:A:966:ASN:ND2	2.42	0.53
4:A:1150:SER:HB3	10:I:46:HIS:HB3	1.91	0.53
6:C:165:LYS:HD2	12:K:10:PHE:HB3	1.90	0.53
2:T:6:DT:H2''	2:T:7:DC:C4	2.44	0.53
4:A:121:LEU:HB3	4:A:141:LEU:HD13	1.91	0.53
4:A:137:ALA:O	4:A:141:LEU:HG	2.09	0.53
4:A:898:ARG:HH12	4:A:930:ASP:HA	1.74	0.53
5:B:193:LYS:HG2	5:B:787:VAL:HG21	1.90	0.53
4:A:602:ASP:OD2	4:A:616:VAL:HG23	2.09	0.52
6:C:142:VAL:HG23	11:J:15:GLY:HA3	1.90	0.52
7:E:61:GLN:HB2	7:E:79:TRP:HE3	1.74	0.52
2:T:6:DT:H2''	2:T:7:DC:C5	2.44	0.52
3:N:7:DA:H2''	3:N:8:DG:H5'	1.91	0.52
4:A:25:GLU:HA	4:A:28:ARG:HE	1.74	0.52
12:K:91:CYS:HA	12:K:94:ILE:HD12	1.91	0.52
13:L:29:TYR:HE1	13:L:58:LYS:HE3	1.73	0.52
4:A:50:ILE:HG23	4:A:52:GLY:H	1.75	0.52
4:A:879:GLU:OE2	4:A:962:ARG:NH2	2.42	0.52
5:B:273:LEU:HB2	5:B:276:ILE:HB	1.90	0.52
4:A:482:PHE:CD2	5:B:836:GLU:HB2	2.44	0.52
4:A:951:GLU:O	4:A:954:TRP:NE1	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:104:GLU:OE2	5:B:120:ARG:NH2	2.39	0.52
6:C:60:ASP:OD2	13:L:60:ARG:NH2	2.42	0.52
4:A:1161:THR:HG23	4:A:1167:GLU:HG2	1.90	0.52
5:B:425:THR:HA	5:B:428:ILE:HD12	1.92	0.52
6:C:178:PHE:HE1	6:C:228:PHE:HB3	1.74	0.52
5:B:825:VAL:HG22	5:B:1010:LEU:HB3	1.91	0.52
5:B:551:PRO:O	5:B:555:ILE:HG12	2.10	0.52
4:A:427:GLN:HB2	4:A:430:TRP:CE2	2.45	0.52
5:B:193:LYS:NZ	13:L:33:GLU:OE2	2.43	0.52
5:B:245:GLU:HA	5:B:249:ARG:HH22	1.75	0.52
6:C:50:GLU:HG3	13:L:66:GLN:HA	1.91	0.52
11:J:41:LEU:HD23	11:J:46:CYS:HB3	1.92	0.52
4:A:92:HIS:CD2	4:A:304:MET:HE3	2.45	0.51
4:A:262:LEU:O	4:A:266:LEU:HG	2.10	0.51
4:A:827:THR:O	4:A:831:THR:HG23	2.10	0.51
4:A:1217:LYS:NZ	4:A:1222:ASN:OD1	2.43	0.51
5:B:25:ILE:H	5:B:651:LEU:HD11	1.75	0.51
5:B:830:TYR:H	5:B:834:ASN:HD21	1.57	0.51
4:A:210:ILE:O	4:A:214:ILE:HG13	2.10	0.51
4:A:265:LYS:HG3	4:A:303:TYR:HB2	1.93	0.51
4:A:705:LYS:HB2	4:A:708:MET:HB3	1.93	0.51
5:B:914:LYS:HB3	5:B:937:ALA:HB3	1.91	0.51
9:H:56:THR:HB	9:H:145:ARG:HB3	1.91	0.51
5:B:1063:GLY:O	6:C:202:PRO:HG3	2.10	0.51
4:A:472:LEU:HD12	4:A:650:GLN:HE21	1.76	0.51
5:B:227:LYS:HA	5:B:236:HIS:HD2	1.74	0.51
6:C:259:LEU:O	6:C:263:THR:HG23	2.11	0.51
6:C:262:LEU:HD11	12:K:87:LEU:HD23	1.91	0.51
10:I:68:LEU:HB3	10:I:84:VAL:HG13	1.92	0.51
13:L:38:LEU:HD22	13:L:56:LEU:HD21	1.91	0.51
4:A:181:LEU:O	4:A:202:LEU:HB2	2.11	0.51
4:A:840:ARG:HE	4:A:1384:VAL:HG23	1.76	0.51
5:B:465:ASN:HB3	5:B:474:SER:HB2	1.93	0.51
5:B:848:ARG:HD2	11:J:8:PHE:HA	1.91	0.51
4:A:351:THR:HG23	5:B:1103:ILE:HG12	1.91	0.51
5:B:754:SER:HB2	5:B:812:LEU:HD11	1.93	0.51
10:I:85:PHE:HB3	10:I:101:PHE:CD2	2.45	0.51
4:A:483:ASP:HB2	5:B:987:LYS:HD3	1.92	0.51
4:A:550:LEU:HD12	4:A:577:ILE:HD13	1.92	0.51
7:E:180:ARG:NH1	7:E:215:MET:O	2.43	0.51
4:A:340:LEU:HD13	4:A:1429:ILE:HG23	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:535:THR:HG21	4:A:617:VAL:HG23	1.92	0.51
13:L:31:CYS:SG	13:L:51:CYS:HB3	2.51	0.51
13:L:47:ARG:HH11	13:L:54:ARG:HE	1.58	0.51
4:A:335:ARG:O	4:A:340:LEU:N	2.35	0.51
4:A:569:LYS:NZ	6:C:222:LYS:HD2	2.25	0.51
4:A:798:GLY:HA2	4:A:815:PHE:CD2	2.46	0.51
4:A:913:LEU:HD22	4:A:915:SER:H	1.75	0.51
4:A:1070:GLN:HE22	5:B:1137:CYS:HA	1.75	0.51
4:A:1329:THR:H	4:A:1335:ILE:HD11	1.75	0.51
7:E:37:LEU:HD23	7:E:42:PHE:HD1	1.75	0.51
9:H:40:LEU:HD21	9:H:42:ILE:HD13	1.91	0.51
9:H:132:LEU:HD12	9:H:132:LEU:H	1.76	0.51
13:L:39:SER:O	13:L:40:LEU:HG	2.10	0.51
5:B:843:GLN:HA	5:B:846:ILE:HD12	1.93	0.50
4:A:131:SER:HA	4:A:134:ARG:HD3	1.93	0.50
4:A:915:SER:O	4:A:919:ILE:N	2.44	0.50
5:B:220:GLY:HA2	5:B:241:ARG:HG3	1.94	0.50
5:B:274:PRO:HG2	5:B:359:GLU:HB3	1.93	0.50
4:A:214:ILE:HB	4:A:219:PHE:HE1	1.76	0.50
4:A:388:LEU:O	4:A:392:VAL:HG23	2.11	0.50
4:A:537:ARG:NH2	4:A:599:SER:O	2.44	0.50
4:A:339:ASN:O	4:A:343:LYS:HG2	2.12	0.50
4:A:497:THR:HG23	5:B:1146:PHE:HB2	1.93	0.50
4:A:569:LYS:HD2	6:C:221:TYR:HB2	1.92	0.50
5:B:203:PHE:HB3	5:B:205:ILE:HD11	1.93	0.50
4:A:75:ASN:OD1	5:B:1116:ARG:NH1	2.45	0.50
4:A:176:LYS:HA	4:A:181:LEU:HA	1.92	0.50
4:A:108:MET:HE3	4:A:210:ILE:CD1	2.35	0.50
4:A:66:LYS:H	4:A:66:LYS:HD2	1.77	0.50
4:A:443:LEU:HD12	4:A:501:LEU:HD11	1.92	0.50
5:B:1072:MET:HG3	5:B:1085:ILE:HB	1.93	0.50
6:C:48:SER:OG	6:C:50:GLU:OE2	2.29	0.50
9:H:97:MET:HE2	9:H:118:PHE:HB3	1.93	0.50
4:A:218:ASP:O	4:A:222:LEU:HG	2.12	0.50
5:B:355:ILE:HG23	5:B:359:GLU:HB2	1.92	0.50
5:B:656:GLY:O	5:B:660:LYS:HG3	2.11	0.50
7:E:158:SER:O	7:E:162:ARG:HG3	2.11	0.50
10:I:58:VAL:HA	10:I:62:ILE:HD12	1.94	0.50
4:A:587:HIS:HB3	4:A:608:ILE:HD13	1.94	0.49
4:A:941:LYS:NZ	4:A:945:GLU:OE2	2.39	0.49
4:A:1035:TYR:CD1	4:A:1037:LEU:HD13	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:954:VAL:O	13:L:56:LEU:N	2.44	0.49
4:A:544:ASP:OD1	4:A:545:GLN:N	2.42	0.49
4:A:555:ASP:OD2	4:A:644:LYS:HE2	2.12	0.49
4:A:598:LEU:O	9:H:122:LEU:HD12	2.12	0.49
4:A:846:GLU:HA	4:A:1066:VAL:HG22	1.94	0.49
5:B:311:LEU:O	5:B:315:LYS:HG3	2.13	0.49
5:B:998:ASP:OD1	6:C:35:ARG:NH2	2.44	0.49
10:I:7:CYS:HB2	10:I:34:TYR:CD2	2.47	0.49
11:J:44:TYR:HA	11:J:47:ARG:HB2	1.94	0.49
4:A:1329:THR:HG22	4:A:1331:SER:H	1.76	0.49
6:C:144:ILE:HD12	6:C:144:ILE:H	1.77	0.49
4:A:214:ILE:HB	4:A:219:PHE:CE1	2.47	0.49
4:A:463:ILE:HG21	4:A:469:ARG:HG3	1.94	0.49
4:A:579:SER:OG	4:A:612:ILE:HG22	2.13	0.49
5:B:600:LEU:HD22	5:B:609:ILE:HD11	1.93	0.49
5:B:1054:GLY:O	5:B:1058:LEU:HG	2.12	0.49
1:R:1:A:H2'	1:R:2:U:C6	2.48	0.49
4:A:140:THR:HA	4:A:143:LYS:HE3	1.95	0.49
4:A:439:ASN:HA	4:A:459:ARG:HD2	1.95	0.49
4:A:674:PRO:HA	4:A:677:ARG:HD3	1.94	0.49
9:H:125:LEU:HG	9:H:130:ARG:NH1	2.27	0.49
4:A:842:VAL:HG11	5:B:1136:ASP:CG	2.37	0.49
5:B:883:LEU:HB2	5:B:932:HIS:HB3	1.94	0.49
2:T:5:DC:H2''	2:T:6:DT:H2'	1.94	0.49
5:B:890:TYR:HD1	5:B:893:LEU:HD12	1.77	0.49
6:C:77:ILE:O	6:C:161:LYS:NZ	2.39	0.49
4:A:287:HIS:O	4:A:290:GLU:HG3	2.13	0.49
4:A:579:SER:HB3	4:A:611:GLN:HA	1.93	0.49
4:A:779:PHE:CE2	4:A:785:PRO:HD3	2.48	0.49
13:L:38:LEU:HD21	13:L:48:CYS:HB3	1.94	0.49
4:A:5:GLN:NE2	4:A:72:GLU:OE1	2.46	0.49
4:A:9:ALA:HB3	5:B:1193:GLN:HG3	1.95	0.49
4:A:23:SER:HB2	4:A:233:TRP:CE2	2.47	0.49
4:A:97:ALA:O	4:A:101:LYS:HG2	2.12	0.49
4:A:356:ASP:OD1	5:B:833:TYR:OH	2.29	0.49
4:A:856:THR:HB	4:A:865:GLN:HB2	1.94	0.49
4:A:901:LEU:HD13	4:A:919:ILE:HG13	1.94	0.49
10:I:78:CYS:CB	10:I:103:CYS:SG	3.00	0.49
4:A:868:TYR:OH	4:A:1366:ARG:HD3	2.12	0.49
4:A:1027:ALA:O	4:A:1031:VAL:N	2.35	0.49
5:B:91:SER:HB2	5:B:133:LYS:HB2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:F:97:ARG:NH1	8:F:100:GLN:OE1	2.41	0.49
5:B:886:LYS:HE3	5:B:886:LYS:HA	1.94	0.48
6:C:36:VAL:HA	6:C:40:GLU:HG2	1.95	0.48
4:A:1118:VAL:HB	4:A:1306:LEU:HB2	1.95	0.48
4:A:1207:LEU:HD11	4:A:1273:LEU:HB2	1.96	0.48
5:B:788:ARG:O	5:B:967:ARG:NH1	2.46	0.48
8:F:89:GLU:HG2	8:F:134:ILE:HD13	1.96	0.48
9:H:93:TYR:CD2	9:H:145:ARG:HB2	2.48	0.48
4:A:1386:ARG:HA	4:A:1390:ASN:HB2	1.95	0.48
9:H:102:TYR:CZ	9:H:115:TYR:HB3	2.47	0.48
4:A:930:ASP:O	4:A:934:LYS:HG2	2.14	0.48
4:A:1115:SER:HA	4:A:1308:THR:O	2.12	0.48
5:B:205:ILE:HG13	5:B:461:LEU:HG	1.95	0.48
5:B:610:ASN:HB3	5:B:613:VAL:HG23	1.94	0.48
4:A:83:HIS:ND1	4:A:85:ASP:OD1	2.46	0.48
4:A:882:SER:O	4:A:1025:ARG:NH2	2.46	0.48
4:A:1099:PRO:O	4:A:1103:GLU:HG3	2.14	0.48
4:A:31:SER:O	5:B:1183:LYS:NZ	2.46	0.48
4:A:1117:THR:OG1	4:A:1328:TYR:O	2.31	0.48
7:E:112:TYR:HE1	7:E:134:THR:HA	1.79	0.48
2:T:10:DT:O2	3:N:10:DG:N2	2.47	0.48
4:A:858:ASN:HD21	4:A:860:LEU:HB2	1.79	0.48
4:A:1282:VAL:HG22	4:A:1308:THR:HG22	1.96	0.48
5:B:701:ILE:HB	5:B:739:THR:OG1	2.13	0.48
4:A:147:VAL:HG23	4:A:169:ASN:C	2.39	0.48
4:A:1109:LYS:H	4:A:1109:LYS:HD2	1.79	0.48
5:B:449:ASN:ND2	5:B:452:THR:HG23	2.28	0.48
5:B:806:THR:HG22	5:B:808:ALA:H	1.79	0.48
7:E:29:PHE:HB2	7:E:65:THR:HG22	1.95	0.48
9:H:112:ILE:HG21	9:H:131:ASN:HB3	1.96	0.48
4:A:105:CYS:CB	4:A:142:CYS:HB3	2.44	0.48
4:A:870:GLU:OE2	4:A:1365:TYR:OH	2.26	0.48
5:B:839:MET:HE2	5:B:1010:LEU:HD21	1.95	0.48
7:E:64:PRO:HD3	7:E:77:SER:H	1.79	0.48
4:A:693:VAL:HG21	4:A:721:PHE:HE2	1.79	0.48
4:A:982:THR:HG21	4:A:984:LYS:HE2	1.96	0.48
4:A:1225:PHE:CE1	4:A:1241:ARG:HB2	2.49	0.48
4:A:1438:THR:HA	8:F:88:TYR:HB3	1.95	0.48
9:H:125:LEU:HB3	9:H:130:ARG:HH12	1.79	0.48
10:I:65:ASP:OD1	10:I:67:THR:OG1	2.31	0.48
12:K:58:PHE:CE2	12:K:60:ALA:HB2	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:19:WVQ:OP3	4:A:337:ARG:NH2	2.47	0.47
2:T:19:WVQ:OP3	2:T:19:WVQ:O3'	2.32	0.47
4:A:779:PHE:HD1	5:B:699:GLU:HG2	1.78	0.47
4:A:786:HIS:HE1	5:B:519:TRP:NE1	2.12	0.47
8:F:81:THR:HB	8:F:136:ARG:HH11	1.79	0.47
12:K:7:PHE:HA	12:K:10:PHE:CE1	2.49	0.47
4:A:42:ASP:OD1	4:A:43:GLU:N	2.47	0.47
4:A:1004:ASN:HD21	4:A:1006:ILE:HB	1.79	0.47
5:B:370:PHE:HA	5:B:373:ARG:NH1	2.29	0.47
9:H:41:ASP:HB3	9:H:121:LEU:HD22	1.96	0.47
4:A:311:GLN:N	4:A:312:PRO:HD3	2.30	0.47
4:A:1138:ILE:HG23	4:A:1282:VAL:HG21	1.96	0.47
4:A:22:PHE:CD2	5:B:1213:THR:HG22	2.48	0.47
5:B:546:SER:HB2	5:B:612:GLU:CD	2.39	0.47
7:E:72:PHE:HE1	7:E:157:SER:HA	1.78	0.47
13:L:41:SER:O	13:L:44:ASP:HB2	2.14	0.47
4:A:380:VAL:HG12	4:A:388:LEU:HD12	1.95	0.47
4:A:451:HIS:HE1	4:A:515:GLN:NE2	2.12	0.47
5:B:236:HIS:CE1	5:B:389:ALA:HA	2.49	0.47
5:B:353:LYS:O	5:B:357:GLN:HG2	2.14	0.47
5:B:489:SER:HA	5:B:492:LEU:HD12	1.97	0.47
5:B:1009:ASP:OD2	11:J:48:ARG:NH2	2.47	0.47
7:E:83:CYS:HB3	7:E:110:PHE:HE1	1.79	0.47
4:A:267:ALA:O	4:A:271:LYS:HG3	2.15	0.47
5:B:983:ARG:NH2	5:B:1028:GLU:OE2	2.46	0.47
7:E:59:SER:HB2	7:E:80:VAL:O	2.15	0.47
12:K:29:ASN:H	12:K:76:GLN:HE21	1.62	0.47
4:A:248:PRO:HD3	5:B:1114:LEU:HD22	1.95	0.47
4:A:889:SER:HB2	4:A:1295:THR:HG22	1.95	0.47
4:A:1006:ILE:HD13	7:E:167:ARG:HG3	1.96	0.47
5:B:69:LEU:HB3	5:B:90:ILE:HD13	1.97	0.47
5:B:269:ILE:HD11	5:B:386:LEU:HD21	1.96	0.47
5:B:642:ASP:HB2	5:B:644:GLU:O	2.15	0.47
5:B:1172:ILE:HD11	5:B:1181:GLU:HB2	1.96	0.47
11:J:2:ILE:HD12	11:J:57:ILE:HG21	1.96	0.47
4:A:845:LEU:O	4:A:1065:GLY:HA3	2.15	0.47
5:B:485:ARG:CZ	5:B:782:LEU:HD11	2.45	0.47
5:B:1180:PHE:HB2	5:B:1191:ILE:HG12	1.96	0.47
2:T:15:DC:H4'	2:T:16:DT:OP1	2.14	0.47
4:A:1431:GLY:HA3	5:B:1197:PRO:HD3	1.97	0.47
1:R:4:G:H2'	1:R:5:A:H8	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:209:ASN:HA	4:A:212:LYS:HE3	1.96	0.47
4:A:592:ASP:O	4:A:603:ASN:ND2	2.48	0.47
4:A:728:LYS:O	4:A:732:LEU:HG	2.15	0.47
9:H:86:ASP:OD1	9:H:87:ARG:N	2.48	0.47
4:A:1074:GLU:O	4:A:1077:THR:OG1	2.27	0.46
5:B:31:TRP:HA	5:B:34:ILE:HD12	1.96	0.46
5:B:363:HIS:HD2	5:B:585:VAL:HG22	1.80	0.46
5:B:449:ASN:HD22	5:B:452:THR:HG23	1.80	0.46
4:A:172:PRO:HB2	4:A:183:GLY:HA3	1.97	0.46
4:A:139:TRP:HA	4:A:142:CYS:HB2	1.96	0.46
4:A:143:LYS:HG3	4:A:144:THR:HG23	1.97	0.46
4:A:356:ASP:HB2	4:A:469:ARG:HH21	1.80	0.46
4:A:605:MET:HE1	4:A:616:VAL:O	2.15	0.46
5:B:120:ARG:NH2	13:L:54:ARG:HD3	2.30	0.46
5:B:957:ASN:ND2	5:B:961:LEU:O	2.48	0.46
8:F:97:ARG:HE	8:F:124:GLU:CD	2.24	0.46
4:A:619:LYS:O	4:A:623:GLY:N	2.49	0.46
5:B:322:PHE:CE1	10:I:13:MET:HG2	2.50	0.46
5:B:414:ALA:O	5:B:418:LYS:HG3	2.16	0.46
5:B:547:VAL:N	5:B:612:GLU:OE1	2.43	0.46
7:E:97:VAL:HG13	7:E:127:ILE:HD11	1.97	0.46
9:H:125:LEU:CG	9:H:130:ARG:HH12	2.29	0.46
2:T:9:DC:H2''	2:T:10:DT:H2'	1.98	0.46
4:A:1352:VAL:HG12	4:A:1368:MET:HE2	1.97	0.46
11:J:28:ASP:HB2	11:J:30:LEU:HG	1.96	0.46
4:A:231:PRO:HA	4:A:234:MET:HE2	1.98	0.46
4:A:711:ARG:HG2	10:I:97:MET:HG3	1.97	0.46
5:B:115:GLN:HA	5:B:118:ARG:HD2	1.98	0.46
6:C:29:MET:HE3	6:C:29:MET:HB2	1.83	0.46
6:C:52:GLU:HA	13:L:64:LEU:HD22	1.98	0.46
6:C:92:CYS:HB3	6:C:95:CYS:HB3	1.96	0.46
10:I:7:CYS:HB2	10:I:34:TYR:HD2	1.81	0.46
4:A:30:ILE:HD12	5:B:1170:THR:HG21	1.97	0.46
4:A:105:CYS:HB2	4:A:142:CYS:HB3	1.98	0.46
4:A:180:LYS:HD3	4:A:181:LEU:N	2.31	0.46
4:A:998:LEU:HB2	4:A:1001:ARG:NH2	2.28	0.46
5:B:345:LYS:HD2	5:B:348:ARG:NH1	2.31	0.46
5:B:405:ARG:HH21	5:B:629:ASP:HB3	1.81	0.46
5:B:848:ARG:NH1	11:J:8:PHE:O	2.48	0.46
6:C:46:ILE:HA	6:C:159:ALA:HA	1.97	0.46
9:H:125:LEU:HG	9:H:130:ARG:NH2	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:997:LEU:HD23	4:A:1053:PHE:CD2	2.50	0.46
4:A:1376:THR:O	7:E:212:ARG:NH2	2.48	0.46
5:B:287:ARG:NH2	5:B:294:ASP:OD1	2.48	0.46
5:B:757:PRO:HG3	5:B:983:ARG:CZ	2.46	0.46
5:B:1166:CYS:HB3	5:B:1185:CYS:SG	2.55	0.46
4:A:42:ASP:HB2	4:A:49:LYS:N	2.31	0.46
4:A:532:ARG:HH12	4:A:745:GLN:HB3	1.80	0.46
4:A:707:GLY:HA3	4:A:1281:ARG:HD2	1.98	0.46
4:A:923:LEU:O	4:A:927:VAL:HG13	2.16	0.46
5:B:68:THR:HA	5:B:90:ILE:O	2.15	0.46
5:B:764:SER:OG	5:B:765:PRO:HD3	2.16	0.46
6:C:145:CYS:SG	6:C:146:LYS:N	2.89	0.46
4:A:662:PHE:HB3	5:B:829:CYS:SG	2.56	0.46
4:A:1410:PHE:HE1	5:B:1210:MET:HG2	1.80	0.46
5:B:102:VAL:HG23	5:B:110:HIS:CE1	2.51	0.46
5:B:681:TRP:CH2	5:B:690:VAL:HG11	2.51	0.46
6:C:62:PHE:CE1	6:C:66:ARG:HD2	2.50	0.46
5:B:431:TYR:HA	5:B:434:ARG:HD3	1.97	0.45
8:F:97:ARG:O	8:F:100:GLN:HG2	2.16	0.45
11:J:32:GLU:O	11:J:36:LEU:HG	2.16	0.45
4:A:942:PHE:O	4:A:946:VAL:HG23	2.16	0.45
4:A:1128:GLN:HG3	4:A:1304:TRP:NE1	2.29	0.45
4:A:1342:GLU:OE1	7:E:200:ARG:HD3	2.16	0.45
5:B:827:ILE:HG12	5:B:1012:ILE:HD11	1.98	0.45
7:E:93:MET:HG2	7:E:120:ALA:HA	1.97	0.45
5:B:273:LEU:HG	5:B:280:ILE:HD11	1.97	0.45
5:B:579:ARG:NH1	5:B:623:GLU:HG3	2.32	0.45
7:E:99:HIS:HA	7:E:102:GLU:HG3	1.98	0.45
13:L:28:LYS:HG3	13:L:40:LEU:HD23	1.99	0.45
2:T:22:DT:H2'	2:T:23:DC:H6	1.82	0.45
4:A:1267:MET:HA	4:A:1271:ILE:HG12	1.98	0.45
5:B:412:LEU:HB3	5:B:466:TRP:NE1	2.32	0.45
7:E:83:CYS:HB3	7:E:110:PHE:CE1	2.51	0.45
4:A:22:PHE:CE2	5:B:1208:MET:HA	2.48	0.45
4:A:90:VAL:HB	4:A:297:GLN:NE2	2.32	0.45
4:A:105:CYS:SG	4:A:114:LEU:N	2.90	0.45
4:A:526:ASP:HB3	4:A:657:LEU:HD23	1.99	0.45
5:B:122:LEU:HD21	5:B:958:GLN:HB2	1.99	0.45
5:B:193:LYS:HB3	5:B:787:VAL:HG11	1.99	0.45
5:B:454:THR:HG22	5:B:458:LYS:HD3	1.99	0.45
6:C:75:MET:O	6:C:246:ARG:NH2	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:E:41:ASP:O	7:E:45:LYS:HG2	2.17	0.45
8:F:109:VAL:HG21	8:F:123:LYS:HG3	1.98	0.45
10:I:26:LEU:HD23	10:I:37:GLU:HA	1.98	0.45
4:A:224:PHE:CD2	4:A:231:PRO:HD3	2.51	0.45
4:A:446:ARG:HH21	4:A:480:ALA:HA	1.81	0.45
4:A:531:ILE:HD12	4:A:653:VAL:HG21	1.98	0.45
4:A:665:GLY:HA3	5:B:1069:PHE:CE1	2.52	0.45
4:A:874:ASP:HB2	4:A:1058:VAL:HA	1.98	0.45
4:A:1095:THR:H	4:A:1113:THR:CG2	2.30	0.45
5:B:280:ILE:HG13	5:B:285:ILE:HD11	1.99	0.45
5:B:839:MET:SD	5:B:980:PHE:HB2	2.57	0.45
5:B:1159:ARG:HD3	5:B:1161:HIS:CE1	2.52	0.45
6:C:101:LEU:HB2	6:C:118:LEU:HG	1.99	0.45
5:B:549:THR:HB	5:B:628:THR:HB	1.98	0.45
5:B:900:ALA:HA	13:L:58:LYS:HD3	1.99	0.45
5:B:992:ILE:HD11	12:K:66:PRO:HB2	1.99	0.45
6:C:66:ARG:O	6:C:70:ILE:HG13	2.16	0.45
4:A:326:ARG:HG3	4:A:1406:VAL:HG21	1.99	0.45
4:A:924:LYS:O	4:A:927:VAL:HG22	2.17	0.45
4:A:939:ASP:O	4:A:943:LEU:HG	2.17	0.45
5:B:360:PHE:CE2	5:B:374:LYS:HB3	2.52	0.45
5:B:637:LEU:HD23	5:B:742:GLU:HA	1.99	0.45
11:J:2:ILE:HG13	11:J:3:VAL:N	2.31	0.45
12:K:14:GLU:HG2	12:K:14:GLU:O	2.17	0.45
4:A:86:LEU:HD23	4:A:86:LEU:H	1.81	0.45
4:A:111:GLY:HA3	4:A:213:HIS:C	2.42	0.45
4:A:849:MET:HE3	4:A:1063:MET:SD	2.57	0.45
4:A:1166:ASP:HA	4:A:1169:ILE:HD12	1.98	0.45
4:A:1413:GLY:HA3	5:B:1212:ILE:HD12	1.99	0.45
5:B:472:ALA:O	5:B:475:SER:OG	2.28	0.45
5:B:834:ASN:O	5:B:1013:ASN:HB2	2.16	0.45
5:B:1067:ARG:HG3	6:C:192:TRP:CZ3	2.52	0.45
5:B:1142:GLY:HA3	8:F:88:TYR:HE1	1.81	0.45
12:K:20:LYS:HD3	12:K:21:ILE:N	2.32	0.45
12:K:91:CYS:O	12:K:95:ILE:HG13	2.17	0.45
2:T:17:DG:H1'	4:A:1386:ARG:HH21	1.82	0.45
4:A:23:SER:HB2	4:A:233:TRP:CZ2	2.52	0.45
5:B:851:PHE:CG	5:B:980:PHE:HE2	2.35	0.45
7:E:144:ILE:HD11	7:E:187:TYR:HB2	1.99	0.45
9:H:89:LEU:HD13	9:H:91:ASP:O	2.17	0.45
9:H:100:THR:HG23	9:H:138:GLU:HA	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:I:52:ILE:H	10:I:52:ILE:HG13	1.61	0.45
13:L:38:LEU:HD13	13:L:56:LEU:HD21	1.98	0.45
4:A:440:ASP:O	4:A:460:VAL:HG23	2.17	0.44
4:A:446:ARG:HG2	4:A:478:TYR:O	2.17	0.44
4:A:533:LYS:HB3	4:A:533:LYS:HE3	1.77	0.44
4:A:1148:ILE:N	4:A:1196:GLU:O	2.50	0.44
5:B:858:SER:HA	5:B:966:VAL:O	2.17	0.44
4:A:767:GLN:HA	4:A:799:PHE:HA	1.99	0.44
4:A:1436:ILE:HD12	5:B:1139:ILE:HG23	1.99	0.44
5:B:234:ILE:HG21	5:B:257:LYS:HB3	1.99	0.44
5:B:824:ILE:O	5:B:1009:ASP:N	2.50	0.44
6:C:10:ILE:HD12	12:K:108:GLU:HB3	1.99	0.44
9:H:17:PRO:HA	9:H:24:CYS:SG	2.57	0.44
4:A:442:VAL:HG21	4:A:489:LEU:HD11	2.00	0.44
4:A:519:PRO:O	4:A:624:SER:HB2	2.17	0.44
4:A:675:THR:HG21	4:A:736:ASN:HB2	1.98	0.44
4:A:1095:THR:HG23	4:A:1113:THR:HG22	1.99	0.44
4:A:1147:THR:HB	10:I:48:LEU:HD12	1.98	0.44
5:B:58:THR:O	5:B:62:ILE:HG12	2.17	0.44
7:E:152:LYS:HD2	7:E:152:LYS:HA	1.89	0.44
10:I:10:CYS:SG	10:I:31:THR:HB	2.58	0.44
11:J:34:THR:O	11:J:38:ARG:HG2	2.17	0.44
4:A:668:ASP:OD2	4:A:742:ASN:N	2.36	0.44
4:A:722:LEU:HD13	4:A:799:PHE:HB2	2.00	0.44
4:A:785:PRO:HG2	5:B:703:ILE:HD11	1.98	0.44
5:B:693:ILE:HG23	5:B:697:GLU:HG2	1.99	0.44
5:B:760:ASP:OD1	5:B:760:ASP:N	2.49	0.44
5:B:822:ASN:O	11:J:48:ARG:NH1	2.50	0.44
6:C:106:GLU:OE1	6:C:106:GLU:N	2.48	0.44
7:E:177:ARG:O	7:E:212:ARG:NH1	2.51	0.44
10:I:78:CYS:HB3	10:I:106:CYS:CB	2.47	0.44
11:J:3:VAL:HG11	11:J:18:TRP:HB2	2.00	0.44
4:A:1197:LEU:HB2	4:A:1209:MET:HE1	2.00	0.44
6:C:84:ARG:HD2	12:K:11:LEU:HD21	1.99	0.44
13:L:34:CYS:HB3	13:L:51:CYS:N	2.33	0.44
4:A:22:PHE:CG	5:B:1213:THR:HG22	2.52	0.44
4:A:442:VAL:O	4:A:457:ALA:HA	2.18	0.44
4:A:667:GLY:HA3	5:B:1067:ARG:HD2	2.00	0.44
4:A:1008:GLN:HB3	4:A:1012:ARG:CZ	2.47	0.44
7:E:46:TYR:HE1	7:E:58:MET:CG	2.31	0.44
1:R:4:G:H2'	1:R:5:A:C8	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:108:MET:HG2	4:A:171:GLN:OE1	2.18	0.44
4:A:463:ILE:HD13	4:A:469:ARG:HG2	2.00	0.44
4:A:1387:HIS:HA	4:A:1391:ARG:HG3	1.99	0.44
1:R:7:A:O3'	5:B:776:GLN:NE2	2.51	0.44
4:A:492:PRO:HB3	4:A:497:THR:HG22	1.98	0.44
4:A:757:ASN:O	4:A:761:MET:HG3	2.17	0.44
4:A:1430:LEU:HB3	4:A:1432:GLN:HG3	1.99	0.44
5:B:121:ASN:ND2	5:B:860:MET:HE2	2.33	0.44
5:B:211:VAL:HG11	5:B:483:LEU:HD12	1.99	0.44
5:B:234:ILE:HG22	5:B:259:TYR:HA	1.98	0.44
7:E:12:LEU:HD22	7:E:137:GLU:OE2	2.18	0.44
7:E:93:MET:HE3	7:E:120:ALA:HB1	2.00	0.44
11:J:45:CYS:HA	11:J:48:ARG:HE	1.82	0.44
2:T:18:DA:H5''	4:A:337:ARG:HH12	1.82	0.44
4:A:527:THR:HG23	4:A:653:VAL:HB	1.99	0.44
4:A:684:ALA:O	4:A:688:LYS:HD3	2.18	0.44
4:A:850:VAL:HG12	4:A:1060:PRO:HA	2.00	0.44
5:B:579:ARG:H	5:B:579:ARG:HG3	1.64	0.44
6:C:66:ARG:NH1	11:J:3:VAL:O	2.49	0.44
10:I:75:CYS:HB3	10:I:110:PHE:CD1	2.53	0.44
11:J:49:MET:O	11:J:53:HIS:HB2	2.18	0.44
4:A:1148:ILE:HD11	4:A:1198:ASP:HA	2.00	0.43
5:B:59:LEU:HD12	5:B:59:LEU:HA	1.86	0.43
5:B:115:GLN:NE2	5:B:193:LYS:O	2.51	0.43
5:B:405:ARG:HD2	5:B:405:ARG:HA	1.89	0.43
5:B:554:ILE:O	5:B:558:LEU:HG	2.18	0.43
5:B:830:TYR:CE2	5:B:1000:PRO:HD3	2.53	0.43
6:C:254:LYS:O	6:C:258:ILE:HG12	2.18	0.43
7:E:99:HIS:O	7:E:102:GLU:HG3	2.18	0.43
7:E:113:GLN:OE1	7:E:113:GLN:N	2.44	0.43
11:J:41:LEU:HB3	11:J:46:CYS:HB2	2.00	0.43
2:T:22:DT:P	4:A:344:ARG:HH22	2.41	0.43
3:N:8:DG:H2''	3:N:9:DA:C8	2.52	0.43
4:A:175:ARG:HA	4:A:175:ARG:HD3	1.87	0.43
4:A:452:LYS:HD2	5:B:1140:ALA:HB1	1.99	0.43
6:C:248:ILE:O	6:C:252:GLN:HG3	2.17	0.43
7:E:68:SER:HB3	7:E:75:MET:SD	2.59	0.43
4:A:153:PRO:HA	4:A:162:VAL:HG13	2.00	0.43
4:A:471:ASN:O	4:A:474:VAL:HG12	2.18	0.43
4:A:635:ARG:NE	4:A:877:HIS:HA	2.33	0.43
4:A:746:MET:HG2	5:B:1015:HIS:CE1	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:897:TYR:CZ	4:A:1030:ARG:HD2	2.54	0.43
4:A:1282:VAL:HG11	4:A:1306:LEU:HD13	2.00	0.43
5:B:262:GLU:HA	5:B:267:ARG:CZ	2.49	0.43
6:C:66:ARG:NH2	6:C:143:LEU:O	2.47	0.43
6:C:94:LYS:HA	6:C:127:ARG:HH12	1.81	0.43
9:H:35:GLN:H	9:H:35:GLN:HG3	1.61	0.43
12:K:57:LEU:N	12:K:76:GLN:O	2.51	0.43
3:N:8:DG:H5''	4:A:175:ARG:HH22	1.82	0.43
4:A:576:GLN:O	4:A:580:VAL:HG23	2.18	0.43
5:B:286:PHE:CE1	5:B:375:ALA:HB1	2.54	0.43
5:B:351:TYR:CZ	5:B:355:ILE:HD11	2.53	0.43
5:B:900:ALA:HB3	13:L:61:THR:HG22	2.00	0.43
6:C:20:PHE:CE1	6:C:230:MET:HB2	2.53	0.43
4:A:114:LEU:HD11	4:A:171:GLN:HG2	2.00	0.43
4:A:205:GLU:O	4:A:208:LEU:HG	2.18	0.43
4:A:760:GLN:HG2	4:A:765:VAL:HA	2.01	0.43
4:A:1030:ARG:O	4:A:1034:GLU:HG2	2.17	0.43
5:B:520:GLY:HA3	5:B:635:ARG:NH1	2.34	0.43
5:B:901:PRO:HG3	5:B:952:VAL:HG23	2.01	0.43
4:A:361:LEU:HB2	4:A:471:ASN:HD22	1.82	0.43
4:A:396:PRO:HG3	4:A:416:ARG:HG2	2.01	0.43
5:B:175:ARG:HG2	5:B:200:GLY:HA3	2.00	0.43
5:B:458:LYS:HB3	5:B:458:LYS:HE3	1.87	0.43
5:B:1099:VAL:O	5:B:1103:ILE:HG13	2.19	0.43
7:E:155:ARG:NE	7:E:194:GLU:OE2	2.52	0.43
1:R:9:G:O2'	4:A:485:ASP:OD1	2.26	0.43
4:A:69:THR:O	5:B:1174:LYS:HG2	2.18	0.43
4:A:115:LEU:HD23	4:A:142:CYS:HA	2.00	0.43
4:A:122:MET:O	4:A:126:LEU:HG	2.18	0.43
4:A:518:LYS:NZ	4:A:519:PRO:O	2.49	0.43
7:E:114:ASN:OD1	7:E:115:ASN:N	2.50	0.43
4:A:94:GLY:HA3	4:A:1410:PHE:CD2	2.54	0.43
4:A:1308:THR:OG1	4:A:1310:GLY:O	2.32	0.43
5:B:954:VAL:HG22	5:B:964:VAL:HG12	2.00	0.43
7:E:23:VAL:HG12	7:E:28:TYR:HB2	2.00	0.43
7:E:156:LEU:HD23	7:E:156:LEU:HA	1.91	0.43
9:H:125:LEU:CB	9:H:130:ARG:HH12	2.32	0.43
4:A:92:HIS:HD2	4:A:304:MET:HE3	1.83	0.43
4:A:242:PRO:HG3	5:B:1209:ALA:HB2	1.99	0.43
4:A:286:HIS:HA	4:A:289:ILE:HD12	2.00	0.43
4:A:566:ILE:HB	9:H:96:VAL:HG12	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:679:ILE:HG12	4:A:729:ALA:HB1	2.00	0.43
4:A:946:VAL:HA	7:E:201:LYS:HE3	2.01	0.43
5:B:333:PHE:O	5:B:334:ILE:HG13	2.19	0.43
5:B:757:PRO:HG2	5:B:984:HIS:CE1	2.53	0.43
6:C:36:VAL:HG23	12:K:41:THR:HG21	2.00	0.43
4:A:224:PHE:HD2	4:A:231:PRO:HD3	1.84	0.43
4:A:345:VAL:HG23	4:A:348:SER:HB3	2.00	0.43
4:A:845:LEU:HD12	4:A:1069:ALA:HB2	2.01	0.43
4:A:1013:ASP:O	7:E:205:SER:HB2	2.19	0.43
4:A:1194:ARG:HG3	4:A:1237:ILE:HG23	2.01	0.43
4:A:1438:THR:OG1	5:B:1142:GLY:O	2.24	0.43
5:B:809:MET:HA	5:B:812:LEU:HB2	2.00	0.43
5:B:899:ILE:O	5:B:952:VAL:HG21	2.19	0.43
6:C:10:ILE:HA	6:C:20:PHE:HA	2.01	0.43
6:C:186:LEU:HB3	6:C:188:HIS:ND1	2.34	0.43
13:L:38:LEU:HD22	13:L:56:LEU:HD11	2.01	0.43
4:A:57:ARG:CB	4:A:68:GLN:HB2	2.49	0.42
4:A:151:ASP:HA	4:A:164:ARG:O	2.18	0.42
4:A:527:THR:O	4:A:531:ILE:N	2.45	0.42
4:A:787:PHE:CE2	4:A:796:SER:HA	2.54	0.42
4:A:1202:MET:HE3	4:A:1202:MET:HB3	1.87	0.42
5:B:611:PRO:HB3	5:B:685:LEU:HD11	2.01	0.42
6:C:163:ILE:HD12	6:C:165:LYS:HB3	2.01	0.42
11:J:1:MET:HE2	11:J:60:PHE:HE2	1.84	0.42
1:R:3:C:H2'	1:R:4:G:C8	2.54	0.42
4:A:620:LYS:HB2	4:A:620:LYS:HE2	1.72	0.42
4:A:789:LYS:HG3	10:I:67:THR:HB	2.00	0.42
4:A:820:GLY:O	4:A:824:LEU:HG	2.18	0.42
4:A:983:ILE:HG23	4:A:1028:THR:HG21	2.02	0.42
5:B:186:GLU:HA	5:B:189:LEU:HD12	2.01	0.42
5:B:216:GLU:OE1	5:B:537:LYS:NZ	2.35	0.42
5:B:582:VAL:HG22	5:B:626:ILE:HD13	2.01	0.42
5:B:701:ILE:HD12	5:B:740:HIS:ND1	2.33	0.42
5:B:726:ALA:HB3	5:B:1051:THR:HG22	2.01	0.42
5:B:1170:THR:OG1	5:B:1182:CYS:SG	2.77	0.42
7:E:65:THR:OG1	7:E:67:GLU:HG2	2.19	0.42
12:K:49:GLU:HG3	12:K:94:ILE:CG1	2.48	0.42
4:A:537:ARG:HG2	4:A:575:LYS:NZ	2.34	0.42
4:A:658:LEU:HD12	5:B:831:SER:N	2.34	0.42
4:A:951:GLU:OE2	4:A:953:ASN:ND2	2.52	0.42
4:A:1111:MET:HE3	4:A:1111:MET:HB2	1.96	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:367:LEU:HD12	5:B:368:GLU:O	2.19	0.42
5:B:555:ILE:HD12	5:B:587:HIS:CE1	2.54	0.42
4:A:129:LYS:H	4:A:129:LYS:HG2	1.70	0.42
5:B:168:GLY:HA2	5:B:450:ALA:HB1	2.01	0.42
5:B:302:CYS:HB2	5:B:310:MET:HG2	2.01	0.42
5:B:605:ARG:HG3	5:B:605:ARG:HH11	1.85	0.42
8:F:81:THR:OG1	8:F:146:TRP:NE1	2.52	0.42
2:T:22:DT:H2'	2:T:23:DC:C6	2.54	0.42
4:A:463:ILE:HD13	4:A:469:ARG:CG	2.50	0.42
5:B:170:LEU:HD12	5:B:171:PRO:HD2	2.02	0.42
5:B:354:ASP:HA	5:B:357:GLN:HE21	1.85	0.42
7:E:61:GLN:HB2	7:E:79:TRP:CE3	2.53	0.42
9:H:99:GLY:HA3	9:H:118:PHE:HA	2.01	0.42
4:A:247:ARG:H	4:A:247:ARG:HG2	1.66	0.42
5:B:709:ASP:OD2	5:B:733:HIS:NE2	2.53	0.42
5:B:721:LEU:HB3	5:B:722:ASP:H	1.55	0.42
5:B:1016:ALA:O	5:B:1020:ARG:HG2	2.19	0.42
10:I:4:PHE:CZ	10:I:13:MET:HE3	2.55	0.42
4:A:265:LYS:HA	4:A:265:LYS:HD3	1.77	0.42
4:A:452:LYS:O	5:B:1141:HIS:NE2	2.53	0.42
4:A:455:MET:O	5:B:1141:HIS:NE2	2.49	0.42
4:A:1290:LYS:HA	4:A:1300:LYS:HA	2.01	0.42
5:B:331:LEU:HA	5:B:334:ILE:HD12	2.01	0.42
5:B:495:LEU:HD23	5:B:495:LEU:HA	1.66	0.42
5:B:1152:MET:O	5:B:1157:ALA:HB2	2.20	0.42
6:C:97:VAL:HG21	6:C:129:ILE:HG22	2.01	0.42
4:A:134:ARG:HH21	4:A:221:SER:HA	1.84	0.42
4:A:672:ASP:H	4:A:736:ASN:ND2	2.12	0.42
5:B:62:ILE:HG23	5:B:418:LYS:HG2	2.02	0.42
5:B:246:LYS:HE3	5:B:246:LYS:HB2	1.84	0.42
5:B:763:GLN:HG3	5:B:765:PRO:HD2	2.00	0.42
5:B:1033:LYS:O	5:B:1037:LEU:HG	2.19	0.42
6:C:205:LYS:O	6:C:208:GLU:HG2	2.19	0.42
4:A:182:VAL:HG12	4:A:201:VAL:HA	2.01	0.42
4:A:426:LEU:HD23	4:A:426:LEU:HA	1.88	0.42
4:A:1094:VAL:HA	4:A:1113:THR:HG21	2.01	0.42
4:A:1121:GLU:OE1	4:A:1130:GLN:NE2	2.53	0.42
5:B:115:GLN:O	5:B:119:LEU:HG	2.20	0.42
5:B:122:LEU:HD23	5:B:122:LEU:HA	1.82	0.42
5:B:293:PRO:HB2	5:B:296:GLU:HB2	2.01	0.42
5:B:310:MET:HE2	5:B:310:MET:HB2	1.89	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:486:TYR:CE2	5:B:1096:ARG:HB3	2.54	0.42
6:C:110:THR:HG22	6:C:146:LYS:HG2	2.00	0.42
9:H:13:SER:N	9:H:27:GLU:O	2.52	0.42
10:I:74:GLU:HB3	10:I:81:ARG:HD2	2.02	0.42
4:A:12:ARG:HB2	5:B:1218:THR:HB	2.02	0.42
4:A:50:ILE:HG23	4:A:52:GLY:N	2.34	0.42
5:B:232:SER:O	5:B:261:ARG:NH1	2.53	0.42
5:B:361:LEU:HD21	5:B:364:ILE:HD12	2.01	0.42
5:B:1067:ARG:HA	5:B:1067:ARG:HD3	1.88	0.42
6:C:147:LEU:HA	6:C:147:LEU:HD23	1.80	0.42
13:L:63:ARG:H	13:L:63:ARG:HG3	1.69	0.42
3:N:2:DC:H1'	3:N:3:DA:C8	2.54	0.41
4:A:98:LYS:HE2	4:A:224:PHE:CZ	2.55	0.41
4:A:110:CYS:HB2	4:A:167:CYS:HB2	2.01	0.41
4:A:436:ILE:HD11	4:A:491:VAL:HG11	2.02	0.41
4:A:663:SER:O	4:A:742:ASN:ND2	2.53	0.41
4:A:698:GLN:HA	10:I:97:MET:O	2.20	0.41
4:A:784:LEU:HD23	4:A:784:LEU:HA	1.89	0.41
4:A:1105:LEU:HB3	4:A:1384:VAL:CG2	2.50	0.41
5:B:294:ASP:HA	5:B:297:ILE:HD12	2.01	0.41
5:B:308:TRP:H	5:B:308:TRP:CD1	2.38	0.41
5:B:400:HIS:O	5:B:404:LYS:HG2	2.20	0.41
5:B:975:GLN:O	5:B:990:ILE:HD12	2.20	0.41
5:B:1020:ARG:HH12	16:B:1302:POP:P1	2.43	0.41
6:C:239:PRO:O	6:C:243:VAL:HG23	2.20	0.41
3:N:7:DA:C6	3:N:8:DG:C6	3.08	0.41
4:A:786:HIS:HE1	5:B:519:TRP:CE2	2.39	0.41
9:H:38:LEU:HD13	9:H:125:LEU:HB2	2.01	0.41
4:A:42:ASP:HB3	4:A:46:THR:C	2.45	0.41
4:A:450:LEU:HD22	4:A:1077:THR:HG21	2.02	0.41
4:A:756:ILE:O	4:A:760:GLN:HG3	2.20	0.41
4:A:956:LEU:HD22	4:A:1021:LEU:HD22	2.01	0.41
4:A:981:LEU:HG	4:A:1039:LYS:HA	2.01	0.41
5:B:261:ARG:HB2	5:B:264:SER:HB3	2.02	0.41
5:B:1072:MET:HE3	5:B:1072:MET:HB3	1.95	0.41
3:N:6:DG:C5	3:N:7:DA:C5	3.09	0.41
4:A:592:ASP:O	4:A:595:THR:OG1	2.35	0.41
4:A:658:LEU:HD12	5:B:831:SER:H	1.86	0.41
4:A:676:MET:O	4:A:680:THR:HG23	2.20	0.41
4:A:814:PHE:CD2	4:A:818:MET:HE2	2.55	0.41
4:A:1079:MET:HG2	4:A:1359:ASP:CG	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1420:ASP:OD2	4:A:1422:ARG:NH2	2.54	0.41
5:B:651:LEU:HD13	5:B:653:VAL:HG23	2.02	0.41
5:B:757:PRO:HG2	5:B:984:HIS:NE2	2.36	0.41
5:B:1023:VAL:O	5:B:1027:ILE:HG13	2.20	0.41
6:C:192:TRP:CZ3	6:C:194:GLU:HG2	2.55	0.41
2:T:22:DT:OP1	4:A:344:ARG:NH1	2.37	0.41
4:A:1120:LEU:HD23	4:A:1124:HIS:HB3	2.03	0.41
5:B:581:PHE:CE2	5:B:586:TRP:HB2	2.56	0.41
5:B:640:VAL:HG13	5:B:710:LEU:HD11	2.02	0.41
6:C:37:MET:HA	6:C:41:ILE:HD11	2.02	0.41
6:C:82:TYR:CD1	6:C:161:LYS:HB3	2.56	0.41
4:A:71:GLN:HE22	5:B:1176:ASN:HD22	1.67	0.41
4:A:528:LEU:HD23	4:A:751:SER:HA	2.03	0.41
4:A:695:LYS:HE3	4:A:695:LYS:HB3	1.98	0.41
4:A:956:LEU:HD13	4:A:1021:LEU:HD22	2.03	0.41
4:A:1436:ILE:O	4:A:1440:ALA:N	2.53	0.41
4:A:1441:PHE:CZ	8:F:89:GLU:HA	2.55	0.41
5:B:308:TRP:HE3	5:B:312:GLU:HG3	1.85	0.41
5:B:996:ARG:NH1	6:C:174:ALA:O	2.53	0.41
5:B:1004:GLU:HB2	5:B:1006:ILE:HG13	2.02	0.41
5:B:1172:ILE:H	5:B:1172:ILE:HG13	1.68	0.41
13:L:47:ARG:HD3	13:L:54:ARG:NE	2.34	0.41
4:A:132:LYS:HA	4:A:132:LYS:HD3	1.60	0.41
4:A:366:VAL:HG22	4:A:468:PHE:HE1	1.86	0.41
4:A:662:PHE:O	5:B:828:ALA:HA	2.21	0.41
4:A:775:ILE:HG21	4:A:815:PHE:CD1	2.56	0.41
4:A:782:ARG:NH1	5:B:701:ILE:O	2.51	0.41
4:A:1191:TRP:CD1	4:A:1191:TRP:H	2.39	0.41
4:A:1336:MET:HE2	4:A:1336:MET:HB3	1.94	0.41
5:B:567:GLU:H	5:B:567:GLU:CD	2.28	0.41
6:C:17:ASN:HA	6:C:232:VAL:O	2.21	0.41
13:L:29:TYR:O	13:L:38:LEU:CB	2.64	0.41
13:L:39:SER:OG	13:L:40:LEU:HD12	2.20	0.41
4:A:53:LEU:HD21	4:A:266:LEU:HD13	2.01	0.41
4:A:532:ARG:HD3	4:A:749:ALA:HB2	2.03	0.41
5:B:953:LEU:HA	13:L:56:LEU:O	2.21	0.41
6:C:77:ILE:HD12	6:C:77:ILE:HA	1.92	0.41
10:I:68:LEU:O	10:I:70:ARG:NH1	2.53	0.41
10:I:97:MET:HE3	10:I:97:MET:HB3	1.89	0.41
1:R:3:C:H2'	1:R:4:G:H8	1.86	0.41
4:A:316:GLN:N	4:A:320:ARG:O	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:399:HIS:CE1	4:A:462:VAL:HG21	2.56	0.41
4:A:711:ARG:NH2	10:I:87:GLN:OE1	2.54	0.41
4:A:956:LEU:HD13	4:A:1021:LEU:HD13	2.01	0.41
4:A:1029:ARG:O	4:A:1033:GLN:HB2	2.21	0.41
5:B:625:LYS:HB2	5:B:625:LYS:HE2	1.85	0.41
6:C:11:ARG:N	6:C:19:ASP:O	2.54	0.41
6:C:143:LEU:HD21	11:J:2:ILE:HD11	2.02	0.41
7:E:147:HIS:CE1	7:E:149:LEU:HG	2.56	0.41
7:E:178:ILE:HB	7:E:212:ARG:HH11	1.86	0.41
9:H:94:ASP:HB3	9:H:146:ARG:NH1	2.36	0.41
9:H:142:LEU:HD22	9:H:144:ILE:HD11	2.03	0.41
12:K:20:LYS:HD3	12:K:20:LYS:C	2.46	0.41
4:A:643:ALA:HA	4:A:646:PHE:HD2	1.86	0.41
4:A:1138:ILE:CG2	4:A:1282:VAL:HG21	2.51	0.41
4:A:1262:LYS:HB3	4:A:1262:LYS:HE3	1.80	0.41
4:A:1398:MET:O	4:A:1401:SER:OG	2.39	0.41
7:E:94:LYS:O	7:E:98:ILE:HG12	2.21	0.41
4:A:53:LEU:HA	4:A:53:LEU:HD23	1.77	0.40
5:B:127:GLY:HA2	5:B:166:PHE:HE1	1.85	0.40
5:B:566:LEU:HD21	5:B:586:TRP:CE2	2.56	0.40
5:B:591:ARG:H	5:B:591:ARG:HG2	1.74	0.40
5:B:1098:MET:HE3	5:B:1098:MET:HB2	1.93	0.40
6:C:262:LEU:HD23	6:C:262:LEU:HA	1.80	0.40
7:E:19:VAL:O	7:E:23:VAL:HG23	2.21	0.40
9:H:93:TYR:CG	9:H:143:LEU:HB3	2.57	0.40
4:A:1111:MET:HB3	4:A:1114:PRO:HG3	2.03	0.40
5:B:546:SER:HA	5:B:612:GLU:OE1	2.21	0.40
5:B:749:LEU:HD22	5:B:753:ALA:HB1	2.03	0.40
5:B:1002:THR:HG23	5:B:1004:GLU:H	1.86	0.40
6:C:246:ARG:O	6:C:250:THR:OG1	2.25	0.40
2:T:8:DT:C2	3:N:12:DG:N2	2.89	0.40
4:A:851:HIS:ND1	8:F:139:PRO:HG3	2.37	0.40
4:A:916:GLY:O	4:A:919:ILE:HG22	2.21	0.40
4:A:1205:LYS:HA	4:A:1205:LYS:HD3	1.72	0.40
5:B:556:THR:O	5:B:560:GLU:HG3	2.21	0.40
5:B:705:MET:HE2	5:B:705:MET:HB2	1.85	0.40
5:B:994:TYR:HD1	5:B:994:TYR:HA	1.76	0.40
6:C:239:PRO:O	6:C:243:VAL:N	2.51	0.40
7:E:48:ASP:OD1	7:E:52:ARG:N	2.54	0.40
7:E:90:VAL:O	7:E:94:LYS:HG3	2.20	0.40
9:H:102:TYR:CE2	9:H:115:TYR:HB3	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:367:PRO:HD2	4:A:370:ILE:HD12	2.04	0.40
5:B:400:HIS:HB3	5:B:403:LYS:HG3	2.03	0.40
5:B:579:ARG:NH1	5:B:621:GLU:O	2.49	0.40
5:B:883:LEU:HD13	5:B:932:HIS:ND1	2.37	0.40
6:C:129:ILE:HD13	6:C:129:ILE:HA	1.84	0.40
10:I:6:PHE:HD1	10:I:13:MET:HA	1.87	0.40
4:A:38:PRO:HB3	4:A:270:LEU:HB3	2.03	0.40
4:A:88:LYS:NZ	4:A:205:GLU:H	2.18	0.40
4:A:588:LEU:O	4:A:606:LEU:HA	2.21	0.40
4:A:786:HIS:CD2	5:B:703:ILE:HG13	2.57	0.40
5:B:528:PRO:HG2	5:B:536:VAL:HB	2.04	0.40
7:E:99:HIS:NE2	7:E:103:LYS:HE2	2.37	0.40
7:E:118:PRO:HA	7:E:121:MET:HG2	2.03	0.40
9:H:77:ARG:NH1	9:H:77:ARG:HB3	2.37	0.40
12:K:49:GLU:HG3	12:K:94:ILE:HG13	2.04	0.40
13:L:34:CYS:N	13:L:51:CYS:HB3	2.36	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:L:39:SER:OG	13:L:42:ARG:O[2_555]	2.16	0.04

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 X-ray entries followed by that with respect to entries of similar resolution.

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	1370/1733 (79%)	1328 (97%)	42 (3%)	0	100	100
5	B	1108/1224 (90%)	1097 (99%)	11 (1%)	0	100	100
6	C	265/318 (83%)	263 (99%)	2 (1%)	0	100	100
7	E	210/215 (98%)	205 (98%)	5 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	F	84/155 (54%)	82 (98%)	2 (2%)	0	100	100
9	H	129/146 (88%)	126 (98%)	3 (2%)	0	100	100
10	I	116/122 (95%)	115 (99%)	1 (1%)	0	100	100
11	J	63/70 (90%)	63 (100%)	0	0	100	100
12	K	112/120 (93%)	111 (99%)	1 (1%)	0	100	100
13	L	41/70 (59%)	35 (85%)	6 (15%)	0	100	100
All	All	3498/4173 (84%)	3425 (98%)	73 (2%)	0	100	100

There are no Ramachandran outliers to report.

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 X-ray entries followed by that with respect to entries of similar resolution.

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	1194/1520 (79%)	1191 (100%)	3 (0%)	86	83
5	B	956/1061 (90%)	955 (100%)	1 (0%)	88	87
6	C	235/274 (86%)	234 (100%)	1 (0%)	84	81
7	E	193/197 (98%)	193 (100%)	0	100	100
8	F	73/137 (53%)	73 (100%)	0	100	100
9	H	116/128 (91%)	116 (100%)	0	100	100
10	I	109/116 (94%)	107 (98%)	2 (2%)	51	68
11	J	60/65 (92%)	59 (98%)	1 (2%)	53	69
12	K	99/102 (97%)	99 (100%)	0	100	100
13	L	37/57 (65%)	36 (97%)	1 (3%)	39	61
All	All	3072/3657 (84%)	3063 (100%)	9 (0%)	86	83

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	A	70	CYS

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Mol	Chain	Res	Type
4	A	77	CYS
4	A	167	CYS
5	B	1163	CYS
6	C	92	CYS
10	I	7	CYS
10	I	103	CYS
11	J	7	CYS
13	L	31	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
4	A	18	GLN
4	A	71	GLN
4	A	286	HIS
4	A	297	GLN
4	A	399	HIS
4	A	517	ASN
4	A	767	GLN
4	A	838	GLN
4	A	854	ASN
4	A	858	ASN
4	A	935	GLN
4	A	953	ASN
4	A	1004	ASN
4	A	1078	GLN
4	A	1188	GLN
4	A	1354	ASN
5	B	110	HIS
5	B	178	ASN
5	B	206	ASN
5	B	357	GLN
5	B	587	HIS
5	B	706	GLN
5	B	734	HIS
5	B	776	GLN
5	B	932	HIS
5	B	1097	HIS
5	B	1161	HIS
6	C	91	HIS
6	C	214	ASN
6	C	252	GLN

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Mol	Chain	Res	Type
7	E	32	GLN
7	E	61	GLN
7	E	63	ASN
7	E	101	GLN
7	E	115	ASN
10	I	22	ASN
10	I	60	GLN
12	K	76	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	R	9/10 (90%)	2 (22%)	0

All (2) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	R	9	G
1	R	10	A

There are no RNA pucker outliers to report.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	WVQ	T	19	2	19,24,25	3.60	7 (36%)	18,33,36	1.74	4 (22%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	WVQ	T	19	2	-	4/6/40/41	0/2/2/2

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	T	19	WVQ	C5-N7	12.69	1.46	1.28
2	T	19	WVQ	C4-N9	4.40	1.45	1.35
2	T	19	WVQ	C2-N2	4.12	1.45	1.34
2	T	19	WVQ	C6-C5	-4.12	1.35	1.47
2	T	19	WVQ	C6-N1	-3.31	1.32	1.38
2	T	19	WVQ	O6-C6	-2.72	1.18	1.23
2	T	19	WVQ	C5-C4	-2.47	1.36	1.43

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	T	19	WVQ	N3-C2-N1	-4.46	119.38	126.44
2	T	19	WVQ	O4'-C1'-N9	-3.69	106.12	110.17
2	T	19	WVQ	N2-C2-N3	2.34	120.29	116.57
2	T	19	WVQ	N2-C2-N1	2.09	120.33	117.09

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	T	19	WVQ	N3-C4-N9-C1'
2	T	19	WVQ	C4'-C5'-O5'-P
2	T	19	WVQ	O4'-C1'-N9-C4
2	T	19	WVQ	O4'-C4'-C5'-O5'

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	T	19	WVQ	2	0

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 10 ligands modelled in this entry, 9 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
16	POP	B	1302	-	6,8,8	0.76	0	12,13,13	0.90	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	POP	B	1302	-	-	3/6/6/6	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
16	B	1302	POP	P1-O-P2-O4
16	B	1302	POP	P1-O-P2-O5
16	B	1302	POP	P1-O-P2-O6

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	B	1302	POP	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	R	10/10 (100%)	0.06	0 100 100	109, 128, 184, 198	0
2	T	23/29 (79%)	0.32	0 100 100	108, 223, 315, 334	0
3	N	13/18 (72%)	0.38	0 100 100	252, 278, 321, 360	0
4	A	1384/1733 (79%)	0.19	15 (1%) 78 52	56, 118, 208, 328	0
5	B	1126/1224 (91%)	0.15	16 (1%) 73 46	58, 113, 182, 292	0
6	C	267/318 (83%)	0.06	1 (0%) 88 70	61, 101, 172, 264	0
7	E	212/215 (98%)	0.21	7 (3%) 49 28	88, 147, 211, 350	0
8	F	86/155 (55%)	-0.05	0 100 100	89, 118, 167, 207	0
9	H	133/146 (91%)	0.14	1 (0%) 82 58	90, 140, 210, 344	0
10	I	118/122 (96%)	0.11	1 (0%) 82 58	83, 132, 190, 304	0
11	J	65/70 (92%)	0.17	1 (1%) 72 44	61, 86, 141, 182	0
12	K	114/120 (95%)	0.20	2 (1%) 67 40	69, 106, 163, 243	0
13	L	43/70 (61%)	0.67	3 (6%) 22 15	87, 192, 292, 409	0
All	All	3594/4230 (84%)	0.17	47 (1%) 75 48	56, 118, 207, 409	0

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	A	1002	GLY	4.7
7	E	112	TYR	4.6
5	B	714	GLU	3.9
13	L	46	VAL	3.7
5	B	775	LYS	3.5
13	L	28	LYS	3.3
7	E	93	MET	3.1
4	A	22	PHE	3.0
4	A	105	CYS	3.0

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Mol	Chain	Res	Type	RSRZ
4	A	1267	MET	3.0
5	B	489	SER	2.8
5	B	819	ALA	2.8
7	E	125	PRO	2.7
13	L	41	SER	2.7
9	H	130	ARG	2.7
5	B	779	GLY	2.6
5	B	446	LEU	2.6
7	E	46	TYR	2.6
4	A	141	LEU	2.6
4	A	303	TYR	2.5
5	B	543	SER	2.5
5	B	832	GLY	2.5
10	I	84	VAL	2.5
4	A	48	ALA	2.5
7	E	139	ALA	2.5
4	A	11	LEU	2.5
4	A	1394	THR	2.5
12	K	71	PHE	2.4
7	E	9	ILE	2.3
4	A	323	LYS	2.3
4	A	181	LEU	2.3
4	A	322	VAL	2.3
5	B	534	GLY	2.2
5	B	1144	ALA	2.2
5	B	751	VAL	2.2
4	A	997	LEU	2.2
5	B	390	LEU	2.2
5	B	648	HIS	2.1
11	J	54	VAL	2.1
7	E	111	VAL	2.1
4	A	56	PRO	2.1
6	C	251	LEU	2.1
12	K	42	LEU	2.1
5	B	75	ALA	2.1
4	A	1010	ALA	2.0
5	B	694	ASP	2.0
5	B	335	GLY	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	WVQ	T	19	23/24	0.64	0.21	127,165,198,210	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
16	POP	B	1302	9/9	0.64	0.08	119,150,174,179	0
15	ZN	A	1801	1/1	0.79	0.11	358,358,358,358	0
15	ZN	I	202	1/1	0.83	0.12	277,277,277,277	0
15	ZN	L	101	1/1	0.89	0.10	364,364,364,364	0
15	ZN	A	1802	1/1	0.91	0.09	185,185,185,185	0
14	MG	R	2001	1/1	0.95	0.08	124,124,124,124	0
15	ZN	I	201	1/1	0.97	0.05	126,126,126,126	0
15	ZN	C	401	1/1	0.97	0.05	100,100,100,100	0
15	ZN	B	1301	1/1	0.98	0.04	172,172,172,172	0
15	ZN	J	101	1/1	0.99	0.11	165,165,165,165	0

6.5 Other polymers [i](#)

There are no such residues in this entry.