



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 23, 2026 – 09:58 AM EDT

PDB ID : 8UKR / pdb_00008ukr
Title : RNA polymerase II elongation complex with Fapy-dG lesion soaking with ATP before chemistry
Authors : Hou, P.; Oh, J.; Wang, D.
Deposited on : 2023-10-15
Resolution : 3.78 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
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
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

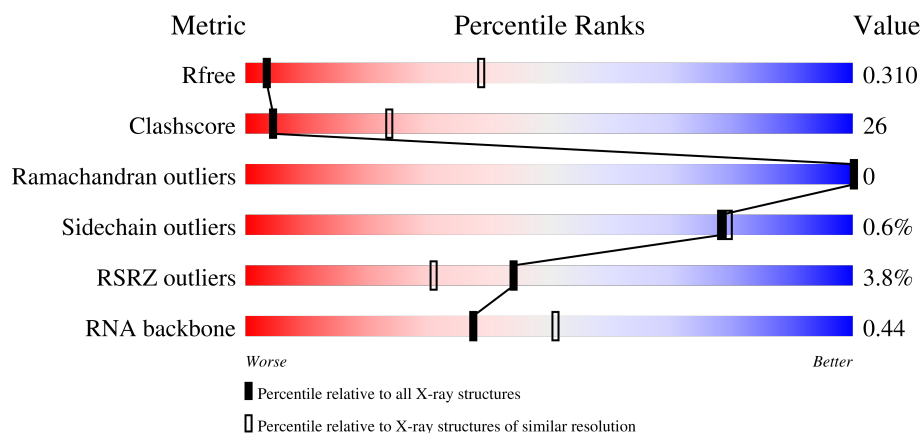
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.78 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	1085 (3.94-3.62)
Clashscore	190562	1029 (3.92-3.64)
Ramachandran outliers	187476	1064 (3.94-3.62)
Sidechain outliers	187428	1059 (3.94-3.62)
RSRZ outliers	180081	1084 (3.94-3.62)
RNA backbone	3983	1002 (4.46-3.10)

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	9	
2	T	29	
3	N	18	
4	A	1733	

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Mol	Chain	Length	Quality of chain
5	B	1224	46%46%8% 4%
6	C	318	46%37%16% 3%
7	E	215	46%53% 3%
8	F	155	28%27%45% 2%
9	H	146	44%47%9%
10	I	122	41%53%
11	J	70	41%50%7% 3%
12	K	120	52%43%5% 6%
13	L	70	24%31%39% 3%

2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 28985 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	9	Total	C	N	O	P	0	0	0
			194	88	40	58	8			

- 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	1123	Total	C	N	O	S	0	0	0
			8859	5607	1552	1647	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
			1724	1094	305	314	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
			952	585	173	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
			332	205	64	59	4			

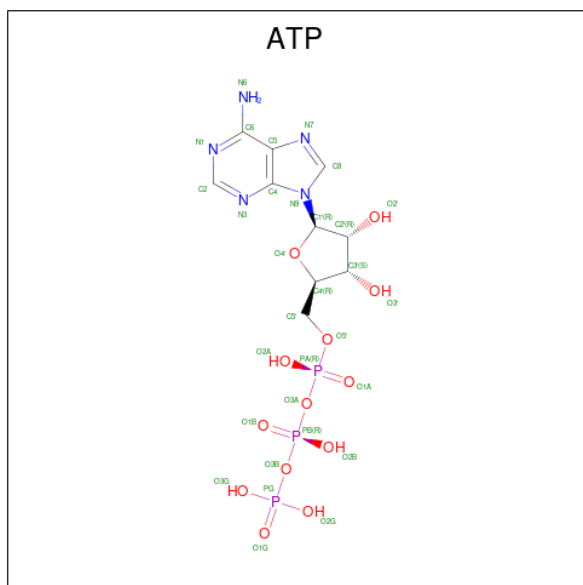
- Molecule 14 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 15 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	A	1	Total Mg 1 1	0	0

- Molecule 16 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $\text{C}_{10}\text{H}_{16}\text{N}_5\text{O}_{13}\text{P}_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
16	B	1	Total 31	C 10	N 5	O 13	P 3	0	0

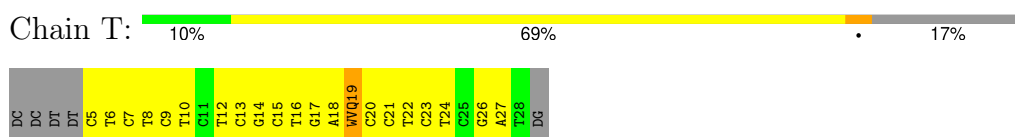
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

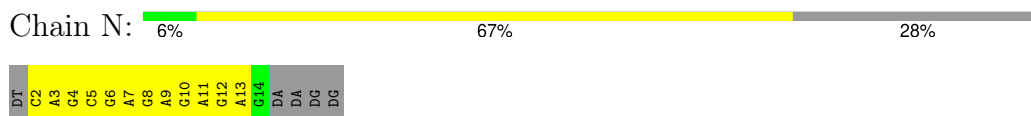
- Molecule 1: RNA



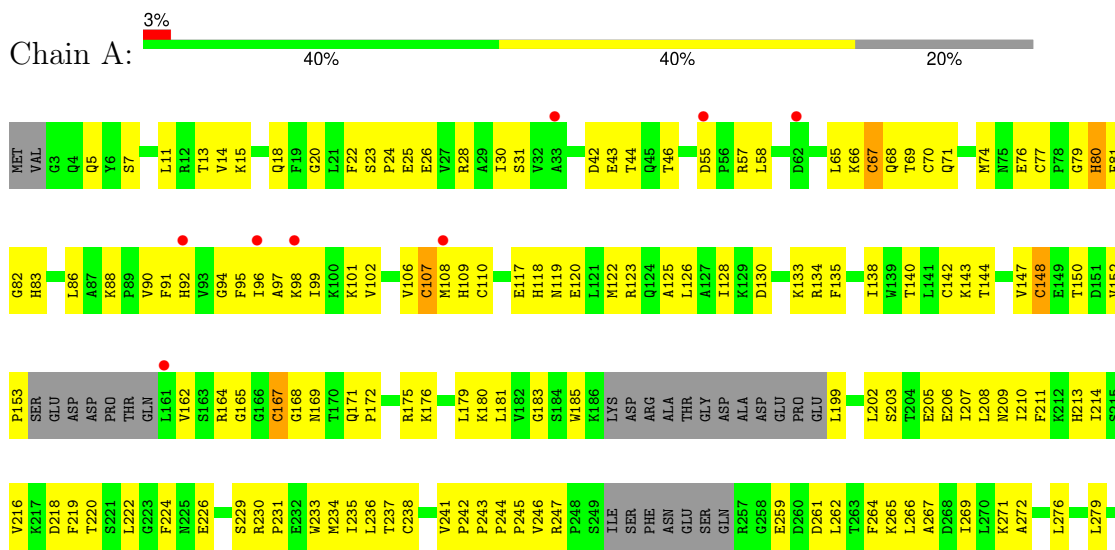
- Molecule 2: tsDNA with Fapy-dG lesion



- Molecule 3: ntsDNA

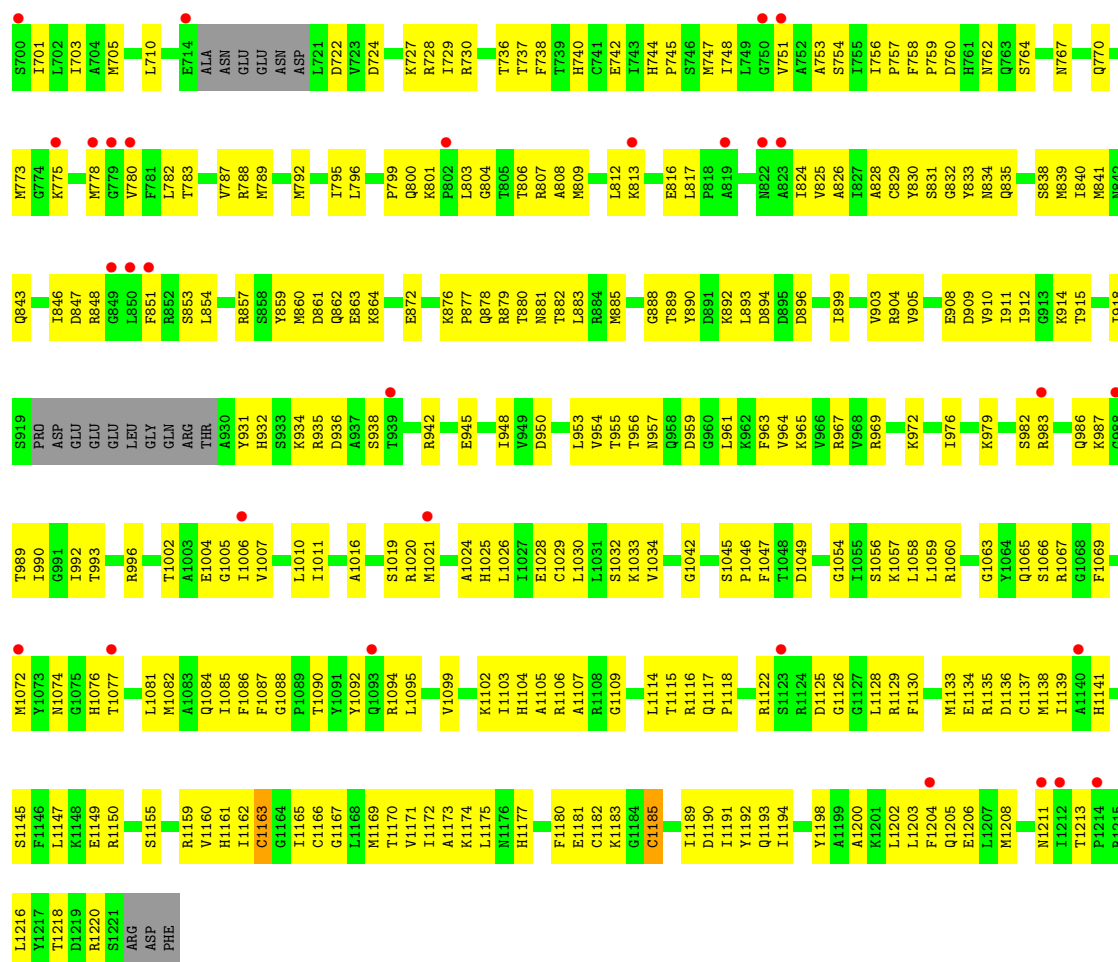


- Molecule 4: DNA-directed RNA polymerase II subunit RPB1

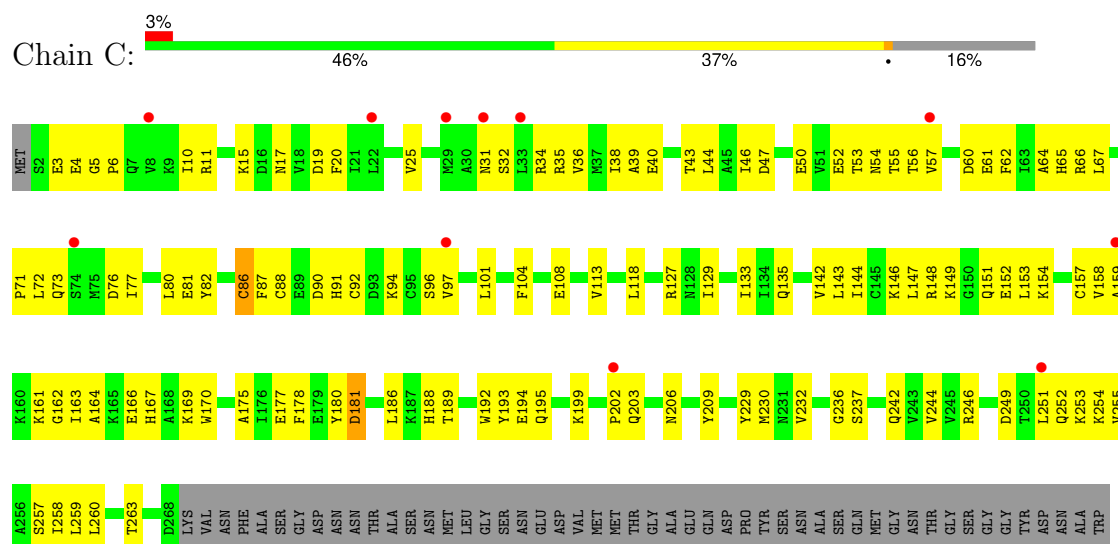


K1290	V1291	P1292	K1300	E1303	L1306	T1307	T1308	G1309	G1310	V1311	M1312	L1313	S1314	E1315	V1316	M1317	D1323	P1324	T1325	R1326	I1327	Y1328	T1329	D1334	I1335	M1336	E1337	V1338	G1339	L1340	I1341	E1342	R1345	A1346	Y1349	K1350	V1355	S1358	D1359	V1363	M1364	Y1365	R1366	H1367	M1368	A1369	L1370	L1371																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																
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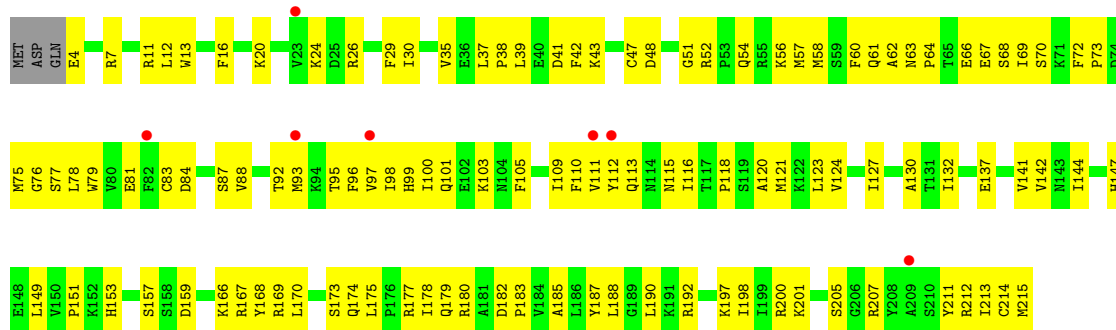


- Molecule 6: DNA-directed RNA polymerase II subunit RPB3

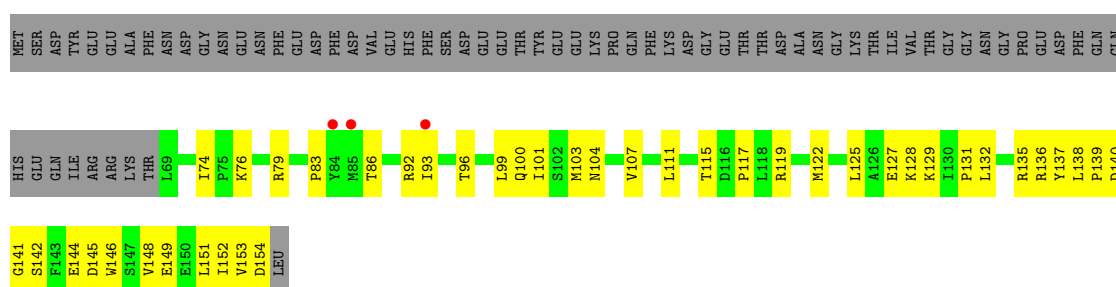
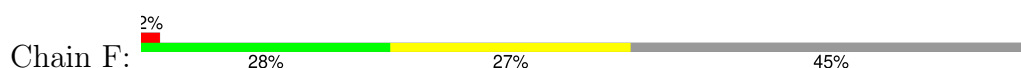


- Molecule 7: DNA-directed RNA polymerases I, II, and III subunit RPABC1

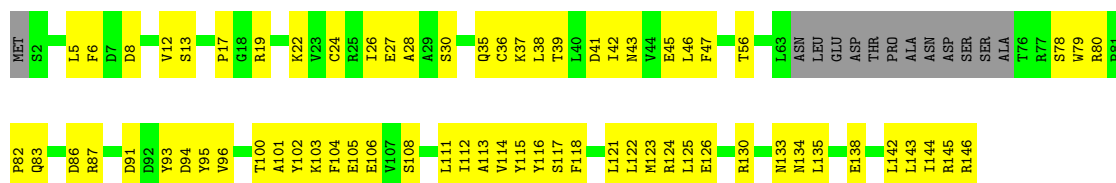




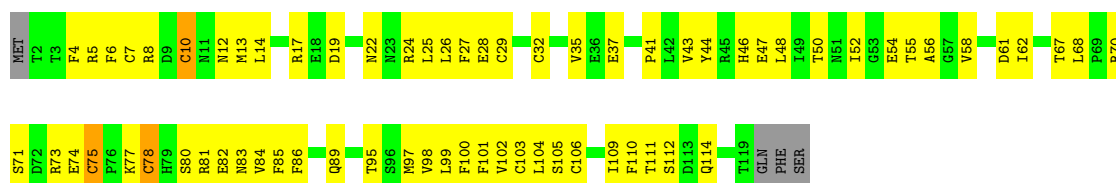
• Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC2



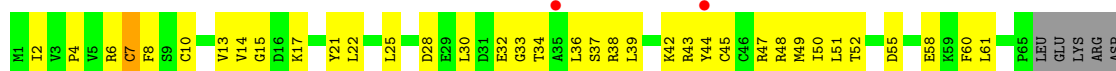
• Molecule 9: DNA-directed RNA polymerases I, II, and III subunit RPABC3



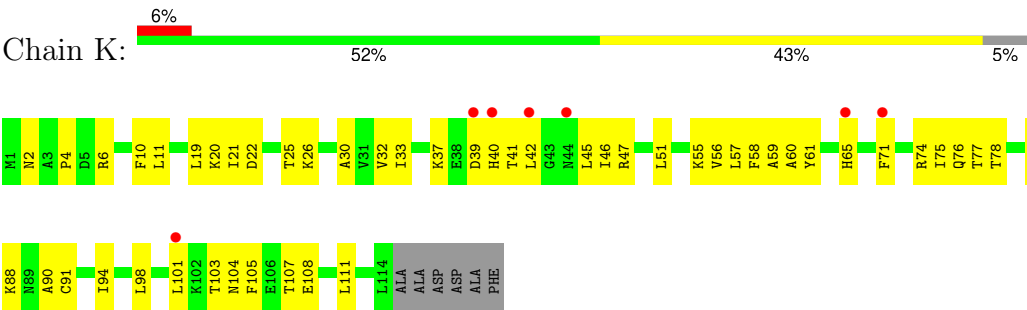
• Molecule 10: DNA-directed RNA polymerase II subunit RPB9



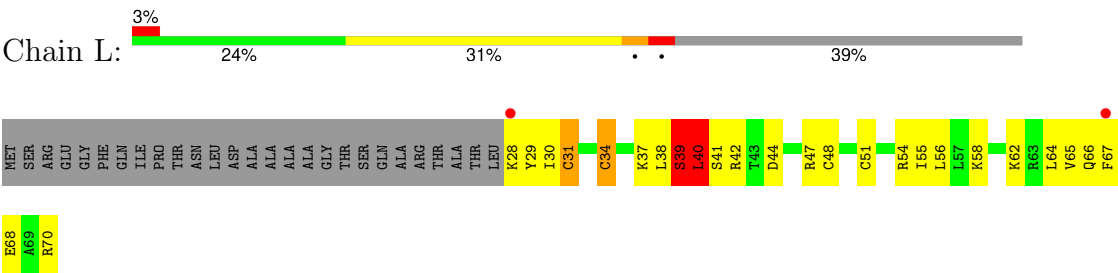
• Molecule 11: DNA-directed RNA polymerases I, II, and III subunit RPABC5



● 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	159.62Å 222.63Å 190.70Å 90.00° 97.69° 90.00°	Depositor
Resolution (Å)	47.96 – 3.78 47.96 – 3.78	Depositor EDS
% Data completeness (in resolution range)	97.6 (47.96-3.78) 97.5 (47.96-3.78)	Depositor EDS
R_{merge}	0.57	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.18 (at 3.77Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.261 , 0.310 0.261 , 0.310	Depositor DCC
R_{free} test set	2000 reflections (2.61%)	wwPDB-VP
Wilson B-factor (Å ²)	112.7	Xtriage
Anisotropy	0.584	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 135.5	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	28985	wwPDB-VP
Average B, all atoms (Å ²)	148.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.62% 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: ZN, MG, ATP, 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	0.19	0/218	0.41	0/339
2	T	0.30	0/507	0.62	0/775
3	N	0.32	0/311	0.50	0/479
4	A	0.23	0/11020	0.51	1/14907 (0.0%)
5	B	0.21	0/9030	0.49	1/12186 (0.0%)
6	C	0.24	1/2139 (0.0%)	0.47	0/2899
7	E	0.26	0/1759	0.51	0/2367
8	F	0.19	0/696	0.46	0/943
9	H	0.21	0/1082	0.53	0/1466
10	I	0.23	0/970	0.55	0/1308
11	J	0.23	0/541	0.48	0/727
12	K	0.25	0/937	0.53	0/1265
13	L	0.97	2/333 (0.6%)	1.05	3/442 (0.7%)
All	All	0.25	3/29543 (0.0%)	0.51	5/40103 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
13	L	0	2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	L	39	SER	C-O	-8.31	1.12	1.24
13	L	40	LEU	CG-CD2	-8.29	1.25	1.52
6	C	181	ASP	C-O	-5.40	1.21	1.23

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	L	39	SER	CA-C-O	-8.54	109.13	120.15
13	L	40	LEU	CB-CG-CD1	8.00	134.70	110.70
13	L	39	SER	CB-CA-C	7.37	122.48	111.06
4	A	622	VAL	N-CA-C	-6.09	106.56	112.29
5	B	1167	GLY	N-CA-C	-5.14	108.74	115.47

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
13	L	39	SER	Peptide
13	L	40	LEU	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	R	194	0	98	7	0
2	T	481	0	262	28	0
3	N	275	0	144	20	0
4	A	10828	0	10875	629	0
5	B	8859	0	8816	486	0
6	C	2101	0	2056	113	0
7	E	1724	0	1751	100	0
8	F	684	0	692	36	0
9	H	1064	0	1029	69	0
10	I	952	0	897	69	0
11	J	532	0	542	33	0
12	K	919	0	929	59	0
13	L	332	0	347	40	1
14	A	2	0	0	0	0
14	B	1	0	0	0	0
14	C	1	0	0	0	0
14	I	2	0	0	0	0
14	J	1	0	0	0	0
14	L	1	0	0	0	0
15	A	1	0	0	0	0
16	B	31	0	12	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	28985	0	28450	1505	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 26.

All (1505) 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:70:CYS:SG	4:A:80:HIS:CE1	2.58	0.96
4:A:613:ILE:HG21	9:H:102:TYR:HB3	1.49	0.93
4:A:881:GLN:HB2	4:A:956:LEU:HD12	1.52	0.92
5:B:892:LYS:NZ	5:B:904:ARG:O	2.07	0.88
4:A:1325:THR:HA	7:E:147:HIS:HA	1.57	0.87
5:B:621:GLU:HG3	5:B:623:GLU:HG3	1.55	0.86
4:A:326:ARG:HG3	4:A:1406:VAL:HG11	1.55	0.85
7:E:69:ILE:HG13	7:E:73:PRO:HA	1.60	0.84
4:A:1139:GLU:HG3	4:A:1282:VAL:HG22	1.60	0.84
7:E:78:LEU:HD11	7:E:109:ILE:HG12	1.61	0.82
5:B:129:PHE:HA	5:B:166:PHE:HA	1.61	0.81
9:H:38:LEU:HA	9:H:124:ARG:O	1.79	0.81
5:B:1056:SER:HB3	5:B:1066:SER:HB2	1.61	0.81
5:B:121:ASN:HA	5:B:207:GLY:HA3	1.61	0.81
4:A:11:LEU:HD12	5:B:1193:GLN:HG2	1.62	0.80
5:B:956:THR:HG22	13:L:54:ARG:HG2	1.62	0.80
4:A:279:LEU:HD21	4:A:289:ILE:HG12	1.63	0.79
4:A:783:THR:O	5:B:516:ASN:ND2	2.13	0.79
5:B:710:LEU:HD21	5:B:738:PHE:HB2	1.64	0.79
5:B:114:PRO:HG3	5:B:181:LEU:HD11	1.65	0.79
6:C:94:LYS:HA	6:C:127:ARG:HH22	1.47	0.79
5:B:228:LYS:HG2	5:B:234:ILE:HG13	1.64	0.79
13:L:47:ARG:HB2	13:L:54:ARG:HG3	1.65	0.78
5:B:102:VAL:HG22	5:B:112:LEU:HB2	1.65	0.77
4:A:122:MET:HE1	4:A:126:LEU:HD12	1.64	0.77
13:L:34:CYS:HB3	13:L:48:CYS:SG	2.24	0.77
13:L:38:LEU:HG	13:L:40:LEU:H	1.49	0.77
2:T:16:DT:O4	3:N:2:DC:N4	2.17	0.77
5:B:72:GLU:HA	5:B:87:LYS:HA	1.67	0.77
11:J:36:LEU:HD13	11:J:47:ARG:HG2	1.65	0.77
4:A:224:PHE:HB3	4:A:229:SER:HB2	1.66	0.76
5:B:123:THR:HG23	5:B:205:ILE:HA	1.67	0.76
7:E:16:PHE:HZ	7:E:58:MET:HB3	1.50	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:128:ILE:HB	4:A:134:ARG:HB2	1.66	0.76
6:C:39:ALA:HA	6:C:164:ALA:HB3	1.67	0.76
4:A:583:PRO:HD3	4:A:645:LEU:HD13	1.67	0.76
4:A:781:ASP:HB3	4:A:790:ASP:H	1.51	0.76
4:A:845:LEU:HA	4:A:848:ILE:HD12	1.66	0.76
4:A:668:ASP:OD2	4:A:742:ASN:N	2.18	0.75
7:E:4:GLU:O	7:E:7:ARG:NH2	2.20	0.75
4:A:70:CYS:SG	4:A:80:HIS:HE1	2.03	0.75
9:H:22:LYS:NZ	9:H:45:GLU:OE1	2.19	0.75
6:C:6:PRO:HB3	6:C:25:VAL:HG22	1.70	0.74
4:A:760:GLN:HB2	5:B:1021:MET:HE1	1.68	0.74
13:L:34:CYS:CB	13:L:48:CYS:SG	2.75	0.74
4:A:542:GLU:OE1	4:A:569:LYS:NZ	2.21	0.74
5:B:50:SER:HB3	5:B:408:LEU:HD23	1.70	0.74
7:E:16:PHE:CZ	7:E:58:MET:HB3	2.22	0.74
4:A:1224:LEU:HD21	4:A:1240:CYS:HB3	1.70	0.74
5:B:1033:LYS:HG2	5:B:1059:LEU:HD11	1.69	0.74
4:A:148:CYS:HB2	4:A:167:CYS:HB2	1.70	0.73
5:B:910:VAL:HG11	5:B:938:SER:HB3	1.69	0.73
4:A:1434:ALA:HB1	4:A:1436:ILE:HD13	1.69	0.73
4:A:607:ILE:HA	4:A:612:ILE:HA	1.70	0.73
7:E:179:GLN:HG3	7:E:182:ASP:HB2	1.71	0.73
4:A:242:PRO:O	4:A:247:ARG:NH1	2.22	0.73
4:A:774:ARG:HG2	4:A:797:LYS:HB3	1.70	0.73
4:A:946:VAL:HA	7:E:201:LYS:HD3	1.69	0.73
5:B:570:VAL:HG23	5:B:573:GLN:HB2	1.69	0.73
4:A:455:MET:HE3	5:B:1138:MET:HE3	1.71	0.73
10:I:22:ASN:HB3	10:I:24:ARG:HB2	1.70	0.73
13:L:29:TYR:CE1	13:L:41:SER:HA	2.23	0.72
5:B:483:LEU:HD21	5:B:491:THR:HG23	1.70	0.72
5:B:428:ILE:HG12	5:B:448:ILE:HG22	1.71	0.72
12:K:47:ARG:HD2	12:K:60:ALA:HA	1.72	0.72
4:A:351:THR:HG23	5:B:1103:ILE:HG12	1.72	0.72
3:N:6:DG:H2''	3:N:7:DA:H5''	1.71	0.72
4:A:361:LEU:HB2	4:A:471:ASN:HD22	1.54	0.72
4:A:1303:GLU:OE1	4:A:1326:ARG:NH2	2.22	0.72
5:B:468:GLU:O	5:B:470:LYS:NZ	2.23	0.72
4:A:899:VAL:HG13	4:A:929:LEU:HD13	1.72	0.71
7:E:47:CYS:HB3	7:E:51:GLY:HA2	1.70	0.71
5:B:904:ARG:HD2	13:L:65:VAL:HG11	1.72	0.71
9:H:37:LYS:H	9:H:126:GLU:HB2	1.56	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:J:10:CYS:SG	11:J:43:ARG:NH1	2.64	0.71
10:I:84:VAL:HG23	10:I:104:LEU:HD21	1.72	0.71
4:A:67:CYS:HB3	4:A:70:CYS:HB2	1.72	0.70
5:B:942:ARG:HB2	5:B:945:GLU:HG3	1.73	0.70
4:A:880:LYS:HE2	4:A:955:PRO:HD3	1.72	0.70
5:B:38:PHE:HZ	5:B:541:LEU:HD13	1.57	0.70
7:E:83:CYS:O	7:E:113:GLN:NE2	2.25	0.70
11:J:17:LYS:HB3	11:J:39:LEU:HD22	1.73	0.70
4:A:901:LEU:HB2	4:A:926:GLN:HB2	1.73	0.70
5:B:35:SER:HB3	5:B:39:ARG:HH21	1.56	0.70
4:A:450:LEU:HD13	4:A:1074:GLU:HB2	1.73	0.70
4:A:452:LYS:HA	5:B:1137:CYS:HB3	1.74	0.70
4:A:483:ASP:HB2	5:B:987:LYS:HG3	1.72	0.70
5:B:950:ASP:OD1	5:B:969:ARG:NH1	2.25	0.70
6:C:52:GLU:HG2	6:C:53:THR:HG23	1.74	0.70
4:A:1421:CYS:HB3	4:A:1430:LEU:HD11	1.72	0.69
11:J:7:CYS:HA	11:J:49:MET:HE3	1.71	0.69
4:A:873:MET:O	4:A:1366:ARG:NH2	2.25	0.69
7:E:42:PHE:HE1	7:E:58:MET:HE1	1.56	0.69
4:A:368:LYS:HG2	4:A:372:LYS:HE2	1.73	0.69
5:B:227:LYS:HA	5:B:236:HIS:HD2	1.57	0.69
4:A:308:ILE:HG13	4:A:312:PRO:HD2	1.74	0.69
10:I:74:GLU:HB3	10:I:81:ARG:HA	1.75	0.69
5:B:1076:HIS:O	6:C:31:ASN:ND2	2.26	0.69
5:B:357:GLN:HG2	5:B:368:GLU:HG3	1.75	0.69
5:B:996:ARG:HG3	5:B:1007:VAL:HG21	1.75	0.69
6:C:76:ASP:HB2	6:C:129:ILE:HG12	1.74	0.69
13:L:40:LEU:HG	13:L:41:SER:N	2.08	0.69
4:A:370:ILE:HG12	5:B:1105:ALA:HB2	1.74	0.68
6:C:31:ASN:OD1	6:C:34:ARG:NH1	2.26	0.68
2:T:8:DT:O2	3:N:12:DG:N2	2.27	0.68
6:C:50:GLU:HB3	13:L:66:GLN:HG2	1.74	0.68
4:A:1027:ALA:O	4:A:1031:VAL:N	2.23	0.68
4:A:286:HIS:HA	4:A:289:ILE:HD12	1.75	0.68
4:A:968:GLN:HA	4:A:973:ILE:HD12	1.76	0.68
4:A:1142:THR:HG23	4:A:1145:SER:H	1.59	0.68
5:B:361:LEU:HD21	5:B:377:PHE:HB3	1.76	0.68
4:A:446:ARG:HD3	4:A:448:PRO:HD2	1.75	0.67
4:A:711:ARG:HD2	10:I:95:THR:HB	1.75	0.67
5:B:780:VAL:HG22	5:B:795:ILE:HG23	1.76	0.67
4:A:407:ARG:HG3	4:A:413:ILE:HD11	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:1104:HIS:NE2	5:B:1126:GLY:O	2.27	0.67
4:A:898:ARG:NH1	4:A:899:VAL:O	2.26	0.67
9:H:115:TYR:CE1	9:H:124:ARG:HD3	2.30	0.67
4:A:363:GLN:HE21	4:A:459:ARG:HH21	1.42	0.67
5:B:308:TRP:H	5:B:308:TRP:CD1	2.10	0.67
5:B:1029:CYS:HG	5:B:1090:THR:HG1	1.42	0.67
4:A:915:SER:O	4:A:919:ILE:N	2.28	0.67
10:I:26:LEU:HD13	10:I:35:VAL:HG11	1.76	0.67
13:L:30:ILE:HG12	13:L:37:LYS:HG3	1.77	0.67
9:H:96:VAL:HA	9:H:142:LEU:O	1.95	0.67
7:E:66:GLU:HA	7:E:69:ILE:HG22	1.76	0.67
5:B:796:LEU:HB3	5:B:799:PRO:HG3	1.76	0.67
7:E:79:TRP:CD1	7:E:103:LYS:HZ3	2.13	0.67
7:E:197:LYS:HD2	7:E:211:TYR:HE1	1.60	0.67
5:B:789:MET:HE2	5:B:967:ARG:HB2	1.76	0.66
13:L:68:GLU:HG2	13:L:70:ARG:H	1.60	0.66
4:A:956:LEU:HD13	4:A:1021:LEU:HD22	1.77	0.66
4:A:208:LEU:HD13	4:A:235:ILE:HD11	1.77	0.66
5:B:237:VAL:HG22	5:B:257:LYS:HB3	1.76	0.66
5:B:724:ASP:HB2	5:B:727:LYS:HD3	1.76	0.66
9:H:93:TYR:HA	9:H:145:ARG:HD3	1.76	0.66
12:K:56:VAL:HG22	12:K:77:THR:HG22	1.77	0.66
4:A:877:HIS:HD2	4:A:1056:SER:HA	1.60	0.66
4:A:1152:ILE:HD12	4:A:1261:LYS:HG2	1.78	0.66
12:K:61:TYR:HB2	12:K:71:PHE:HE1	1.60	0.66
11:J:45:CYS:HB2	11:J:48:ARG:NH2	2.10	0.65
7:E:103:LYS:HB3	7:E:105:PHE:CD2	2.31	0.65
7:E:118:PRO:HA	7:E:121:MET:HG2	1.78	0.65
5:B:680:THR:HG23	5:B:683:SER:H	1.59	0.65
12:K:57:LEU:N	12:K:76:GLN:O	2.30	0.65
4:A:704:ALA:HB2	4:A:710:LEU:HD13	1.79	0.65
8:F:136:ARG:HB2	8:F:144:GLU:HG3	1.77	0.65
5:B:277:LYS:HG3	5:B:278:GLN:HG3	1.79	0.65
6:C:36:VAL:HA	6:C:40:GLU:HG2	1.79	0.65
10:I:82:GLU:HB3	10:I:104:LEU:HG	1.79	0.65
5:B:653:VAL:HA	5:B:689:LEU:HD13	1.79	0.65
4:A:701:LEU:HD21	10:I:114:GLN:HB2	1.78	0.65
6:C:178:PHE:HE1	6:C:180:TYR:HB3	1.62	0.65
4:A:269:ILE:HG13	4:A:299:HIS:HB3	1.79	0.64
5:B:1160:VAL:HG23	5:B:1194:ILE:HG13	1.79	0.64
5:B:1072:MET:HG3	5:B:1085:ILE:HB	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:17:DG:H4'	4:A:1403:GLU:HG2	1.80	0.64
3:N:11:DA:H2''	3:N:12:DG:C8	2.32	0.64
5:B:475:SER:OG	5:B:476:ARG:NH1	2.31	0.64
4:A:91:PHE:HB3	4:A:235:ILE:HG22	1.80	0.64
3:N:3:DA:H1'	3:N:4:DG:H5'	1.79	0.64
5:B:276:ILE:HD11	5:B:355:ILE:HD13	1.78	0.64
4:A:58:LEU:HB3	4:A:244:PRO:HG2	1.80	0.64
5:B:273:LEU:HB2	5:B:276:ILE:HB	1.78	0.64
6:C:11:ARG:HH12	6:C:229:TYR:HB3	1.63	0.64
7:E:127:ILE:HG22	7:E:130:ALA:H	1.62	0.64
4:A:207:ILE:HA	4:A:210:ILE:HD12	1.80	0.63
5:B:693:ILE:HG21	5:B:701:ILE:HD13	1.80	0.63
4:A:1342:GLU:OE1	7:E:200:ARG:NH1	2.31	0.63
13:L:28:LYS:HE3	13:L:41:SER:HB3	1.79	0.63
12:K:30:ALA:HA	12:K:75:ILE:O	1.98	0.63
4:A:563:PRO:HB2	4:A:566:ILE:HG12	1.80	0.63
5:B:604:ARG:NH1	5:B:613:VAL:O	2.31	0.63
7:E:99:HIS:O	7:E:103:LYS:HG2	1.99	0.63
9:H:116:TYR:O	9:H:123:MET:HB3	1.97	0.63
13:L:31:CYS:HB3	13:L:34:CYS:SG	2.38	0.63
4:A:765:VAL:HG22	4:A:800:VAL:HB	1.80	0.63
4:A:761:MET:O	4:A:803:SER:OG	2.16	0.63
4:A:822:GLU:HA	4:A:825:ILE:HD12	1.80	0.63
7:E:68:SER:HB3	7:E:75:MET:HE2	1.80	0.63
2:T:6:DT:H2''	2:T:7:DC:C5	2.33	0.62
6:C:36:VAL:HG13	6:C:40:GLU:HB2	1.81	0.62
6:C:64:ALA:HA	6:C:67:LEU:HD12	1.81	0.62
5:B:426:LYS:O	5:B:430:ARG:HG3	1.98	0.62
5:B:1171:VAL:HB	5:B:1182:CYS:HB2	1.80	0.62
6:C:36:VAL:HG21	6:C:251:LEU:HD13	1.82	0.62
4:A:23:SER:HB2	4:A:233:TRP:CE2	2.34	0.62
4:A:91:PHE:O	4:A:297:GLN:NE2	2.32	0.62
4:A:875:ALA:HB2	4:A:1366:ARG:HD3	1.81	0.62
12:K:61:TYR:HB2	12:K:71:PHE:CE1	2.34	0.62
5:B:1054:GLY:HA2	5:B:1057:LYS:HD2	1.80	0.62
5:B:613:VAL:HG22	5:B:628:THR:HA	1.80	0.62
5:B:883:LEU:HB2	5:B:932:HIS:HB3	1.81	0.62
4:A:357:PRO:HG3	4:A:472:LEU:HD11	1.80	0.62
5:B:261:ARG:HB2	5:B:264:SER:HB2	1.80	0.62
5:B:736:THR:HG23	5:B:737:THR:HG23	1.82	0.62
5:B:1029:CYS:HB3	5:B:1088:GLY:HA3	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:E:24:LYS:HD3	7:E:30:ILE:HG22	1.82	0.62
4:A:660:ASN:HA	5:B:1082:MET:HB3	1.80	0.62
4:A:667:GLY:HA3	5:B:1067:ARG:HD2	1.81	0.62
4:A:672:ASP:H	4:A:736:ASN:HD21	1.47	0.62
5:B:582:VAL:HG22	5:B:626:ILE:HB	1.80	0.62
5:B:1116:ARG:HG3	5:B:1198:TYR:CD2	2.35	0.62
13:L:29:TYR:CZ	13:L:41:SER:HA	2.35	0.62
4:A:590:ARG:HH12	4:A:592:ASP:CG	2.07	0.62
5:B:562:GLY:O	5:B:590:HIS:ND1	2.33	0.62
6:C:88:CYS:HB3	6:C:92:CYS:HB3	1.82	0.61
6:C:108:GLU:HG2	6:C:149:LYS:HE3	1.81	0.61
9:H:94:ASP:OD2	9:H:146:ARG:HG3	2.00	0.61
4:A:407:ARG:HH22	4:A:411:ASP:HB3	1.65	0.61
4:A:1242:VAL:HG12	4:A:1243:VAL:HG12	1.82	0.61
6:C:52:GLU:HA	13:L:64:LEU:HD13	1.82	0.61
12:K:10:PHE:CD2	12:K:11:LEU:HD13	2.35	0.61
12:K:55:LYS:HB3	12:K:78:THR:HG22	1.81	0.61
5:B:697:GLU:O	5:B:701:ILE:HG23	2.00	0.61
5:B:431:TYR:HA	5:B:434:ARG:HE	1.65	0.61
5:B:880:THR:HB	5:B:931:TYR:HE1	1.65	0.61
5:B:1174:LYS:HB2	5:B:1177:HIS:HB2	1.82	0.61
4:A:526:ASP:HB3	4:A:657:LEU:HD23	1.82	0.61
7:E:173:SER:HA	7:E:177:ARG:HH21	1.66	0.61
9:H:106:GLU:HB3	9:H:112:ILE:HD13	1.82	0.61
10:I:73:ARG:O	10:I:83:ASN:ND2	2.34	0.61
11:J:37:SER:OG	11:J:42:LYS:NZ	2.33	0.61
4:A:14:VAL:HG11	5:B:1216:LEU:HB3	1.82	0.61
4:A:682:THR:OG1	4:A:728:LYS:NZ	2.34	0.61
4:A:767:GLN:HA	4:A:799:PHE:HA	1.81	0.61
9:H:138:GLU:OE1	9:H:138:GLU:N	2.28	0.61
10:I:26:LEU:HA	10:I:37:GLU:HA	1.82	0.61
11:J:58:GLU:HA	11:J:61:LEU:HD12	1.81	0.61
1:R:2:U:H2'	1:R:3:C:C6	2.36	0.61
4:A:575:LYS:O	4:A:579:SER:OG	2.18	0.61
4:A:335:ARG:O	4:A:340:LEU:N	2.30	0.60
4:A:900:ASP:H	4:A:906:HIS:HB3	1.66	0.60
12:K:51:LEU:HD22	12:K:59:ALA:HB3	1.81	0.60
4:A:176:LYS:HG3	4:A:181:LEU:HG	1.83	0.60
4:A:946:VAL:HG13	7:E:201:LYS:HG2	1.83	0.60
5:B:55:VAL:HA	5:B:59:LEU:HD12	1.83	0.60
5:B:800:GLN:HB3	11:J:52:THR:HB	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:298:LEU:HD11	5:B:318:VAL:HG21	1.84	0.60
7:E:43:LYS:O	7:E:47:CYS:N	2.30	0.60
7:E:48:ASP:OD1	7:E:52:ARG:N	2.23	0.60
4:A:1188:GLN:HE22	4:A:1241:ARG:HH11	1.50	0.60
5:B:751:VAL:HG23	5:B:812:LEU:HD22	1.83	0.60
4:A:265:LYS:O	4:A:269:ILE:HD12	2.01	0.60
9:H:101:ALA:HA	9:H:116:TYR:HA	1.82	0.60
12:K:47:ARG:HD3	12:K:61:TYR:HD2	1.65	0.60
2:T:26:DG:H3'	2:T:27:DA:H8	1.67	0.60
4:A:960:ILE:HG21	4:A:1025:ARG:HB3	1.82	0.60
4:A:1424:VAL:HG22	4:A:1436:ILE:HD11	1.82	0.60
5:B:36:ALA:HA	5:B:39:ARG:HD2	1.82	0.60
6:C:203:GLN:OE1	6:C:203:GLN:N	2.31	0.60
10:I:7:CYS:SG	10:I:32:CYS:HB2	2.41	0.60
4:A:143:LYS:HG3	4:A:144:THR:HG23	1.83	0.60
5:B:915:THR:HG21	5:B:934:LYS:HE3	1.83	0.60
5:B:1072:MET:HB2	5:B:1081:LEU:HD12	1.84	0.60
6:C:55:THR:OG1	6:C:152:GLU:N	2.34	0.60
6:C:177:GLU:O	6:C:230:MET:HA	2.01	0.60
7:E:64:PRO:HD3	7:E:77:SER:H	1.67	0.60
4:A:381:THR:HA	8:F:104:ASN:HD21	1.66	0.60
5:B:605:ARG:NH2	5:B:641:GLU:OE2	2.32	0.60
5:B:703:ILE:HG22	5:B:740:HIS:HB2	1.83	0.60
2:T:6:DT:H4'	2:T:7:DC:H5'	1.84	0.59
4:A:42:ASP:HB3	4:A:46:THR:HB	1.82	0.59
4:A:550:LEU:HD12	4:A:577:ILE:HD13	1.84	0.59
4:A:1009:ASN:HA	4:A:1012:ARG:HE	1.67	0.59
5:B:896:ASP:OD2	13:L:28:LYS:NZ	2.35	0.59
7:E:144:ILE:HD11	7:E:187:TYR:HB2	1.84	0.59
8:F:96:THR:HG22	8:F:100:GLN:HE21	1.66	0.59
4:A:994:GLN:HE22	4:A:1023:ARG:HE	1.48	0.59
12:K:30:ALA:HB2	12:K:76:GLN:HG2	1.83	0.59
4:A:560:ILE:H	9:H:78:SER:HB2	1.67	0.59
4:A:702:LEU:HD13	4:A:710:LEU:HD11	1.84	0.59
5:B:979:LYS:HD2	5:B:1095:LEU:HG	1.85	0.59
5:B:1084:GLN:OE1	6:C:189:THR:OG1	2.21	0.59
4:A:120:GLU:HA	4:A:123:ARG:HE	1.67	0.59
7:E:185:ALA:HA	7:E:190:LEU:HD12	1.83	0.59
5:B:38:PHE:CZ	5:B:541:LEU:HD13	2.37	0.59
5:B:354:ASP:O	5:B:358:LYS:HG2	2.01	0.59
7:E:205:SER:OG	7:E:207:ARG:O	2.18	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:851:HIS:ND1	8:F:139:PRO:HG3	2.17	0.59
5:B:778:MET:HE2	5:B:1094:ARG:HB3	1.85	0.59
9:H:12:VAL:HG21	9:H:26:ILE:HD12	1.84	0.59
4:A:57:ARG:O	4:A:68:GLN:N	2.35	0.59
6:C:142:VAL:HG23	11:J:15:GLY:HA3	1.85	0.59
3:N:4:DG:H2"	3:N:5:DC:C5	2.38	0.59
4:A:126:LEU:O	4:A:134:ARG:NE	2.36	0.59
4:A:537:ARG:HG3	4:A:575:LYS:HZ3	1.67	0.59
4:A:1323:ASP:OD2	4:A:1325:THR:OG1	2.19	0.59
8:F:76:LYS:HD2	8:F:79:ARG:HD2	1.83	0.59
4:A:859:SER:HA	4:A:1422:ARG:HE	1.68	0.59
5:B:40:GLU:OE1	5:B:680:THR:OG1	2.20	0.59
5:B:658:ILE:HG22	5:B:662:MET:HE2	1.85	0.59
7:E:88:VAL:HG12	7:E:92:THR:OG1	2.03	0.59
8:F:128:LYS:HD2	8:F:149:GLU:HA	1.85	0.59
4:A:1207:LEU:HG	4:A:1274:ARG:HH21	1.68	0.59
5:B:828:ALA:O	5:B:834:ASN:ND2	2.36	0.59
6:C:32:SER:HA	12:K:41:THR:OG1	2.03	0.59
4:A:1035:TYR:CE2	4:A:1037:LEU:HD22	2.37	0.58
5:B:1163:CYS:SG	5:B:1166:CYS:N	2.67	0.58
9:H:105:GLU:HG3	9:H:113:ALA:HB3	1.85	0.58
13:L:31:CYS:CB	13:L:34:CYS:SG	2.91	0.58
4:A:666:ILE:O	4:A:669:THR:OG1	2.18	0.58
5:B:128:LEU:HB2	5:B:168:GLY:O	2.03	0.58
6:C:54:ASN:OD1	6:C:56:THR:HG22	2.04	0.58
11:J:32:GLU:O	11:J:36:LEU:HG	2.03	0.58
4:A:128:ILE:H	4:A:134:ARG:HH21	1.51	0.58
5:B:853:SER:O	5:B:972:LYS:HB2	2.04	0.58
5:B:860:MET:HB2	5:B:965:LYS:HG3	1.86	0.58
6:C:195:GLN:HB2	6:C:199:LYS:NZ	2.18	0.58
8:F:125:LEU:HD21	8:F:153:VAL:HG21	1.84	0.58
4:A:781:ASP:HB3	4:A:790:ASP:N	2.17	0.58
4:A:786:HIS:CE1	5:B:703:ILE:HG13	2.38	0.58
4:A:352:VAL:HB	5:B:1099:VAL:HG12	1.86	0.58
4:A:529:CYS:O	4:A:533:LYS:HG3	2.03	0.58
7:E:13:TRP:HB2	7:E:42:PHE:CE2	2.39	0.58
8:F:127:GLU:HB3	8:F:129:LYS:HG2	1.85	0.58
4:A:110:CYS:SG	4:A:168:GLY:N	2.68	0.58
5:B:44:VAL:HG11	5:B:495:LEU:HD13	1.86	0.58
5:B:601:ARG:O	5:B:605:ARG:HD3	2.04	0.58
5:B:639:ILE:HD11	5:B:691:GLU:HB2	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:839:ARG:O	4:A:843:LYS:HG2	2.04	0.58
5:B:728:ARG:HD2	5:B:730:ARG:HH21	1.66	0.58
4:A:24:PRO:HB3	4:A:238:CYS:H	1.66	0.58
4:A:326:ARG:HB2	4:A:1406:VAL:HG21	1.85	0.58
4:A:662:PHE:O	5:B:828:ALA:HA	2.04	0.58
5:B:60:GLN:NE2	5:B:94:LYS:HB3	2.19	0.58
7:E:127:ILE:HB	7:E:132:ILE:HD11	1.86	0.58
5:B:758:PHE:HB2	5:B:1024:ALA:HB1	1.86	0.57
4:A:427:GLN:HG3	4:A:428:TYR:H	1.69	0.57
5:B:1114:LEU:HG	5:B:1202:LEU:HD11	1.87	0.57
4:A:1194:ARG:HA	4:A:1238:ILE:O	2.04	0.57
4:A:527:THR:HG21	4:A:650:GLN:HG2	1.85	0.57
4:A:705:LYS:HB2	4:A:708:MET:HE3	1.85	0.57
4:A:1111:MET:HB3	4:A:1114:PRO:HG3	1.86	0.57
5:B:829:CYS:HA	5:B:834:ASN:HD21	1.69	0.57
9:H:43:ASN:HB3	9:H:46:LEU:HB2	1.85	0.57
4:A:396:PRO:HG3	4:A:416:ARG:HG2	1.85	0.57
6:C:3:GLU:HB2	12:K:104:ASN:HD21	1.69	0.57
12:K:25:THR:HG22	12:K:26:LYS:HG3	1.87	0.57
4:A:1120:LEU:HG	4:A:1124:HIS:HB3	1.86	0.57
5:B:681:TRP:CH2	5:B:690:VAL:HG11	2.39	0.57
12:K:20:LYS:HZ3	12:K:22:ASP:HB2	1.69	0.57
2:T:15:DC:H1'	2:T:16:DT:C6	2.40	0.57
4:A:463:ILE:HD13	4:A:469:ARG:HG2	1.87	0.57
5:B:753:ALA:HA	5:B:756:ILE:HD12	1.86	0.57
9:H:35:GLN:HE21	9:H:111:LEU:HD11	1.69	0.57
9:H:30:SER:HB2	9:H:36:CYS:HB3	1.87	0.56
4:A:830:LYS:HZ1	4:A:1081:LEU:HB2	1.69	0.56
7:E:29:PHE:HB3	7:E:63:ASN:HB3	1.87	0.56
4:A:711:ARG:CZ	10:I:97:MET:HG2	2.35	0.56
5:B:37:PHE:HB2	5:B:681:TRP:CE3	2.40	0.56
5:B:329:THR:HA	5:B:332:ASP:HB3	1.88	0.56
5:B:457:LEU:O	5:B:461:LEU:HD12	2.04	0.56
6:C:81:GLU:HG2	6:C:86:CYS:HB2	1.87	0.56
6:C:101:LEU:HB2	6:C:118:LEU:HD23	1.88	0.56
10:I:75:CYS:HB2	10:I:110:PHE:CD1	2.39	0.56
1:R:4:G:H2'	1:R:5:A:C8	2.39	0.56
4:A:755:PHE:HA	4:A:758:ILE:HD12	1.87	0.56
4:A:902:LEU:HG	4:A:926:GLN:HG2	1.88	0.56
5:B:579:ARG:NH2	5:B:621:GLU:O	2.39	0.56
4:A:877:HIS:CD2	4:A:1056:SER:HA	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1239:ARG:HH12	4:A:1241:ARG:HE	1.53	0.56
5:B:459:TYR:CE1	5:B:468:GLU:HA	2.41	0.56
5:B:619:ILE:HG22	10:I:62:ILE:HG13	1.88	0.56
5:B:657:HIS:CD2	5:B:689:LEU:HD11	2.40	0.56
3:N:4:DG:H2"	3:N:5:DC:C6	2.40	0.56
4:A:122:MET:HE3	4:A:122:MET:C	2.31	0.56
4:A:998:LEU:O	4:A:1001:ARG:NH2	2.38	0.56
5:B:29:ASP:HB3	5:B:658:ILE:HG21	1.88	0.56
5:B:355:ILE:HG23	5:B:359:GLU:HB2	1.87	0.56
4:A:602:ASP:OD2	4:A:616:VAL:HG23	2.06	0.56
5:B:68:THR:HB	5:B:70:ILE:HD11	1.86	0.56
5:B:483:LEU:HD22	5:B:485:ARG:HD3	1.87	0.56
4:A:130:ASP:HB3	4:A:133:LYS:HD2	1.88	0.56
5:B:64:CYS:HA	5:B:67:SER:HB3	1.88	0.56
5:B:635:ARG:HH22	5:B:742:GLU:CD	2.14	0.56
4:A:1051:ALA:O	4:A:1055:ARG:HG2	2.06	0.55
5:B:612:GLU:O	5:B:632:ARG:NH1	2.34	0.55
5:B:953:LEU:HD11	13:L:55:ILE:HB	1.87	0.55
5:B:956:THR:CG2	13:L:54:ARG:HG2	2.36	0.55
7:E:179:GLN:HA	7:E:215:MET:OXT	2.06	0.55
10:I:68:LEU:O	10:I:70:ARG:NH1	2.39	0.55
4:A:967:ALA:HB2	4:A:1044:TRP:CZ3	2.41	0.55
5:B:1115:THR:HB	5:B:1117:GLN:HG3	1.87	0.55
7:E:72:PHE:CE1	7:E:157:SER:HA	2.42	0.55
7:E:120:ALA:HA	7:E:123:LEU:HD12	1.87	0.55
4:A:203:SER:HB2	4:A:206:GLU:HB2	1.88	0.55
4:A:587:HIS:HE1	4:A:969:GLN:HG2	1.70	0.55
10:I:100:PHE:HD1	10:I:111:THR:HG23	1.71	0.55
4:A:348:SER:HB2	5:B:1128:LEU:HB2	1.88	0.55
5:B:1099:VAL:O	5:B:1103:ILE:HG13	2.05	0.55
10:I:85:PHE:HB2	10:I:99:LEU:HD22	1.88	0.55
10:I:103:CYS:HB3	10:I:105:SER:O	2.07	0.55
13:L:29:TYR:OH	13:L:41:SER:HA	2.06	0.55
4:A:728:LYS:O	4:A:732:LEU:HG	2.07	0.55
5:B:541:LEU:HD12	5:B:542:MET:HG2	1.87	0.55
4:A:344:ARG:O	5:B:1155:SER:OG	2.22	0.55
9:H:13:SER:N	9:H:27:GLU:O	2.40	0.55
6:C:10:ILE:HA	6:C:20:PHE:HA	1.88	0.55
4:A:28:ARG:HH22	4:A:237:THR:HG1	1.55	0.55
4:A:265:LYS:HE3	4:A:322:VAL:HG11	1.89	0.55
4:A:391:LEU:HD22	4:A:400:PRO:HB2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:456:MET:HE3	4:A:507:VAL:HG22	1.89	0.55
4:A:1239:ARG:HH22	4:A:1241:ARG:HH21	1.55	0.55
5:B:258:LEU:HD11	5:B:267:ARG:HB3	1.88	0.55
6:C:167:HIS:CD2	13:L:70:ARG:HB3	2.41	0.55
4:A:1116:LEU:HB2	4:A:1311:VAL:HG22	1.88	0.55
6:C:46:ILE:HA	6:C:159:ALA:HA	1.88	0.55
6:C:94:LYS:HA	6:C:127:ARG:NH2	2.19	0.55
7:E:178:ILE:HG23	7:E:214:CYS:HA	1.89	0.55
4:A:303:TYR:CE1	4:A:325:ILE:HD11	2.42	0.54
4:A:528:LEU:O	4:A:531:ILE:HG22	2.08	0.54
4:A:684:ALA:O	4:A:688:LYS:HG2	2.07	0.54
5:B:384:ARG:HA	5:B:387:LEU:HD12	1.89	0.54
4:A:1013:ASP:HB3	7:E:207:ARG:HB3	1.88	0.54
4:A:1212:VAL:O	4:A:1216:ILE:HG13	2.07	0.54
5:B:281:PRO:HD2	5:B:284:ILE:HD12	1.89	0.54
5:B:955:THR:HB	13:L:55:ILE:HA	1.88	0.54
5:B:101:MET:HE2	5:B:109:THR:HG21	1.89	0.54
5:B:830:TYR:H	5:B:834:ASN:HD21	1.56	0.54
5:B:1135:ARG:O	5:B:1139:ILE:HG13	2.07	0.54
3:N:2:DC:H2"	3:N:3:DA:H5"	1.90	0.54
4:A:117:GLU:HG2	4:A:122:MET:CE	2.37	0.54
4:A:803:SER:HB3	4:A:806:ARG:HG3	1.90	0.54
4:A:1161:THR:OG1	4:A:1167:GLU:HG2	2.08	0.54
7:E:67:GLU:CD	7:E:67:GLU:H	2.15	0.54
10:I:75:CYS:HB3	10:I:78:CYS:SG	2.47	0.54
10:I:75:CYS:SG	10:I:77:LYS:N	2.78	0.54
4:A:450:LEU:HA	4:A:838:GLN:HE21	1.72	0.54
4:A:774:ARG:CZ	4:A:797:LYS:HG3	2.37	0.54
4:A:1154:TYR:HB2	4:A:1191:TRP:CE3	2.42	0.54
5:B:405:ARG:NH1	5:B:632:ARG:HB3	2.22	0.54
5:B:889:THR:OG1	5:B:909:ASP:OD1	2.23	0.54
4:A:109:HIS:CG	4:A:169:ASN:HB3	2.43	0.54
4:A:523:ILE:HB	4:A:622:VAL:HG22	1.90	0.54
4:A:1189:SER:HB3	4:A:1242:VAL:HB	1.87	0.54
4:A:1329:THR:HB	4:A:1335:ILE:HG12	1.89	0.54
4:A:1426:GLU:O	4:A:1430:LEU:HG	2.07	0.54
9:H:118:PHE:CE2	9:H:142:LEU:HD12	2.42	0.54
12:K:90:ALA:O	12:K:94:ILE:HG13	2.07	0.54
13:L:39:SER:C	13:L:44:ASP:OD2	2.50	0.54
4:A:120:GLU:HB2	4:A:123:ARG:HH21	1.72	0.54
4:A:262:LEU:O	4:A:266:LEU:HG	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:739:ASP:N	4:A:739:ASP:OD1	2.40	0.54
5:B:857:ARG:HG2	5:B:859:TYR:CZ	2.42	0.54
6:C:148:ARG:HB3	6:C:151:GLN:CD	2.33	0.54
7:E:37:LEU:HD12	7:E:38:PRO:HD2	1.89	0.54
4:A:1341:ILE:HG13	4:A:1376:THR:HG23	1.90	0.54
2:T:17:DG:P	4:A:330:LYS:HZ1	2.30	0.54
4:A:438:ASP:HA	4:A:460:VAL:HG12	1.89	0.54
5:B:545:ILE:HG23	5:B:631:GLY:HA2	1.90	0.54
5:B:1181:GLU:N	5:B:1181:GLU:OE1	2.41	0.54
6:C:92:CYS:SG	6:C:94:LYS:HG3	2.47	0.54
4:A:183:GLY:O	4:A:199:LEU:N	2.41	0.54
4:A:367:PRO:HG2	4:A:370:ILE:HD12	1.90	0.54
4:A:741:ASN:OD1	4:A:744:LYS:HB2	2.07	0.54
4:A:1122:PRO:HD3	4:A:1323:ASP:HB2	1.88	0.54
4:A:1279:ILE:HG21	4:A:1282:VAL:HG13	1.90	0.54
4:A:1291:VAL:HG22	4:A:1292:PRO:HD2	1.89	0.54
5:B:854:LEU:HD12	5:B:854:LEU:H	1.72	0.54
6:C:6:PRO:HB2	12:K:101:LEU:HD12	1.89	0.54
8:F:101:ILE:HB	8:F:117:PRO:HB3	1.90	0.54
10:I:5:ARG:HB3	10:I:14:LEU:HD12	1.89	0.54
11:J:6:ARG:HG3	11:J:13:VAL:HA	1.88	0.54
11:J:21:TYR:HB2	11:J:39:LEU:HD11	1.90	0.54
12:K:20:LYS:NZ	12:K:22:ASP:HB2	2.23	0.54
12:K:58:PHE:O	12:K:75:ILE:HA	2.08	0.54
4:A:230:ARG:HG3	4:A:233:TRP:CD2	2.43	0.53
4:A:527:THR:O	4:A:653:VAL:HG11	2.08	0.53
5:B:120:ARG:HB3	5:B:122:LEU:HD13	1.90	0.53
11:J:28:ASP:HB2	11:J:30:LEU:HG	1.89	0.53
4:A:1166:ASP:O	4:A:1170:ILE:HG12	2.08	0.53
9:H:47:PHE:HB2	9:H:95:TYR:CD2	2.43	0.53
4:A:1191:TRP:HZ3	10:I:43:VAL:HG13	1.73	0.53
5:B:288:ALA:O	5:B:327:ARG:NH2	2.40	0.53
5:B:754:SER:HB2	5:B:812:LEU:HD11	1.91	0.53
5:B:835:GLN:O	5:B:838:SER:OG	2.26	0.53
5:B:864:LYS:H	5:B:872:GLU:HB2	1.72	0.53
7:E:79:TRP:HB2	7:E:105:PHE:HD2	1.72	0.53
4:A:172:PRO:HB3	4:A:185:TRP:CG	2.43	0.53
4:A:361:LEU:HA	4:A:471:ASN:HB2	1.88	0.53
5:B:878:GLN:HE22	5:B:880:THR:HG23	1.72	0.53
7:E:64:PRO:HB3	7:E:76:GLY:HA2	1.90	0.53
11:J:8:PHE:H	11:J:49:MET:HE3	1.72	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:383:TYR:HD2	8:F:115:THR:HG1	1.55	0.53
5:B:899:ILE:HD11	5:B:905:VAL:HG11	1.89	0.53
5:B:1159:ARG:HD3	5:B:1161:HIS:CE1	2.43	0.53
6:C:195:GLN:HB2	6:C:199:LYS:HZ3	1.74	0.53
6:C:254:LYS:HE3	12:K:42:LEU:HD22	1.90	0.53
4:A:328:ARG:HD3	4:A:335:ARG:HH12	1.72	0.53
7:E:69:ILE:HA	7:E:72:PHE:O	2.07	0.53
4:A:30:ILE:HG23	5:B:1170:THR:HG23	1.89	0.53
4:A:472:LEU:HD13	5:B:835:GLN:OE1	2.09	0.53
4:A:218:ASP:O	4:A:222:LEU:HG	2.09	0.53
4:A:374:LEU:HA	5:B:1107:ALA:HB2	1.90	0.53
4:A:452:LYS:N	4:A:1070:GLN:OE1	2.41	0.53
4:A:942:PHE:O	4:A:946:VAL:HG23	2.09	0.53
4:A:1188:GLN:HE22	4:A:1241:ARG:NH1	2.06	0.53
5:B:37:PHE:O	5:B:41:LYS:HG2	2.08	0.53
5:B:175:ARG:HG2	5:B:200:GLY:HA3	1.90	0.53
5:B:796:LEU:HD23	5:B:799:PRO:HA	1.91	0.53
4:A:91:PHE:CD1	4:A:96:ILE:HD12	2.43	0.53
4:A:381:THR:H	4:A:384:ASN:HB3	1.74	0.53
4:A:666:ILE:HG22	5:B:1026:LEU:HB3	1.90	0.53
4:A:806:ARG:O	5:B:728:ARG:HG2	2.08	0.53
7:E:20:LYS:HD2	7:E:35:VAL:HA	1.90	0.53
4:A:23:SER:HB3	4:A:26:GLU:HB2	1.90	0.53
4:A:150:THR:HG22	4:A:167:CYS:H	1.74	0.53
4:A:606:LEU:O	4:A:613:ILE:N	2.42	0.53
5:B:915:THR:HB	5:B:934:LYS:HB3	1.90	0.53
7:E:79:TRP:HE1	7:E:96:PHE:HE1	1.56	0.53
4:A:180:LYS:NZ	4:A:202:LEU:O	2.35	0.52
4:A:442:VAL:HG21	4:A:489:LEU:HD11	1.91	0.52
5:B:566:LEU:HD11	5:B:586:TRP:CD2	2.44	0.52
10:I:17:ARG:HG2	10:I:28:GLU:OE2	2.08	0.52
2:T:14:DG:H2''	2:T:15:DC:H5'	1.91	0.52
4:A:140:THR:HA	4:A:143:LYS:HE2	1.91	0.52
4:A:445:ASN:C	4:A:487:MET:HE3	2.35	0.52
4:A:524:VAL:O	4:A:527:THR:OG1	2.25	0.52
4:A:635:ARG:NH2	4:A:877:HIS:H	2.06	0.52
4:A:820:GLY:O	4:A:824:LEU:HG	2.08	0.52
5:B:390:LEU:HD13	5:B:392:ARG:NH2	2.23	0.52
4:A:219:PHE:HD2	4:A:226:GLU:HB2	1.75	0.52
4:A:372:LYS:HA	4:A:435:HIS:CD2	2.45	0.52
4:A:1346:ALA:O	4:A:1350:LYS:HG2	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:1180:PHE:HD2	5:B:1191:ILE:HG21	1.74	0.52
6:C:10:ILE:HG12	6:C:20:PHE:HB3	1.91	0.52
9:H:93:TYR:CD2	9:H:145:ARG:HB2	2.44	0.52
4:A:18:GLN:HE22	4:A:1416:ALA:HB1	1.75	0.52
4:A:715:GLU:OE2	4:A:774:ARG:NH2	2.39	0.52
6:C:163:ILE:HG22	6:C:166:GLU:HG3	1.91	0.52
8:F:119:ARG:HA	8:F:122:MET:HE2	1.92	0.52
9:H:37:LYS:O	9:H:125:LEU:HA	2.09	0.52
4:A:1400:CYS:HB2	4:A:1405:THR:HG23	1.91	0.52
5:B:745:PRO:HB2	5:B:1047:PHE:CD2	2.44	0.52
6:C:71:PRO:HB2	6:C:133:ILE:HD13	1.91	0.52
6:C:242:GLN:O	6:C:246:ARG:HG3	2.09	0.52
9:H:17:PRO:HA	9:H:24:CYS:SG	2.49	0.52
10:I:54:GLU:HB2	10:I:100:PHE:CE2	2.44	0.52
12:K:84:LYS:O	12:K:88:LYS:HG2	2.08	0.52
4:A:243:PRO:HB2	4:A:245:PRO:HD2	1.92	0.52
5:B:476:ARG:HB2	5:B:479:VAL:HG22	1.92	0.52
10:I:50:THR:HB	10:I:52:ILE:HG22	1.92	0.52
5:B:566:LEU:HD11	5:B:586:TRP:CG	2.45	0.52
5:B:899:ILE:O	13:L:58:LYS:HD2	2.10	0.52
5:B:1189:ILE:HD12	5:B:1190:ASP:N	2.25	0.52
8:F:136:ARG:HH21	8:F:151:LEU:HD22	1.74	0.52
4:A:667:GLY:O	4:A:670:ILE:HG22	2.10	0.52
7:E:93:MET:SD	7:E:112:TYR:OH	2.63	0.52
7:E:120:ALA:O	7:E:124:VAL:HG23	2.09	0.52
12:K:20:LYS:C	12:K:20:LYS:HD2	2.35	0.52
2:T:9:DC:C6	2:T:10:DT:H72	2.45	0.51
4:A:818:MET:HG2	5:B:514:LEU:HB3	1.91	0.51
4:A:1166:ASP:HB3	4:A:1239:ARG:HE	1.76	0.51
4:A:1207:LEU:HG	4:A:1274:ARG:NH2	2.25	0.51
4:A:1311:VAL:HG21	4:A:1329:THR:HG23	1.93	0.51
5:B:597:MET:HE3	5:B:617:ARG:HB2	1.90	0.51
4:A:86:LEU:HD11	4:A:90:VAL:HG22	1.91	0.51
4:A:578:LEU:O	4:A:582:ILE:HG13	2.10	0.51
4:A:1066:VAL:HG12	4:A:1070:GLN:HE21	1.74	0.51
9:H:5:LEU:HD12	9:H:135:LEU:HD23	1.92	0.51
9:H:80:ARG:HH11	9:H:83:GLN:HE22	1.56	0.51
9:H:80:ARG:HH11	9:H:83:GLN:NE2	2.09	0.51
4:A:1213:GLY:HA2	4:A:1216:ILE:HD12	1.92	0.51
4:A:1268:LEU:HD13	10:I:48:LEU:HD11	1.93	0.51
4:A:1290:LYS:HA	4:A:1300:LYS:HA	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1313:LEU:HB3	4:A:1338:VAL:HG21	1.92	0.51
5:B:287:ARG:NH1	5:B:321:GLY:O	2.44	0.51
6:C:162:GLY:HA3	6:C:170:TRP:CE2	2.45	0.51
6:C:258:ILE:HG23	12:K:19:LEU:HD11	1.92	0.51
10:I:44:TYR:CE2	10:I:46:HIS:HB2	2.44	0.51
4:A:442:VAL:O	4:A:457:ALA:HA	2.10	0.51
5:B:806:THR:HB	5:B:809:MET:HG3	1.92	0.51
10:I:19:ASP:HB3	10:I:22:ASN:HB2	1.93	0.51
4:A:92:HIS:HB3	4:A:95:PHE:CD2	2.46	0.51
4:A:236:LEU:HD21	5:B:1211:ASN:HB2	1.92	0.51
4:A:383:TYR:OH	8:F:101:ILE:HG22	2.10	0.51
5:B:170:LEU:HD12	5:B:171:PRO:HD2	1.91	0.51
5:B:210:LYS:HE2	5:B:482:VAL:HG22	1.92	0.51
5:B:1171:VAL:HA	5:B:1182:CYS:HA	1.93	0.51
8:F:140:ASP:OD1	8:F:141:GLY:N	2.44	0.51
13:L:68:GLU:O	13:L:70:ARG:HG3	2.11	0.51
4:A:1035:TYR:CD2	4:A:1037:LEU:HB2	2.45	0.51
5:B:193:LYS:HE2	5:B:787:VAL:HG11	1.93	0.51
5:B:426:LYS:HG3	5:B:430:ARG:HE	1.76	0.51
5:B:948:ILE:HD13	6:C:61:GLU:OE2	2.11	0.51
7:E:13:TRP:NE1	7:E:37:LEU:O	2.44	0.51
10:I:10:CYS:HB3	10:I:32:CYS:SG	2.50	0.51
4:A:930:ASP:O	4:A:934:LYS:HG2	2.10	0.51
5:B:25:ILE:HG12	5:B:651:LEU:HD22	1.92	0.51
5:B:69:LEU:HD13	5:B:429:PHE:HD1	1.76	0.51
5:B:218:SER:OG	5:B:241:ARG:NH1	2.43	0.51
4:A:69:THR:HB	5:B:1172:ILE:HD11	1.91	0.51
4:A:138:ILE:O	4:A:142:CYS:HB2	2.10	0.51
4:A:513:SER:OG	4:A:515:GLN:O	2.19	0.51
4:A:690:VAL:HG11	4:A:794:PRO:HD3	1.93	0.51
4:A:845:LEU:HD22	4:A:1370:LEU:HD22	1.93	0.51
4:A:1143:LEU:HD23	4:A:1267:MET:HG2	1.93	0.51
5:B:400:HIS:NE2	5:B:699:GLU:OE2	2.44	0.51
5:B:953:LEU:O	5:B:964:VAL:HA	2.11	0.51
5:B:1004:GLU:HB2	5:B:1006:ILE:HD12	1.93	0.51
5:B:1065:GLN:HG2	5:B:1067:ARG:H	1.75	0.51
7:E:112:TYR:CD2	7:E:116:ILE:HG12	2.46	0.51
5:B:1082:MET:HA	6:C:189:THR:HA	1.92	0.51
8:F:93:ILE:HD12	8:F:132:LEU:HD13	1.93	0.51
1:R:4:G:H2'	1:R:5:A:H8	1.76	0.51
4:A:164:ARG:HD2	4:A:165:GLY:N	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1075:PRO:O	4:A:1079:MET:N	2.43	0.51
5:B:825:VAL:HG22	5:B:1010:LEU:HB3	1.93	0.51
7:E:61:GLN:HG3	7:E:62:ALA:N	2.26	0.51
9:H:39:THR:HB	9:H:124:ARG:HB3	1.93	0.51
4:A:519:PRO:O	4:A:624:SER:HB2	2.11	0.50
7:E:54:GLN:HB2	7:E:57:MET:CE	2.40	0.50
11:J:36:LEU:HA	11:J:39:LEU:HD12	1.92	0.50
4:A:666:ILE:HD11	5:B:1067:ARG:HA	1.93	0.50
7:E:62:ALA:HB3	7:E:78:LEU:HB3	1.93	0.50
4:A:7:SER:HB2	5:B:1159:ARG:NH1	2.26	0.50
4:A:65:LEU:HD21	4:A:66:LYS:HZ2	1.75	0.50
1:R:3:C:H2'	1:R:4:G:C8	2.46	0.50
4:A:404:TYR:HD1	4:A:414:ASP:HA	1.75	0.50
4:A:418:SER:HB3	4:A:421:ALA:HB2	1.94	0.50
5:B:122:LEU:HD11	5:B:957:ASN:HB2	1.94	0.50
5:B:770:GLN:HA	5:B:773:MET:HE2	1.92	0.50
5:B:1054:GLY:O	5:B:1058:LEU:HG	2.10	0.50
9:H:56:THR:HB	9:H:145:ARG:HB3	1.94	0.50
12:K:56:VAL:HA	12:K:77:THR:HA	1.91	0.50
4:A:687:LYS:NZ	4:A:795:GLU:OE1	2.43	0.50
10:I:100:PHE:CD1	10:I:111:THR:HG23	2.47	0.50
4:A:209:ASN:O	4:A:213:HIS:ND1	2.45	0.50
4:A:385:ILE:O	4:A:389:THR:HG23	2.12	0.50
4:A:464:PRO:HB2	12:K:4:PRO:HD3	1.94	0.50
4:A:1079:MET:SD	4:A:1359:ASP:HB2	2.52	0.50
5:B:345:LYS:HE3	5:B:348:ARG:HD3	1.93	0.50
5:B:620:ARG:HH12	10:I:68:LEU:HD21	1.77	0.50
5:B:1165:ILE:HB	5:B:1185:CYS:SG	2.51	0.50
5:B:1169:MET:HG2	5:B:1208:MET:HE1	1.92	0.50
4:A:88:LYS:HZ1	4:A:205:GLU:H	1.59	0.50
4:A:344:ARG:HB2	5:B:1118:PRO:HB2	1.93	0.50
4:A:963:ILE:HD12	4:A:1049:ILE:HG12	1.93	0.50
5:B:69:LEU:HD13	5:B:429:PHE:CD1	2.46	0.50
5:B:1002:THR:HG23	5:B:1005:GLY:H	1.77	0.50
9:H:105:GLU:O	9:H:113:ALA:N	2.38	0.50
12:K:55:LYS:HB3	12:K:78:THR:CG2	2.42	0.50
4:A:483:ASP:O	5:B:989:THR:HG23	2.11	0.50
4:A:671:ALA:HB3	4:A:676:MET:HE2	1.94	0.50
4:A:924:LYS:O	4:A:927:VAL:HG22	2.11	0.50
5:B:282:ILE:HA	5:B:285:ILE:HD12	1.93	0.50
5:B:409:ALA:HA	5:B:412:LEU:HD12	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:425:THR:HA	5:B:428:ILE:HD12	1.93	0.50
5:B:428:ILE:O	5:B:432:MET:HG2	2.12	0.50
5:B:824:ILE:HG12	11:J:48:ARG:NH1	2.27	0.50
4:A:854:ASN:HB2	4:A:1000:LEU:HD11	1.93	0.50
4:A:913:LEU:HD22	4:A:915:SER:H	1.75	0.50
5:B:807:ARG:HG2	5:B:1045:SER:HB2	1.94	0.50
5:B:1170:THR:HB	5:B:1182:CYS:SG	2.52	0.50
9:H:6:PHE:HB2	9:H:133:ASN:HB3	1.94	0.50
4:A:108:MET:H	4:A:171:GLN:CD	2.17	0.49
4:A:404:TYR:HA	4:A:415:LEU:HD23	1.93	0.49
6:C:10:ILE:HD11	12:K:105:PHE:CE2	2.47	0.49
9:H:93:TYR:CD2	9:H:143:LEU:HB3	2.47	0.49
4:A:523:ILE:HG23	4:A:527:THR:OG1	2.13	0.49
4:A:567:LYS:HG2	9:H:93:TYR:O	2.12	0.49
4:A:761:MET:HG3	5:B:1021:MET:HE3	1.94	0.49
4:A:800:VAL:HG13	4:A:812:GLU:CD	2.37	0.49
4:A:845:LEU:HD12	4:A:1069:ALA:HB2	1.94	0.49
4:A:1191:TRP:CD1	4:A:1191:TRP:H	2.31	0.49
5:B:380:TYR:O	5:B:384:ARG:HG2	2.12	0.49
5:B:635:ARG:HG3	5:B:637:LEU:HD11	1.93	0.49
5:B:661:LEU:HG	5:B:679:TYR:CD2	2.47	0.49
12:K:55:LYS:HB2	12:K:81:TYR:CD2	2.48	0.49
4:A:537:ARG:HG2	9:H:121:LEU:HD23	1.94	0.49
5:B:286:PHE:HA	5:B:289:LEU:HD12	1.93	0.49
5:B:637:LEU:HD13	5:B:693:ILE:HD13	1.94	0.49
4:A:1239:ARG:HH12	4:A:1241:ARG:NE	2.10	0.49
5:B:294:ASP:HA	5:B:297:ILE:HD12	1.94	0.49
9:H:114:VAL:HG21	9:H:134:ASN:CG	2.38	0.49
10:I:78:CYS:HB3	10:I:105:SER:O	2.13	0.49
4:A:474:VAL:O	4:A:478:TYR:HD2	1.95	0.49
4:A:537:ARG:HH12	9:H:122:LEU:HD12	1.76	0.49
4:A:846:GLU:HA	4:A:1066:VAL:HG22	1.95	0.49
4:A:939:ASP:O	4:A:943:LEU:HG	2.13	0.49
4:A:1257:ASP:OD2	4:A:1261:LYS:NZ	2.36	0.49
8:F:135:ARG:NH1	8:F:145:ASP:OD1	2.46	0.49
9:H:19:ARG:HG2	9:H:19:ARG:HH11	1.77	0.49
4:A:1224:LEU:HD21	4:A:1240:CYS:CB	2.40	0.49
5:B:43:LEU:HG	5:B:496:ARG:HE	1.78	0.49
6:C:80:LEU:HG	6:C:94:LYS:O	2.12	0.49
10:I:75:CYS:HB2	10:I:110:PHE:CG	2.48	0.49
4:A:5:GLN:HG2	5:B:1175:LEU:HD22	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:528:LEU:HG	4:A:749:ALA:HB1	1.94	0.49
4:A:744:LYS:O	4:A:748:MET:HG3	2.13	0.49
5:B:349:ILE:O	5:B:353:LYS:HG3	2.13	0.49
6:C:4:GLU:OE2	6:C:5:GLY:N	2.45	0.49
7:E:151:PRO:HD2	7:E:153:HIS:HE1	1.78	0.49
4:A:67:CYS:SG	4:A:77:CYS:HB2	2.52	0.49
4:A:99:ILE:HG23	4:A:211:PHE:CZ	2.48	0.49
4:A:328:ARG:HD2	5:B:1206:GLU:OE1	2.13	0.49
4:A:898:ARG:HH22	4:A:929:LEU:HB3	1.76	0.49
5:B:312:GLU:HA	5:B:315:LYS:HD3	1.95	0.49
5:B:788:ARG:O	5:B:967:ARG:NH1	2.46	0.49
5:B:1016:ALA:O	5:B:1020:ARG:HG3	2.13	0.49
4:A:25:GLU:CD	4:A:25:GLU:H	2.21	0.49
4:A:399:HIS:HD2	4:A:435:HIS:HB3	1.78	0.49
4:A:506:ALA:HB1	4:A:508:PRO:HD2	1.94	0.49
4:A:1045:VAL:O	4:A:1049:ILE:HG13	2.12	0.49
4:A:1060:PRO:HD2	8:F:86:THR:HG22	1.95	0.49
4:A:1446:ASP:HB2	8:F:131:PRO:HB2	1.94	0.49
5:B:841:MET:HE2	5:B:990:ILE:HG21	1.94	0.49
5:B:954:VAL:HA	5:B:963:PHE:O	2.13	0.49
6:C:162:GLY:HA3	6:C:170:TRP:CD2	2.48	0.49
10:I:54:GLU:HG2	10:I:55:THR:HG23	1.95	0.49
12:K:42:LEU:HG	12:K:46:ILE:HD11	1.95	0.49
13:L:30:ILE:HA	13:L:37:LYS:HA	1.94	0.49
4:A:356:ASP:CG	12:K:65:HIS:HE2	2.21	0.48
4:A:445:ASN:OD1	4:A:455:MET:HG2	2.13	0.48
4:A:586:ILE:HD13	4:A:633:VAL:HG22	1.95	0.48
4:A:1329:THR:H	4:A:1335:ILE:HD11	1.77	0.48
4:A:1438:THR:HA	4:A:1441:PHE:CZ	2.48	0.48
9:H:86:ASP:OD1	9:H:87:ARG:NH2	2.37	0.48
10:I:83:ASN:HA	10:I:104:LEU:HD23	1.95	0.48
4:A:230:ARG:HG3	4:A:233:TRP:CE2	2.48	0.48
4:A:353:ILE:HG22	4:A:468:PHE:HB2	1.95	0.48
4:A:368:LYS:O	4:A:372:LYS:HG3	2.13	0.48
4:A:456:MET:HE3	4:A:507:VAL:HG13	1.94	0.48
4:A:1105:LEU:HB3	4:A:1384:VAL:HG21	1.94	0.48
5:B:453:ILE:O	5:B:457:LEU:HG	2.13	0.48
5:B:586:TRP:CD1	5:B:588:GLY:H	2.31	0.48
5:B:680:THR:HG23	5:B:683:SER:N	2.27	0.48
16:B:1302:ATP:H2'	16:B:1302:ATP:O1A	2.13	0.48
13:L:40:LEU:N	13:L:44:ASP:OD2	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:3:C:H2'	1:R:4:G:H8	1.77	0.48
4:A:67:CYS:CB	4:A:70:CYS:HB2	2.42	0.48
4:A:97:ALA:O	4:A:101:LYS:HG2	2.13	0.48
4:A:1001:ARG:HH11	8:F:83:PRO:HD2	1.78	0.48
7:E:42:PHE:CE1	7:E:58:MET:HE1	2.45	0.48
4:A:135:PHE:CD1	4:A:222:LEU:HA	2.48	0.48
5:B:640:VAL:HG11	5:B:710:LEU:HD13	1.95	0.48
5:B:1162:ILE:O	5:B:1192:TYR:HB2	2.12	0.48
7:E:180:ARG:HH21	7:E:192:ARG:HD2	1.78	0.48
4:A:43:GLU:HG2	4:A:44:THR:HG23	1.94	0.48
4:A:1027:ALA:HB3	4:A:1030:ARG:HB2	1.95	0.48
4:A:1363:VAL:HB	4:A:1368:MET:HE3	1.95	0.48
5:B:544:CYS:HB2	5:B:634:TYR:CE2	2.48	0.48
5:B:953:LEU:HD21	13:L:55:ILE:HG22	1.95	0.48
6:C:175:ALA:HB2	11:J:43:ARG:NH1	2.29	0.48
7:E:54:GLN:O	7:E:58:MET:HG2	2.14	0.48
4:A:932:GLU:O	4:A:936:LEU:HG	2.14	0.48
6:C:52:GLU:HB3	6:C:154:LYS:HB2	1.96	0.48
10:I:6:PHE:O	10:I:8:ARG:NH2	2.46	0.48
4:A:14:VAL:HA	5:B:1218:THR:HA	1.95	0.48
4:A:388:LEU:O	4:A:392:VAL:HG23	2.14	0.48
4:A:761:MET:HA	4:A:804:TYR:HB2	1.94	0.48
4:A:1239:ARG:NH1	4:A:1241:ARG:HE	2.11	0.48
4:A:1390:ASN:HD21	4:A:1403:GLU:H	1.62	0.48
6:C:108:GLU:HA	6:C:149:LYS:HD2	1.96	0.48
6:C:167:HIS:HA	12:K:6:ARG:HH21	1.79	0.48
7:E:166:LYS:HE3	7:E:167:ARG:HD3	1.95	0.48
4:A:446:ARG:HD2	4:A:478:TYR:O	2.14	0.48
4:A:741:ASN:HA	6:C:192:TRP:HE1	1.78	0.48
4:A:951:GLU:O	4:A:954:TRP:NE1	2.47	0.48
4:A:961:ARG:HB3	4:A:1025:ARG:HH12	1.78	0.48
4:A:992:ASP:O	4:A:996:ASN:ND2	2.46	0.48
5:B:31:TRP:CH2	5:B:807:ARG:HB2	2.49	0.48
5:B:903:VAL:HG12	5:B:905:VAL:HG13	1.96	0.48
5:B:1174:LYS:HD3	5:B:1177:HIS:CD2	2.49	0.48
6:C:10:ILE:H	12:K:108:GLU:CD	2.22	0.48
7:E:180:ARG:HE	7:E:192:ARG:HB3	1.79	0.48
2:T:17:DG:H2'	2:T:18:DA:C4	2.49	0.48
4:A:679:ILE:O	4:A:683:ILE:HG12	2.14	0.48
4:A:726:ARG:HG3	4:A:727:ASP:N	2.28	0.48
4:A:901:LEU:HD13	4:A:919:ILE:HG13	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1209:MET:SD	4:A:1236:LEU:HB3	2.54	0.48
5:B:861:ASP:HB3	5:B:912:ILE:HG21	1.96	0.48
4:A:544:ASP:HB2	12:K:47:ARG:HH22	1.78	0.48
4:A:546:VAL:O	4:A:550:LEU:HD13	2.14	0.48
4:A:1161:THR:H	4:A:1167:GLU:CD	2.22	0.48
6:C:62:PHE:O	6:C:66:ARG:HG3	2.14	0.48
6:C:101:LEU:HB2	6:C:118:LEU:CD2	2.44	0.48
7:E:11:ARG:HD2	7:E:141:VAL:HG21	1.95	0.48
8:F:127:GLU:CB	8:F:129:LYS:HG2	2.44	0.48
2:T:12:DT:H2'	2:T:13:DC:C6	2.49	0.47
4:A:446:ARG:HG3	4:A:480:ALA:HB2	1.96	0.47
4:A:666:ILE:HG13	4:A:667:GLY:N	2.28	0.47
4:A:1100:ARG:HE	4:A:1104:ILE:HD11	1.79	0.47
4:A:1315:GLU:OE1	4:A:1315:GLU:N	2.47	0.47
4:A:1444:MET:HE3	4:A:1444:MET:HA	1.96	0.47
5:B:276:ILE:HG23	5:B:335:GLY:HA2	1.95	0.47
5:B:382:ILE:O	5:B:386:LEU:HD23	2.14	0.47
5:B:986:GLN:HB3	5:B:1020:ARG:CD	2.44	0.47
6:C:91:HIS:HB3	6:C:96:SER:OG	2.14	0.47
4:A:340:LEU:HD21	5:B:1200:ALA:N	2.29	0.47
4:A:961:ARG:O	4:A:965:GLN:HG3	2.14	0.47
5:B:564:GLU:O	5:B:588:GLY:HA3	2.15	0.47
4:A:597:LEU:HB3	9:H:102:TYR:HE2	1.79	0.47
4:A:737:LEU:O	4:A:744:LYS:NZ	2.40	0.47
4:A:899:VAL:HG21	4:A:908:LEU:HG	1.96	0.47
5:B:46:GLN:OE1	5:B:47:GLN:N	2.47	0.47
5:B:186:GLU:OE1	5:B:187:SER:N	2.46	0.47
5:B:393:LYS:HA	5:B:393:LYS:HD3	1.67	0.47
11:J:36:LEU:HD11	11:J:51:LEU:HD11	1.95	0.47
3:N:7:DA:C6	3:N:8:DG:C6	3.02	0.47
4:A:216:VAL:O	4:A:220:THR:HG23	2.14	0.47
5:B:28:GLU:OE1	5:B:807:ARG:NH1	2.48	0.47
5:B:483:LEU:CD2	5:B:491:THR:HG23	2.41	0.47
5:B:1116:ARG:HG3	5:B:1198:TYR:CG	2.49	0.47
12:K:45:LEU:HD12	12:K:45:LEU:HA	1.45	0.47
4:A:108:MET:HG3	4:A:109:HIS:CD2	2.48	0.47
4:A:1340:GLY:HA2	7:E:183:PRO:HD2	1.96	0.47
5:B:405:ARG:HH11	5:B:632:ARG:HB3	1.80	0.47
7:E:52:ARG:HA	7:E:52:ARG:NE	2.30	0.47
7:E:93:MET:HE1	7:E:132:ILE:HG21	1.95	0.47
10:I:56:ALA:HB3	10:I:89:GLN:HG3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:22:PHE:CD2	5:B:1213:THR:HG22	2.49	0.47
4:A:231:PRO:HA	4:A:234:MET:HE2	1.97	0.47
4:A:353:ILE:HG21	4:A:487:MET:HB2	1.96	0.47
4:A:626:ASN:HD21	4:A:879:GLU:HA	1.78	0.47
4:A:929:LEU:HD21	4:A:983:ILE:HG23	1.96	0.47
4:A:1035:TYR:HE2	4:A:1037:LEU:HD22	1.79	0.47
5:B:314:LEU:O	5:B:318:VAL:HG23	2.13	0.47
5:B:351:TYR:CZ	5:B:355:ILE:HD11	2.50	0.47
4:A:353:ILE:HD13	4:A:487:MET:SD	2.55	0.47
4:A:535:THR:HG21	4:A:617:VAL:HG23	1.96	0.47
4:A:687:LYS:NZ	4:A:794:PRO:HG2	2.30	0.47
4:A:827:THR:O	4:A:831:THR:HG23	2.14	0.47
4:A:899:VAL:HG23	4:A:906:HIS:O	2.14	0.47
4:A:975:HIS:HA	4:A:1036:ARG:HG2	1.95	0.47
4:A:997:LEU:O	4:A:1011:GLN:NE2	2.46	0.47
4:A:1051:ALA:HA	4:A:1054:LEU:HD12	1.97	0.47
4:A:1336:MET:HG3	4:A:1341:ILE:HA	1.96	0.47
5:B:322:PHE:CE1	10:I:13:MET:HG2	2.50	0.47
5:B:349:ILE:HG22	5:B:353:LYS:HE3	1.95	0.47
5:B:851:PHE:CD1	5:B:1094:ARG:HB2	2.49	0.47
5:B:957:ASN:ND2	5:B:959:ASP:H	2.13	0.47
6:C:244:VAL:HG11	12:K:105:PHE:CZ	2.50	0.47
8:F:148:VAL:HA	8:F:151:LEU:HD12	1.96	0.47
10:I:58:VAL:HA	10:I:62:ILE:HD12	1.97	0.47
10:I:101:PHE:HE1	10:I:112:SER:HB3	1.78	0.47
11:J:43:ARG:HB3	11:J:45:CYS:SG	2.54	0.47
2:T:12:DT:O2	3:N:8:DG:N2	2.47	0.47
4:A:787:PHE:CE2	4:A:796:SER:HA	2.50	0.47
4:A:1288:ASP:CG	4:A:1300:LYS:HD3	2.39	0.47
4:A:1355:VAL:O	4:A:1358:SER:OG	2.29	0.47
5:B:313:MET:HE3	5:B:313:MET:HB3	1.77	0.47
5:B:577:ALA:HB1	5:B:589:VAL:HB	1.96	0.47
5:B:1063:GLY:O	6:C:202:PRO:HG3	2.15	0.47
10:I:6:PHE:CD2	10:I:13:MET:HA	2.50	0.47
1:R:7:A:H2'	1:R:8:G:H8	1.80	0.47
4:A:172:PRO:HG3	4:A:185:TRP:CE2	2.50	0.47
4:A:531:ILE:O	4:A:535:THR:OG1	2.31	0.47
4:A:587:HIS:CE1	4:A:969:GLN:HG2	2.50	0.47
4:A:1198:ASP:OD2	4:A:1201:ALA:N	2.45	0.47
5:B:115:GLN:HG2	5:B:193:LYS:HB2	1.96	0.47
5:B:792:MET:HG2	5:B:857:ARG:HD3	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:82:TYR:CD1	6:C:161:LYS:HB3	2.50	0.47
3:N:8:DG:C6	3:N:9:DA:C6	3.03	0.47
4:A:202:LEU:HB3	4:A:207:ILE:HD11	1.96	0.47
4:A:267:ALA:O	4:A:271:LYS:HG3	2.14	0.47
5:B:51:PHE:O	5:B:55:VAL:HG23	2.15	0.47
5:B:243:ALA:HB2	5:B:251:ILE:HD13	1.96	0.47
5:B:806:THR:HG23	5:B:1045:SER:HA	1.95	0.47
5:B:862:GLN:O	5:B:914:LYS:HE2	2.14	0.47
6:C:144:ILE:HD12	6:C:144:ILE:H	1.80	0.47
3:N:6:DG:C6	3:N:7:DA:C6	3.03	0.46
4:A:125:ALA:O	4:A:134:ARG:HG3	2.14	0.46
4:A:537:ARG:H	4:A:537:ARG:HD3	1.80	0.46
4:A:687:LYS:HZ2	4:A:794:PRO:HG2	1.79	0.46
4:A:1169:ILE:HA	4:A:1172:LEU:HD12	1.97	0.46
4:A:1282:VAL:HA	4:A:1307:GLU:O	2.15	0.46
5:B:234:ILE:HD12	5:B:237:VAL:HG23	1.97	0.46
5:B:236:HIS:CE1	5:B:389:ALA:HA	2.49	0.46
4:A:122:MET:HE3	4:A:123:ARG:N	2.30	0.46
4:A:873:MET:HE3	4:A:1056:SER:HB3	1.97	0.46
4:A:961:ARG:HB3	4:A:1025:ARG:NH1	2.31	0.46
4:A:994:GLN:NE2	4:A:1023:ARG:HE	2.12	0.46
4:A:1099:PRO:O	4:A:1103:GLU:HG3	2.16	0.46
4:A:1221:LYS:NZ	4:A:1223:ASP:OD1	2.48	0.46
5:B:60:GLN:HA	5:B:60:GLN:OE1	2.16	0.46
5:B:384:ARG:HH22	5:B:621:GLU:CD	2.23	0.46
6:C:254:LYS:HB3	12:K:42:LEU:HD22	1.98	0.46
4:A:526:ASP:HB2	5:B:835:GLN:NE2	2.31	0.46
5:B:54:PHE:HA	5:B:58:THR:HB	1.96	0.46
7:E:175:LEU:HD23	7:E:213:ILE:HB	1.98	0.46
2:T:13:DC:C2	2:T:14:DG:N7	2.83	0.46
2:T:14:DG:C6	3:N:4:DG:C6	3.03	0.46
4:A:1154:TYR:HA	4:A:1191:TRP:HA	1.98	0.46
5:B:1106:ARG:NH1	5:B:1118:PRO:HB3	2.30	0.46
13:L:38:LEU:HD12	13:L:39:SER:H	1.80	0.46
3:N:12:DG:H2"	3:N:13:DA:N7	2.30	0.46
4:A:128:ILE:HD12	4:A:134:ARG:HA	1.97	0.46
4:A:147:VAL:HG22	4:A:148:CYS:O	2.14	0.46
4:A:340:LEU:HD13	4:A:1429:ILE:HG23	1.97	0.46
4:A:849:MET:HE2	4:A:1063:MET:HE1	1.98	0.46
5:B:883:LEU:HB3	5:B:935:ARG:HG2	1.98	0.46
6:C:15:LYS:NZ	6:C:236:GLY:HA3	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:I:71:SER:HB3	10:I:83:ASN:OD1	2.16	0.46
4:A:388:LEU:HD13	4:A:391:LEU:HD12	1.97	0.46
4:A:420:ARG:HG2	4:A:424:ILE:HG22	1.96	0.46
4:A:856:THR:OG1	4:A:868:TYR:HB2	2.16	0.46
4:A:947:PHE:HB2	4:A:950:GLY:HA2	1.98	0.46
4:A:1055:ARG:NH2	8:F:154:ASP:OD2	2.49	0.46
5:B:745:PRO:O	5:B:748:ILE:HG12	2.16	0.46
7:E:79:TRP:HB2	7:E:105:PHE:CD2	2.51	0.46
9:H:5:LEU:O	9:H:133:ASN:HB3	2.15	0.46
9:H:42:ILE:HD12	9:H:42:ILE:HA	1.82	0.46
12:K:55:LYS:O	12:K:78:THR:N	2.47	0.46
4:A:92:HIS:CE1	4:A:94:GLY:H	2.34	0.46
4:A:405:VAL:HG23	4:A:415:LEU:HD21	1.98	0.46
4:A:665:GLY:HA3	5:B:1069:PHE:CZ	2.51	0.46
4:A:864:ILE:HG22	4:A:865:GLN:HG2	1.98	0.46
4:A:1034:GLU:HB2	4:A:1035:TYR:CD1	2.50	0.46
5:B:118:ARG:NH2	5:B:194:GLU:OE1	2.49	0.46
5:B:728:ARG:NH1	5:B:1047:PHE:HA	2.31	0.46
5:B:872:GLU:HB3	5:B:914:LYS:HD2	1.98	0.46
1:R:4:G:C2	2:T:26:DG:C2	3.04	0.46
4:A:150:THR:O	4:A:164:ARG:HB3	2.15	0.46
5:B:287:ARG:NH2	5:B:294:ASP:OD2	2.49	0.46
5:B:298:LEU:HD23	5:B:311:LEU:HD22	1.97	0.46
5:B:324:ILE:HD12	5:B:329:THR:HB	1.98	0.46
5:B:557:PHE:CZ	5:B:603:LEU:HD11	2.51	0.46
6:C:11:ARG:N	6:C:19:ASP:O	2.48	0.46
7:E:41:ASP:OD1	7:E:41:ASP:N	2.49	0.46
9:H:41:ASP:CG	9:H:122:LEU:H	2.24	0.46
2:T:22:DT:H2'	2:T:23:DC:C6	2.51	0.46
4:A:74:MET:HB3	4:A:74:MET:HE2	1.58	0.46
4:A:357:PRO:HG2	5:B:831:SER:O	2.16	0.46
4:A:369:SER:OG	12:K:2:ASN:ND2	2.49	0.46
4:A:512:VAL:HA	4:A:519:PRO:HA	1.98	0.46
4:A:844:ALA:HA	4:A:1389:PHE:CE1	2.51	0.46
4:A:1192:LEU:C	4:A:1260:LEU:HD21	2.41	0.46
6:C:32:SER:HA	12:K:41:THR:HG1	1.81	0.46
7:E:96:PHE:CZ	7:E:100:ILE:HD11	2.51	0.46
8:F:74:ILE:HG21	8:F:144:GLU:HB3	1.98	0.46
5:B:101:MET:O	5:B:169:ARG:NH1	2.49	0.46
6:C:181:ASP:CG	6:C:186:LEU:HB2	2.41	0.46
8:F:107:VAL:HG11	8:F:111:LEU:HD21	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:24:DT:OP1	5:B:1122:ARG:NH2	2.48	0.45
4:A:15:LYS:HG2	5:B:1218:THR:O	2.15	0.45
4:A:259:GLU:HB3	4:A:264:PHE:CE1	2.51	0.45
4:A:310:GLY:C	4:A:312:PRO:HD3	2.42	0.45
4:A:332:LYS:HA	4:A:337:ARG:HG2	1.98	0.45
4:A:374:LEU:HD13	4:A:491:VAL:HG21	1.98	0.45
4:A:814:PHE:CZ	5:B:514:LEU:HG	2.51	0.45
5:B:215:GLN:OE1	5:B:476:ARG:HD3	2.16	0.45
5:B:598:GLU:O	5:B:602:THR:HG23	2.16	0.45
5:B:640:VAL:HG12	5:B:649:LYS:HG2	1.97	0.45
5:B:879:ARG:HA	5:B:885:MET:SD	2.56	0.45
5:B:1025:HIS:CE1	5:B:1090:THR:HG21	2.50	0.45
6:C:77:ILE:N	6:C:129:ILE:HD11	2.31	0.45
4:A:381:THR:HA	8:F:104:ASN:ND2	2.30	0.45
4:A:443:LEU:O	4:A:489:LEU:HA	2.16	0.45
5:B:199:MET:SD	5:B:199:MET:N	2.88	0.45
5:B:360:PHE:CE2	5:B:374:LYS:HB3	2.52	0.45
5:B:650:GLU:HG3	5:B:651:LEU:HG	1.99	0.45
5:B:1019:SER:HG	16:B:1302:ATP:HO3'	1.58	0.45
10:I:58:VAL:HG21	10:I:109:ILE:HD11	1.99	0.45
4:A:24:PRO:HG3	4:A:236:LEU:HA	1.97	0.45
4:A:81:PHE:CZ	5:B:1208:MET:HB2	2.51	0.45
4:A:96:ILE:HA	4:A:99:ILE:HB	1.98	0.45
4:A:404:TYR:CD1	4:A:414:ASP:HA	2.51	0.45
4:A:620:LYS:HE2	4:A:620:LYS:HB2	1.59	0.45
5:B:468:GLU:N	5:B:468:GLU:OE1	2.49	0.45
10:I:10:CYS:SG	10:I:12:ASN:ND2	2.83	0.45
10:I:22:ASN:CG	10:I:24:ARG:HE	2.24	0.45
4:A:387:ARG:O	4:A:391:LEU:HG	2.16	0.45
4:A:579:SER:OG	4:A:612:ILE:HG22	2.16	0.45
4:A:916:GLY:O	4:A:919:ILE:HG22	2.16	0.45
4:A:1008:GLN:O	4:A:1012:ARG:HG3	2.17	0.45
4:A:1188:GLN:HA	4:A:1243:VAL:C	2.42	0.45
5:B:103:ASN:HA	5:B:109:THR:HA	1.99	0.45
5:B:1034:VAL:HG23	5:B:1059:LEU:HD13	1.99	0.45
6:C:147:LEU:HD22	6:C:151:GLN:HB3	1.99	0.45
7:E:168:TYR:HB3	7:E:170:LEU:HD23	1.97	0.45
9:H:47:PHE:HB2	9:H:95:TYR:CE2	2.51	0.45
13:L:38:LEU:HD23	13:L:40:LEU:O	2.16	0.45
4:A:80:HIS:CE1	5:B:1172:ILE:HG21	2.52	0.45
4:A:98:LYS:O	4:A:102:VAL:HG12	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1012:ARG:O	4:A:1016:THR:OG1	2.34	0.45
5:B:133:LYS:HE2	5:B:133:LYS:HA	1.99	0.45
5:B:446:LEU:HG	5:B:447:ALA:H	1.82	0.45
5:B:656:GLY:O	5:B:660:LYS:HG3	2.16	0.45
5:B:744:HIS:HB3	5:B:747:MET:HG2	1.99	0.45
5:B:801:LYS:N	11:J:52:THR:O	2.35	0.45
6:C:259:LEU:O	6:C:263:THR:HG23	2.16	0.45
4:A:185:TRP:HB2	4:A:199:LEU:HD12	1.99	0.45
4:A:685:GLU:O	4:A:689:LYS:HG2	2.16	0.45
4:A:1194:ARG:HG3	4:A:1237:ILE:HD11	1.98	0.45
5:B:576:ASP:HA	5:B:622:LYS:HZ3	1.82	0.45
5:B:579:ARG:HG2	5:B:586:TRP:CZ2	2.52	0.45
5:B:638:PHE:O	5:B:740:HIS:HB3	2.17	0.45
5:B:841:MET:HB3	5:B:846:ILE:HD11	1.98	0.45
6:C:17:ASN:HA	6:C:232:VAL:O	2.15	0.45
6:C:73:GLN:N	6:C:133:ILE:HD11	2.32	0.45
6:C:77:ILE:HD12	6:C:80:LEU:HB3	1.98	0.45
6:C:194:GLU:HG3	6:C:195:GLN:HG2	1.98	0.45
7:E:93:MET:HE1	7:E:96:PHE:HD2	1.81	0.45
13:L:40:LEU:HD23	13:L:42:ARG:H	1.81	0.45
4:A:82:GLY:HA3	4:A:241:VAL:HB	1.99	0.45
4:A:478:TYR:CE1	4:A:487:MET:HE1	2.52	0.45
4:A:1197:LEU:HD12	4:A:1209:MET:SD	2.57	0.45
5:B:499:ASN:HA	5:B:536:VAL:HG22	1.99	0.45
5:B:848:ARG:HB3	11:J:8:PHE:HD1	1.81	0.45
5:B:1060:ARG:HD3	5:B:1066:SER:HB3	1.99	0.45
5:B:1087:PHE:HD2	11:J:44:TYR:HH	1.64	0.45
4:A:24:PRO:HB3	4:A:238:CYS:N	2.31	0.45
4:A:219:PHE:HE2	4:A:230:ARG:HH21	1.64	0.45
4:A:1162:VAL:HG21	10:I:41:PRO:HG2	1.99	0.45
5:B:541:LEU:HD12	5:B:542:MET:N	2.31	0.45
5:B:953:LEU:HA	13:L:56:LEU:O	2.17	0.45
5:B:1060:ARG:HD3	5:B:1066:SER:H	1.82	0.45
5:B:1138:MET:HE2	5:B:1141:HIS:HD2	1.82	0.45
6:C:186:LEU:HB3	6:C:188:HIS:CD2	2.52	0.45
7:E:151:PRO:HB2	7:E:198:ILE:HG23	1.98	0.45
4:A:180:LYS:HD3	4:A:181:LEU:N	2.32	0.45
4:A:360:GLU:OE2	4:A:651:LYS:NZ	2.45	0.45
4:A:718:VAL:HA	4:A:721:PHE:CD2	2.51	0.45
5:B:363:HIS:CE1	5:B:364:ILE:HG12	2.51	0.45
5:B:483:LEU:HD23	5:B:484:ASN:N	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:758:PHE:HB2	5:B:1024:ALA:CB	2.46	0.45
5:B:881:ASN:HB3	5:B:934:LYS:HE2	1.98	0.45
5:B:1159:ARG:HG3	5:B:1193:GLN:HE21	1.82	0.45
6:C:90:ASP:C	6:C:91:HIS:CG	2.94	0.45
7:E:54:GLN:HB2	7:E:57:MET:HE2	1.98	0.45
10:I:54:GLU:HG2	10:I:55:THR:N	2.32	0.45
10:I:86:PHE:HE1	10:I:102:VAL:HG23	1.82	0.45
4:A:497:THR:HG21	5:B:1149:GLU:OE2	2.17	0.45
4:A:956:LEU:HD23	4:A:956:LEU:HA	1.78	0.45
4:A:1129:GLU:HA	4:A:1132:LYS:HD2	1.98	0.45
4:A:1312:ASN:O	4:A:1316:VAL:HG23	2.17	0.45
6:C:259:LEU:HD21	12:K:91:CYS:HB2	1.99	0.45
13:L:62:LYS:HE3	13:L:62:LYS:HA	1.99	0.45
4:A:243:PRO:HG2	4:A:246:VAL:HG23	1.99	0.44
5:B:104:GLU:HG2	5:B:110:HIS:CD2	2.53	0.44
5:B:426:LYS:NZ	5:B:430:ARG:HG2	2.31	0.44
5:B:816:GLU:OE1	5:B:816:GLU:N	2.49	0.44
6:C:46:ILE:HD12	6:C:72:LEU:HD11	1.98	0.44
6:C:60:ASP:HB2	13:L:67:PHE:HE2	1.82	0.44
7:E:147:HIS:CE1	7:E:149:LEU:HG	2.51	0.44
9:H:30:SER:CB	9:H:36:CYS:HB3	2.46	0.44
11:J:4:PRO:O	11:J:14:VAL:HG23	2.17	0.44
4:A:487:MET:HE2	4:A:487:MET:HB3	1.61	0.44
4:A:518:LYS:HB2	4:A:624:SER:O	2.17	0.44
4:A:569:LYS:HG3	4:A:570:PRO:HD2	1.98	0.44
4:A:842:VAL:HG11	5:B:1136:ASP:CG	2.42	0.44
5:B:860:MET:HA	5:B:964:VAL:O	2.18	0.44
7:E:168:TYR:CB	7:E:170:LEU:HD23	2.46	0.44
2:T:20:DC:H2"	2:T:21:DC:H6	1.82	0.44
4:A:450:LEU:HA	4:A:838:GLN:NE2	2.32	0.44
4:A:629:LEU:O	4:A:633:VAL:HG23	2.18	0.44
5:B:611:PRO:CG	5:B:685:LEU:HD21	2.47	0.44
5:B:1220:ARG:HD3	5:B:1220:ARG:C	2.42	0.44
4:A:102:VAL:O	4:A:106:VAL:HG12	2.17	0.44
4:A:880:LYS:HA	4:A:954:TRP:O	2.17	0.44
4:A:959:ASN:O	4:A:963:ILE:HG13	2.17	0.44
4:A:1018:PHE:CE1	4:A:1021:LEU:HD23	2.53	0.44
4:A:1216:ILE:HG22	4:A:1220:PHE:CE2	2.52	0.44
5:B:31:TRP:HA	5:B:34:ILE:HD12	1.99	0.44
5:B:833:TYR:O	5:B:838:SER:OG	2.29	0.44
6:C:91:HIS:ND1	6:C:158:VAL:HG11	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:163:ILE:HG21	12:K:10:PHE:CE1	2.53	0.44
7:E:64:PRO:HD3	7:E:77:SER:N	2.32	0.44
4:A:591:PHE:HD1	4:A:595:THR:HB	1.82	0.44
4:A:852:TYR:HB2	8:F:137:TYR:O	2.17	0.44
4:A:1020:CYS:HA	4:A:1023:ARG:HD2	2.00	0.44
4:A:1377:THR:O	7:E:212:ARG:NH2	2.51	0.44
5:B:217:ARG:HH12	5:B:405:ARG:HG2	1.81	0.44
5:B:259:TYR:OH	5:B:279:ASP:OD2	2.20	0.44
5:B:420:LEU:HD21	5:B:456:GLY:HA3	1.99	0.44
5:B:423:LYS:HD2	5:B:452:THR:HG21	1.99	0.44
5:B:554:ILE:O	5:B:558:LEU:HG	2.17	0.44
5:B:795:ILE:O	5:B:853:SER:HA	2.18	0.44
5:B:806:THR:HG23	5:B:1046:PRO:HD3	1.99	0.44
5:B:847:ASP:O	6:C:65:HIS:HE1	2.00	0.44
5:B:888:GLY:HA2	5:B:908:GLU:HB3	1.99	0.44
5:B:1060:ARG:HD3	5:B:1066:SER:N	2.33	0.44
6:C:57:VAL:HG11	11:J:60:PHE:HB3	1.98	0.44
7:E:159:ASP:OD1	7:E:159:ASP:N	2.50	0.44
11:J:30:LEU:HD23	11:J:30:LEU:HA	1.87	0.44
4:A:118:HIS:HD2	4:A:152:VAL:HG23	1.83	0.44
4:A:179:LEU:HD11	4:A:294:SER:HA	1.99	0.44
4:A:231:PRO:HA	4:A:234:MET:HG3	2.00	0.44
4:A:452:LYS:O	5:B:1141:HIS:NE2	2.49	0.44
4:A:786:HIS:CG	5:B:703:ILE:HG13	2.53	0.44
4:A:1116:LEU:HB3	4:A:1308:THR:OG1	2.17	0.44
4:A:1220:PHE:CE2	4:A:1224:LEU:HD22	2.51	0.44
8:F:83:PRO:HB2	8:F:152:ILE:HD13	1.98	0.44
12:K:37:LYS:HA	12:K:37:LYS:HD3	1.79	0.44
4:A:119:ASN:OD1	4:A:120:GLU:N	2.50	0.44
4:A:396:PRO:CG	4:A:416:ARG:HG2	2.47	0.44
4:A:598:LEU:O	9:H:122:LEU:HD13	2.18	0.44
4:A:994:GLN:HE22	4:A:1023:ARG:NE	2.14	0.44
4:A:1150:SER:OG	10:I:46:HIS:HB3	2.17	0.44
4:A:1342:GLU:O	4:A:1345:ARG:HG2	2.17	0.44
5:B:519:TRP:CD1	5:B:519:TRP:C	2.95	0.44
5:B:1204:PHE:O	5:B:1208:MET:HG3	2.18	0.44
10:I:6:PHE:H	10:I:8:ARG:NH2	2.15	0.44
12:K:39:ASP:OD1	12:K:41:THR:HG22	2.18	0.44
4:A:380:VAL:HG22	4:A:430:TRP:O	2.18	0.44
4:A:420:ARG:O	4:A:424:ILE:HG23	2.17	0.44
4:A:471:ASN:OD1	4:A:472:LEU:N	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:537:ARG:HH12	9:H:122:LEU:CD1	2.30	0.44
5:B:762:ASN:ND2	5:B:1024:ALA:HB3	2.33	0.44
6:C:54:ASN:OD1	6:C:153:LEU:HD13	2.18	0.44
7:E:98:ILE:HD13	7:E:101:GLN:HE22	1.83	0.44
9:H:91:ASP:HB2	9:H:93:TYR:HD1	1.82	0.44
12:K:20:LYS:HD2	12:K:21:ILE:N	2.33	0.44
2:T:17:DG:H2'	2:T:18:DA:N9	2.33	0.44
4:A:354:SER:O	4:A:469:ARG:HA	2.18	0.44
4:A:597:LEU:HD12	9:H:102:TYR:HD2	1.83	0.44
5:B:489:SER:HA	5:B:492:LEU:HD12	2.00	0.44
5:B:899:ILE:HD12	5:B:911:ILE:HA	2.00	0.44
7:E:177:ARG:HG2	7:E:215:MET:SD	2.58	0.44
9:H:6:PHE:CE2	9:H:8:ASP:HB2	2.52	0.44
12:K:11:LEU:C	12:K:37:LYS:HG3	2.42	0.44
4:A:71:GLN:HB3	5:B:1174:LYS:HG2	2.00	0.43
4:A:211:PHE:HB3	4:A:231:PRO:HB2	2.00	0.43
4:A:315:LEU:HA	4:A:321:PRO:HA	2.00	0.43
4:A:1154:TYR:HB2	4:A:1191:TRP:CD2	2.52	0.43
4:A:1161:THR:HB	4:A:1239:ARG:HH21	1.83	0.43
4:A:1207:LEU:HD13	4:A:1212:VAL:HG22	2.00	0.43
4:A:1282:VAL:HG12	4:A:1308:THR:HA	2.00	0.43
4:A:1317:MET:HE3	7:E:142:VAL:HB	2.00	0.43
4:A:1349:TYR:CE2	4:A:1365:TYR:HD1	2.36	0.43
5:B:403:LYS:H	5:B:403:LYS:HG2	1.65	0.43
5:B:454:THR:O	5:B:458:LYS:HG3	2.18	0.43
5:B:778:MET:HE1	5:B:853:SER:HB3	1.99	0.43
5:B:803:LEU:HD13	5:B:1032:SER:HB3	1.99	0.43
8:F:76:LYS:HA	8:F:79:ARG:HD3	2.00	0.43
4:A:694:THR:O	4:A:698:GLN:HG3	2.18	0.43
5:B:103:ASN:ND2	5:B:107:GLY:O	2.50	0.43
5:B:185:THR:O	5:B:189:LEU:N	2.46	0.43
6:C:97:VAL:HG21	6:C:129:ILE:HG22	1.99	0.43
9:H:95:TYR:HB3	9:H:144:ILE:HD13	2.00	0.43
10:I:71:SER:HB2	10:I:85:PHE:CD1	2.53	0.43
4:A:389:THR:HG22	4:A:426:LEU:HD23	1.99	0.43
4:A:698:GLN:OE1	10:I:99:LEU:HD12	2.19	0.43
4:A:786:HIS:ND1	5:B:703:ILE:HG13	2.32	0.43
4:A:947:PHE:HB3	4:A:949:ASP:OD1	2.19	0.43
4:A:1300:LYS:HE3	4:A:1300:LYS:HB3	1.62	0.43
5:B:541:LEU:HD11	5:B:747:MET:SD	2.58	0.43
5:B:579:ARG:HB3	5:B:581:PHE:HE1	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:611:PRO:HG2	5:B:685:LEU:HD21	2.01	0.43
5:B:764:SER:HA	5:B:767:ASN:HD22	1.83	0.43
5:B:839:MET:HB2	5:B:1010:LEU:HD21	2.00	0.43
7:E:95:THR:HG22	7:E:99:HIS:CE1	2.53	0.43
7:E:110:PHE:HD1	7:E:111:VAL:N	2.16	0.43
4:A:466:SER:HB2	5:B:1103:ILE:HD11	2.00	0.43
4:A:540:PHE:HB3	4:A:571:LEU:HD12	2.00	0.43
4:A:1119:TYR:HD1	4:A:1327:ILE:HA	1.82	0.43
5:B:982:SER:OG	5:B:986:GLN:HG2	2.17	0.43
5:B:1074:ASN:HB3	5:B:1077:THR:OG1	2.18	0.43
4:A:77:CYS:SG	4:A:79:GLY:N	2.91	0.43
4:A:706:HIS:NE2	4:A:1139:GLU:OE2	2.50	0.43
4:A:825:ILE:O	4:A:829:VAL:HG23	2.18	0.43
4:A:884:ASP:OD2	4:A:1030:ARG:NH2	2.51	0.43
4:A:1207:LEU:HD11	4:A:1273:LEU:HB2	2.00	0.43
4:A:1425:SER:O	4:A:1429:ILE:HG12	2.19	0.43
5:B:41:LYS:NZ	5:B:692:TYR:OH	2.51	0.43
5:B:1016:ALA:HB1	5:B:1020:ARG:NH1	2.34	0.43
6:C:251:LEU:O	6:C:255:VAL:HG23	2.19	0.43
7:E:147:HIS:HE1	7:E:149:LEU:HG	1.82	0.43
12:K:103:THR:O	12:K:107:THR:HG23	2.19	0.43
3:N:12:DG:H2"	3:N:13:DA:C8	2.54	0.43
4:A:98:LYS:HE2	4:A:98:LYS:HB2	1.92	0.43
4:A:845:LEU:O	4:A:1065:GLY:HA3	2.19	0.43
4:A:1381:LEU:HD23	4:A:1381:LEU:HA	1.84	0.43
5:B:120:ARG:NH2	13:L:54:ARG:HB2	2.34	0.43
5:B:311:LEU:O	5:B:315:LYS:HG3	2.18	0.43
5:B:599:THR:O	5:B:603:LEU:HG	2.18	0.43
6:C:6:PRO:CB	12:K:101:LEU:HD12	2.49	0.43
6:C:46:ILE:HG12	6:C:157:CYS:HB3	2.00	0.43
8:F:83:PRO:HA	8:F:146:TRP:CZ3	2.54	0.43
11:J:33:GLY:HA2	11:J:36:LEU:HD12	2.01	0.43
12:K:10:PHE:CE2	12:K:11:LEU:HD13	2.53	0.43
13:L:29:TYR:HE1	13:L:41:SER:HA	1.78	0.43
4:A:447:GLN:HE22	4:A:488:ASN:HD21	1.66	0.43
4:A:500:GLU:CD	5:B:1145:SER:HB3	2.44	0.43
4:A:544:ASP:OD1	4:A:545:GLN:N	2.50	0.43
4:A:576:GLN:O	4:A:580:VAL:HG23	2.18	0.43
4:A:848:ILE:HD13	4:A:1370:LEU:HD21	2.00	0.43
4:A:1165:GLU:O	4:A:1169:ILE:HG12	2.19	0.43
5:B:298:LEU:HG	5:B:314:LEU:HD13	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:918:ILE:HG13	5:B:935:ARG:HD2	2.00	0.43
5:B:959:ASP:HB2	5:B:961:LEU:HD12	2.01	0.43
9:H:12:VAL:HA	9:H:28:ALA:HA	2.00	0.43
3:N:2:DC:H1'	3:N:3:DA:C8	2.54	0.43
4:A:175:ARG:NH1	4:A:176:LYS:O	2.52	0.43
4:A:209:ASN:HB3	4:A:213:HIS:HE1	1.83	0.43
6:C:15:LYS:NZ	6:C:135:GLN:HE21	2.16	0.43
10:I:68:LEU:HB3	10:I:84:VAL:HG13	2.01	0.43
10:I:85:PHE:HB3	10:I:101:PHE:CD2	2.54	0.43
2:T:8:DT:C2	3:N:12:DG:N2	2.87	0.43
4:A:181:LEU:O	4:A:202:LEU:HB2	2.18	0.43
4:A:303:TYR:CZ	4:A:325:ILE:HD11	2.54	0.43
4:A:449:SER:OG	5:B:1133:MET:HB3	2.18	0.43
4:A:862:ASN:OD1	7:E:174:GLN:HA	2.18	0.43
4:A:994:GLN:HE21	4:A:1022:LEU:HD23	1.84	0.43
5:B:783:THR:HA	11:J:60:PHE:HE1	1.84	0.43
6:C:44:LEU:HB2	6:C:77:ILE:HD13	2.01	0.43
11:J:2:ILE:HD12	11:J:2:ILE:HA	1.86	0.43
12:K:59:ALA:HA	12:K:74:ARG:O	2.19	0.43
2:T:8:DT:H2''	2:T:9:DC:C6	2.54	0.43
4:A:325:ILE:O	4:A:329:LEU:HG	2.19	0.43
4:A:344:ARG:HA	5:B:1129:ARG:HA	2.00	0.43
4:A:492:PRO:HB3	4:A:497:THR:HG22	2.01	0.43
5:B:228:LYS:HG3	5:B:232:SER:OG	2.19	0.43
5:B:431:TYR:HD1	5:B:434:ARG:HH21	1.65	0.43
5:B:619:ILE:HG21	10:I:61:ASP:HB2	2.01	0.43
5:B:832:GLY:HA2	5:B:835:GLN:HG3	2.00	0.43
5:B:840:ILE:HG23	5:B:992:ILE:HG23	2.00	0.43
6:C:47:ASP:OD1	13:L:70:ARG:NH1	2.51	0.43
9:H:35:GLN:HB3	9:H:111:LEU:HD11	2.00	0.43
9:H:82:PRO:HA	9:H:87:ARG:NH1	2.34	0.43
10:I:29:CYS:SG	10:I:32:CYS:N	2.84	0.43
10:I:29:CYS:HB3	10:I:32:CYS:O	2.19	0.43
11:J:22:LEU:O	11:J:25:LEU:HG	2.19	0.43
4:A:107:CYS:HA	4:A:171:GLN:CD	2.44	0.42
4:A:117:GLU:O	4:A:122:MET:HE2	2.20	0.42
4:A:126:LEU:HA	4:A:138:ILE:HD11	2.00	0.42
4:A:399:HIS:CD2	4:A:435:HIS:HB3	2.54	0.42
4:A:582:ILE:HD13	4:A:607:ILE:HD13	2.00	0.42
4:A:1119:TYR:CE2	4:A:1287:TYR:HE2	2.37	0.42
4:A:1148:ILE:HD11	4:A:1198:ASP:HA	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1207:LEU:H	4:A:1274:ARG:HH21	1.67	0.42
5:B:128:LEU:O	5:B:167:ILE:N	2.52	0.42
5:B:257:LYS:HE2	5:B:259:TYR:OH	2.18	0.42
5:B:547:VAL:H	5:B:612:GLU:CD	2.27	0.42
5:B:760:ASP:OD1	5:B:760:ASP:N	2.51	0.42
5:B:885:MET:HA	5:B:936:ASP:CB	2.49	0.42
7:E:26:ARG:O	7:E:75:MET:HE1	2.19	0.42
4:A:700:ASN:HB2	10:I:98:VAL:HG22	2.02	0.42
4:A:765:VAL:CG2	4:A:800:VAL:HB	2.49	0.42
4:A:786:HIS:CE1	5:B:705:MET:SD	3.12	0.42
5:B:25:ILE:HG21	5:B:653:VAL:HG13	2.01	0.42
5:B:210:LYS:NZ	5:B:462:ALA:HA	2.34	0.42
5:B:693:ILE:HG23	5:B:697:GLU:HG2	2.01	0.42
5:B:727:LYS:HG3	5:B:1049:ASP:OD1	2.20	0.42
5:B:756:ILE:HG21	5:B:767:ASN:OD1	2.18	0.42
5:B:759:PRO:HD2	5:B:1046:PRO:HG3	2.01	0.42
6:C:206:ASN:HA	6:C:209:TYR:CD2	2.54	0.42
6:C:252:GLN:HE21	12:K:98:LEU:HB3	1.84	0.42
7:E:93:MET:HE2	7:E:124:VAL:HA	2.00	0.42
8:F:99:LEU:O	8:F:103:MET:HG2	2.20	0.42
2:T:8:DT:OP2	2:T:8:DT:H2'	2.19	0.42
4:A:31:SER:O	5:B:1183:LYS:NZ	2.33	0.42
4:A:272:ALA:O	4:A:276:LEU:HD23	2.18	0.42
4:A:596:THR:OG1	4:A:599:SER:N	2.45	0.42
4:A:881:GLN:CD	4:A:959:ASN:HA	2.43	0.42
4:A:1081:LEU:HD12	4:A:1081:LEU:HA	1.83	0.42
5:B:217:ARG:NH1	5:B:405:ARG:HG2	2.34	0.42
5:B:234:ILE:H	5:B:234:ILE:HG12	1.58	0.42
5:B:681:TRP:NE1	5:B:692:TYR:OH	2.52	0.42
9:H:130:ARG:HG2	9:H:134:ASN:HD22	1.85	0.42
10:I:5:ARG:HD2	10:I:5:ARG:HA	1.87	0.42
4:A:82:GLY:CA	4:A:241:VAL:HB	2.49	0.42
4:A:703:THR:O	4:A:705:LYS:NZ	2.52	0.42
4:A:739:ASP:HB3	9:H:19:ARG:HH12	1.84	0.42
4:A:949:ASP:HA	4:A:1290:LYS:HE2	2.01	0.42
4:A:1215:ARG:O	4:A:1219:THR:HG23	2.19	0.42
4:A:1398:MET:HE2	4:A:1423:GLY:HA3	2.01	0.42
4:A:1435:PRO:C	4:A:1436:ILE:HD12	2.44	0.42
5:B:99:LYS:HA	5:B:99:LYS:HD2	1.91	0.42
5:B:399:ASP:OD2	5:B:510:LYS:HG3	2.19	0.42
5:B:582:VAL:HA	5:B:626:ILE:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:806:THR:HG22	5:B:808:ALA:H	1.84	0.42
9:H:100:THR:HA	9:H:138:GLU:O	2.20	0.42
9:H:104:PHE:CE2	9:H:134:ASN:HB3	2.54	0.42
4:A:13:THR:HG23	4:A:15:LYS:HE3	2.01	0.42
4:A:69:THR:O	5:B:1174:LYS:HE3	2.20	0.42
4:A:181:LEU:HD13	4:A:207:ILE:HD13	2.02	0.42
4:A:492:PRO:HA	5:B:1149:GLU:OE2	2.20	0.42
4:A:666:ILE:HD13	5:B:1030:LEU:HD22	2.01	0.42
4:A:777:PHE:CD1	4:A:783:THR:HG23	2.53	0.42
4:A:881:GLN:O	4:A:953:ASN:HA	2.19	0.42
4:A:1278:ASN:HB2	4:A:1312:ASN:HB2	2.02	0.42
5:B:308:TRP:HH2	10:I:47:GLU:HG3	1.84	0.42
5:B:427:ASP:HA	5:B:430:ARG:CD	2.50	0.42
5:B:466:TRP:HD1	5:B:476:ARG:NH1	2.17	0.42
10:I:78:CYS:HB2	10:I:80:SER:HB3	2.00	0.42
4:A:76:GLU:CD	5:B:1159:ARG:HH21	2.27	0.42
4:A:386:ASP:O	4:A:389:THR:OG1	2.37	0.42
4:A:857:ARG:HD3	4:A:861:GLY:O	2.20	0.42
4:A:1035:TYR:CE2	4:A:1037:LEU:HB2	2.54	0.42
5:B:701:ILE:HG13	5:B:703:ILE:HG23	2.00	0.42
5:B:863:GLU:HB2	5:B:961:LEU:HB3	2.02	0.42
7:E:87:SER:HA	7:E:115:ASN:O	2.19	0.42
12:K:107:THR:O	12:K:111:LEU:HD13	2.18	0.42
4:A:20:GLY:O	5:B:1213:THR:N	2.39	0.42
4:A:346:ASP:HB3	4:A:347:PHE:CD2	2.55	0.42
5:B:21:GLU:O	5:B:654:ARG:HB3	2.19	0.42
5:B:406:LEU:HD23	5:B:406:LEU:HA	1.76	0.42
5:B:890:TYR:HD1	5:B:893:LEU:HD12	1.83	0.42
5:B:1019:SER:OG	16:B:1302:ATP:O3'	2.27	0.42
6:C:118:LEU:HD23	6:C:118:LEU:HA	1.80	0.42
7:E:56:LYS:NZ	7:E:84:ASP:HB2	2.34	0.42
9:H:117:SER:HA	9:H:121:LEU:O	2.19	0.42
11:J:55:ASP:HB3	11:J:58:GLU:OE1	2.19	0.42
3:N:9:DA:C6	3:N:10:DG:C6	3.08	0.42
4:A:683:ILE:HG21	4:A:801:GLU:HB2	2.02	0.42
4:A:1281:ARG:NH2	4:A:1309:ASP:OD1	2.51	0.42
4:A:1323:ASP:OD2	4:A:1326:ARG:HB2	2.19	0.42
4:A:1439:GLY:HA2	8:F:92:ARG:NH2	2.34	0.42
5:B:600:LEU:O	5:B:609:ILE:HD12	2.20	0.42
5:B:860:MET:HE3	5:B:860:MET:HB3	1.78	0.42
7:E:83:CYS:HB2	7:E:110:PHE:CE1	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:K:58:PHE:HB3	12:K:76:GLN:HB2	2.01	0.42
4:A:403:LYS:HE2	4:A:403:LYS:HB2	1.72	0.42
4:A:662:PHE:CE2	4:A:746:MET:HE2	2.55	0.42
5:B:894:ASP:HB2	5:B:896:ASP:OD1	2.19	0.42
5:B:982:SER:HB3	5:B:1092:TYR:CZ	2.55	0.42
6:C:43:THR:HB	6:C:170:TRP:O	2.20	0.42
6:C:91:HIS:CE1	6:C:158:VAL:HG11	2.55	0.42
7:E:66:GLU:HA	7:E:69:ILE:CG2	2.46	0.42
4:A:357:PRO:HG2	5:B:832:GLY:HA3	2.02	0.42
4:A:369:SER:H	12:K:2:ASN:HD21	1.68	0.42
4:A:802:ASN:OD1	5:B:729:ILE:N	2.43	0.42
4:A:1289:ARG:HD2	4:A:1290:LYS:O	2.19	0.42
6:C:249:ASP:HB3	6:C:253:LYS:NZ	2.35	0.42
11:J:34:THR:O	11:J:38:ARG:HG2	2.20	0.42
12:K:20:LYS:O	12:K:33:ILE:HA	2.19	0.42
4:A:153:PRO:HA	4:A:162:VAL:HB	2.02	0.41
4:A:782:ARG:NH2	5:B:701:ILE:O	2.48	0.41
5:B:197:PHE:HD2	5:B:817:LEU:HD12	1.84	0.41
5:B:813:LYS:HA	5:B:813:LYS:HD2	1.86	0.41
5:B:882:THR:OG1	5:B:885:MET:SD	2.72	0.41
5:B:976:ILE:HG12	5:B:992:ILE:HA	2.02	0.41
7:E:67:GLU:O	7:E:70:SER:OG	2.30	0.41
4:A:102:VAL:HG13	4:A:211:PHE:CZ	2.55	0.41
4:A:380:VAL:HA	4:A:384:ASN:HD22	1.86	0.41
4:A:563:PRO:HG3	4:A:572:TRP:CZ2	2.55	0.41
4:A:830:LYS:O	4:A:834:THR:OG1	2.30	0.41
4:A:840:ARG:HG2	4:A:1402:PHE:CE1	2.55	0.41
4:A:863:VAL:HG23	7:E:170:LEU:HD11	2.03	0.41
4:A:1140:HIS:HA	4:A:1275:GLY:HA3	2.02	0.41
5:B:186:GLU:HA	5:B:189:LEU:HB2	2.02	0.41
5:B:894:ASP:OD1	5:B:894:ASP:N	2.53	0.41
5:B:983:ARG:NH2	5:B:1028:GLU:OE2	2.53	0.41
5:B:1010:LEU:HD23	5:B:1011:ILE:N	2.35	0.41
6:C:35:ARG:HH12	12:K:40:HIS:HB2	1.85	0.41
9:H:37:LYS:N	9:H:126:GLU:HB2	2.30	0.41
13:L:38:LEU:HD22	13:L:56:LEU:HD11	2.00	0.41
2:T:19:WVQ:O4'	4:A:832:ALA:HA	2.20	0.41
4:A:31:SER:HB3	4:A:83:HIS:CD2	2.55	0.41
4:A:55:ASP:O	4:A:58:LEU:HB2	2.21	0.41
4:A:396:PRO:HA	4:A:435:HIS:CE1	2.55	0.41
4:A:560:ILE:HG22	9:H:79:TRP:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:605:MET:HE1	4:A:617:VAL:HA	2.01	0.41
5:B:360:PHE:CE1	5:B:361:LEU:HD13	2.55	0.41
5:B:876:LYS:HD2	5:B:877:PRO:HD2	2.01	0.41
7:E:52:ARG:HA	7:E:52:ARG:CZ	2.50	0.41
9:H:125:LEU:C	9:H:130:ARG:HH21	2.27	0.41
10:I:26:LEU:HB2	10:I:35:VAL:HG12	2.02	0.41
2:T:5:DC:H1'	2:T:6:DT:H5'	2.02	0.41
4:A:643:ALA:O	4:A:646:PHE:HB2	2.20	0.41
4:A:706:HIS:HE2	4:A:1139:GLU:CD	2.27	0.41
4:A:840:ARG:HG2	4:A:1402:PHE:CZ	2.55	0.41
4:A:1220:PHE:CD2	4:A:1224:LEU:HB3	2.55	0.41
5:B:59:LEU:O	5:B:63:ILE:HG12	2.21	0.41
5:B:367:LEU:HD12	5:B:368:GLU:H	1.84	0.41
5:B:1106:ARG:HD2	5:B:1125:ASP:O	2.21	0.41
5:B:1180:PHE:CD2	5:B:1191:ILE:HG21	2.55	0.41
6:C:169:LYS:HE2	13:L:70:ARG:HG2	2.02	0.41
6:C:181:ASP:OD2	6:C:186:LEU:HB2	2.20	0.41
7:E:188:LEU:HB2	7:E:190:LEU:HG	2.02	0.41
4:A:210:ILE:O	4:A:214:ILE:HG13	2.21	0.41
4:A:335:ARG:HA	4:A:339:ASN:HB2	2.02	0.41
4:A:900:ASP:HB3	4:A:906:HIS:ND1	2.35	0.41
4:A:938:LYS:HD3	4:A:938:LYS:C	2.46	0.41
4:A:959:ASN:OD1	4:A:961:ARG:HG2	2.21	0.41
5:B:175:ARG:CG	5:B:200:GLY:HA3	2.50	0.41
5:B:1173:ALA:HB1	5:B:1180:PHE:CD1	2.56	0.41
6:C:72:LEU:O	6:C:237:SER:HB2	2.20	0.41
6:C:77:ILE:O	6:C:161:LYS:NZ	2.47	0.41
6:C:258:ILE:HD12	12:K:19:LEU:HD21	2.02	0.41
10:I:17:ARG:HD3	10:I:17:ARG:HA	1.80	0.41
2:T:10:DT:C2	3:N:10:DG:N2	2.89	0.41
4:A:261:ASP:HA	4:A:264:PHE:CD2	2.55	0.41
4:A:265:LYS:CG	4:A:303:TYR:HB2	2.50	0.41
4:A:605:MET:HA	4:A:614:PHE:O	2.20	0.41
4:A:807:GLY:C	5:B:728:ARG:HD3	2.46	0.41
4:A:837:ILE:O	4:A:841:LEU:HG	2.20	0.41
4:A:1004:ASN:HB3	4:A:1007:ILE:HB	2.01	0.41
4:A:1159:ARG:O	4:A:1170:ILE:HG21	2.20	0.41
4:A:1221:LYS:O	4:A:1222:ASN:HB2	2.20	0.41
4:A:1329:THR:HG21	4:A:1334:ASP:HB2	2.02	0.41
4:A:1412:ALA:HA	4:A:1415:SER:HB2	2.03	0.41
5:B:581:PHE:O	5:B:625:LYS:HA	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:843:GLN:HB2	5:B:993:THR:HB	2.02	0.41
5:B:1147:LEU:HD23	5:B:1147:LEU:HA	1.81	0.41
6:C:91:HIS:HB3	6:C:96:SER:CB	2.50	0.41
8:F:128:LYS:HA	8:F:128:LYS:HD3	1.90	0.41
9:H:108:SER:HB3	9:H:111:LEU:HB2	2.03	0.41
10:I:97:MET:HE2	10:I:97:MET:HB3	1.83	0.41
4:A:11:LEU:HA	5:B:1193:GLN:HB3	2.03	0.41
4:A:464:PRO:HG2	4:A:465:TYR:CD1	2.55	0.41
4:A:740:LEU:HD11	6:C:193:TYR:H	1.86	0.41
4:A:774:ARG:CG	4:A:797:LYS:HB3	2.47	0.41
4:A:789:LYS:HB2	10:I:67:THR:O	2.21	0.41
4:A:1037:LEU:HD12	4:A:1037:LEU:HA	1.77	0.41
4:A:1157:ASP:HB3	4:A:1160:SER:OG	2.20	0.41
5:B:68:THR:HA	5:B:90:ILE:O	2.20	0.41
5:B:490:SER:HA	5:B:775:LYS:HD3	2.03	0.41
5:B:696:GLU:HA	5:B:699:GLU:HG3	2.03	0.41
7:E:72:PHE:CZ	7:E:157:SER:HA	2.56	0.41
10:I:17:ARG:O	10:I:25:LEU:HD12	2.21	0.41
3:N:6:DG:H2'	3:N:6:DG:OP2	2.21	0.41
4:A:30:ILE:HD12	5:B:1170:THR:HG21	2.03	0.41
4:A:549:MET:HE1	4:A:656:TRP:HD1	1.85	0.41
4:A:648:ASN:O	4:A:652:VAL:HG23	2.20	0.41
4:A:986:ILE:HD12	4:A:1028:THR:HG23	2.01	0.41
4:A:1030:ARG:HG2	4:A:1034:GLU:HG3	2.02	0.41
5:B:70:ILE:HD12	5:B:89:GLU:HB2	2.02	0.41
5:B:246:LYS:HD3	5:B:246:LYS:HA	1.77	0.41
5:B:592:ASN:O	5:B:595:ARG:HG2	2.20	0.41
5:B:722:ASP:OD1	5:B:722:ASP:N	2.54	0.41
5:B:757:PRO:HD3	5:B:983:ARG:HD2	2.02	0.41
5:B:976:ILE:HG23	5:B:990:ILE:O	2.21	0.41
5:B:1130:PHE:CE1	5:B:1134:GLU:HB3	2.56	0.41
6:C:52:GLU:HA	13:L:64:LEU:CD1	2.50	0.41
6:C:143:LEU:HD21	6:C:146:LYS:HG3	2.02	0.41
6:C:257:SER:HA	6:C:260:LEU:HG	2.03	0.41
7:E:13:TRP:CE3	7:E:39:LEU:HB2	2.56	0.41
9:H:39:THR:O	9:H:123:MET:HA	2.21	0.41
2:T:23:DC:H5''	5:B:1122:ARG:HG3	2.01	0.41
4:A:86:LEU:HD23	4:A:86:LEU:H	1.86	0.41
4:A:276:LEU:HD21	4:A:292:ALA:C	2.46	0.41
4:A:420:ARG:O	4:A:423:ASP:N	2.52	0.41
4:A:689:LYS:HA	4:A:689:LYS:HD3	1.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:693:VAL:HG21	4:A:721:PHE:CE2	2.56	0.41
4:A:777:PHE:HD1	4:A:783:THR:N	2.19	0.41
5:B:121:ASN:ND2	5:B:860:MET:HE2	2.36	0.41
5:B:195:CYS:HB3	5:B:782:LEU:HD13	2.02	0.41
5:B:234:ILE:HD12	5:B:237:VAL:CG2	2.50	0.41
5:B:258:LEU:HG	5:B:267:ARG:NH2	2.36	0.41
5:B:566:LEU:HD21	5:B:586:TRP:CZ2	2.55	0.41
5:B:582:VAL:HB	5:B:587:HIS:NE2	2.35	0.41
5:B:597:MET:SD	5:B:624:LEU:HD11	2.61	0.41
5:B:804:GLY:HA2	5:B:1042:GLY:O	2.21	0.41
5:B:1065:GLN:OE1	5:B:1069:PHE:HB2	2.20	0.41
5:B:1106:ARG:NE	5:B:1109:GLY:HA3	2.36	0.41
5:B:1161:HIS:HA	5:B:1192:TYR:O	2.21	0.41
5:B:1163:CYS:SG	5:B:1165:ILE:N	2.94	0.41
6:C:35:ARG:HA	6:C:38:ILE:HD12	2.03	0.41
9:H:37:LYS:HA	9:H:37:LYS:HD3	1.66	0.41
10:I:14:LEU:HD13	10:I:27:PHE:HB3	2.03	0.41
11:J:42:LYS:HD3	11:J:42:LYS:HA	1.80	0.41
12:K:77:THR:HG21	12:K:83:PRO:HA	2.02	0.41
4:A:389:THR:HA	4:A:426:LEU:HD21	2.03	0.41
4:A:850:VAL:HG23	4:A:1064:VAL:HG13	2.02	0.41
6:C:86:CYS:SG	6:C:87:PHE:N	2.93	0.41
4:A:244:PRO:HA	4:A:247:ARG:HG2	2.02	0.40
4:A:335:ARG:HD3	5:B:1203:LEU:HB2	2.02	0.40
4:A:975:HIS:HA	4:A:1036:ARG:CG	2.52	0.40
4:A:1135:ARG:HD3	4:A:1282:VAL:HG23	2.02	0.40
5:B:95:ILE:HD12	5:B:130:VAL:HG13	2.04	0.40
5:B:780:VAL:O	5:B:817:LEU:HD22	2.20	0.40
5:B:860:MET:HG3	5:B:965:LYS:HE3	2.02	0.40
5:B:861:ASP:O	5:B:964:VAL:HG22	2.21	0.40
7:E:97:VAL:HG13	7:E:127:ILE:HG12	2.03	0.40
9:H:83:GLN:HB2	9:H:86:ASP:HB3	2.03	0.40
10:I:75:CYS:HB3	10:I:103:CYS:SG	2.61	0.40
4:A:91:PHE:CE1	4:A:96:ILE:HD12	2.56	0.40
4:A:981:LEU:HD23	4:A:985:ASP:HB2	2.02	0.40
4:A:1028:THR:O	4:A:1032:LEU:HG	2.21	0.40
4:A:1220:PHE:O	4:A:1221:LYS:HB3	2.22	0.40
5:B:190:TYR:CE2	5:B:196:PRO:HG2	2.55	0.40
5:B:324:ILE:HG23	5:B:329:THR:OG1	2.20	0.40
5:B:365:THR:HG21	5:B:370:PHE:CD2	2.56	0.40
5:B:1060:ARG:HD2	5:B:1060:ARG:HA	1.75	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:1102:LYS:HD2	5:B:1102:LYS:HA	1.89	0.40
7:E:12:LEU:HD22	7:E:137:GLU:OE2	2.20	0.40
7:E:79:TRP:NE1	7:E:81:GLU:HB2	2.36	0.40
2:T:16:DT:H1'	2:T:17:DG:N9	2.36	0.40
4:A:508:PRO:HB3	4:A:639:PRO:HB2	2.02	0.40
4:A:852:TYR:CE1	8:F:136:ARG:HD2	2.56	0.40
5:B:635:ARG:HG3	5:B:637:LEU:CD1	2.50	0.40
5:B:1150:ARG:HA	5:B:1150:ARG:HD2	1.84	0.40
6:C:104:PHE:HB2	6:C:152:GLU:HG3	2.03	0.40
6:C:113:VAL:O	6:C:143:LEU:HA	2.21	0.40
7:E:103:LYS:HB3	7:E:105:PHE:CG	2.56	0.40
8:F:76:LYS:HA	8:F:79:ARG:CD	2.51	0.40
9:H:142:LEU:HD22	9:H:144:ILE:CD1	2.51	0.40
4:A:199:LEU:HD23	4:A:199:LEU:HA	1.89	0.40
4:A:556:TRP:HZ3	12:K:74:ARG:NH2	2.19	0.40
4:A:662:PHE:HB3	5:B:829:CYS:SG	2.61	0.40
4:A:1035:TYR:HD2	4:A:1037:LEU:HB2	1.87	0.40
4:A:1191:TRP:HH2	10:I:25:LEU:HD13	1.85	0.40
5:B:69:LEU:HD12	5:B:90:ILE:HD13	2.02	0.40
5:B:839:MET:HG3	5:B:990:ILE:HA	2.04	0.40
5:B:1205:GLN:HA	5:B:1208:MET:HG3	2.03	0.40
7:E:58:MET:O	7:E:60:PHE:HD2	2.05	0.40
8:F:138:LEU:HD12	8:F:142:SER:O	2.22	0.40
9:H:93:TYR:CG	9:H:143:LEU:HB3	2.56	0.40
4:A:340:LEU:HA	4:A:340:LEU:HD23	1.83	0.40
4:A:677:ARG:O	4:A:681:GLU:HG3	2.20	0.40
4:A:1009:ASN:CG	4:A:1012:ARG:HH21	2.29	0.40
4:A:1138:ILE:HD11	4:A:1316:VAL:HG22	2.03	0.40
5:B:693:ILE:HG23	5:B:697:GLU:HB3	2.04	0.40
5:B:826:ALA:HA	5:B:1086:PHE:O	2.22	0.40
6:C:164:ALA:HA	6:C:167:HIS:O	2.22	0.40
7:E:169:ARG:HB3	8:F:140:ASP:HB3	2.02	0.40
9:H:91:ASP:HB2	9:H:93:TYR:CD1	2.57	0.40
9:H:103:LYS:O	9:H:115:TYR:HB2	2.21	0.40
10:I:4:PHE:CE1	10:I:13:MET:HB2	2.57	0.40
11:J:14:VAL:HB	11:J:50:ILE:HD11	2.03	0.40
12:K:32:VAL:HG12	12:K:74:ARG:HG3	2.03	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:O	13:L:39:SER:O[2_555]	1.95	0.25

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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%)	1337 (98%)	33 (2%)	0	100	100
5	B	1103/1224 (90%)	1085 (98%)	18 (2%)	0	100	100
6	C	265/318 (83%)	261 (98%)	4 (2%)	0	100	100
7	E	210/215 (98%)	207 (99%)	3 (1%)	0	100	100
8	F	84/155 (54%)	81 (96%)	3 (4%)	0	100	100
9	H	129/146 (88%)	128 (99%)	1 (1%)	0	100	100
10	I	116/122 (95%)	112 (97%)	4 (3%)	0	100	100
11	J	63/70 (90%)	63 (100%)	0	0	100	100
12	K	112/120 (93%)	110 (98%)	2 (2%)	0	100	100
13	L	41/70 (59%)	37 (90%)	4 (10%)	0	100	100
All	All	3493/4173 (84%)	3421 (98%)	72 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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%)	1189 (100%)	5 (0%)	84	83
5	B	955/1061 (90%)	952 (100%)	3 (0%)	86	84
6	C	235/274 (86%)	234 (100%)	1 (0%)	84	83
7	E	192/197 (98%)	192 (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	110/116 (95%)	106 (96%)	4 (4%)	31	53
11	J	60/65 (92%)	59 (98%)	1 (2%)	53	67
12	K	99/102 (97%)	99 (100%)	0	100	100
13	L	36/57 (63%)	33 (92%)	3 (8%)	10	34
All	All	3070/3657 (84%)	3053 (99%)	17 (1%)	78	79

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

Mol	Chain	Res	Type
4	A	67	CYS
4	A	80	HIS
4	A	107	CYS
4	A	148	CYS
4	A	167	CYS
5	B	101	MET
5	B	1163	CYS
5	B	1185	CYS
6	C	86	CYS
10	I	10	CYS
10	I	75	CYS
10	I	78	CYS
10	I	106	CYS
11	J	7	CYS
13	L	31	CYS
13	L	34	CYS
13	L	51	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
4	A	18	GLN
4	A	54	ASN

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Mol	Chain	Res	Type
4	A	109	HIS
4	A	313	GLN
4	A	358	ASN
4	A	447	GLN
4	A	589	GLN
4	A	742	ASN
4	A	854	ASN
4	A	1009	ASN
4	A	1393	ASN
5	B	103	ASN
5	B	236	HIS
5	B	255	GLN
5	B	306	ASN
5	B	465	ASN
5	B	592	ASN
5	B	657	HIS
5	B	767	ASN
5	B	770	GLN
5	B	1025	HIS
5	B	1177	HIS
5	B	1187	ASN
5	B	1193	GLN
5	B	1195	HIS
6	C	135	GLN
7	E	115	ASN
7	E	174	GLN
9	H	21	ASN
9	H	35	GLN
9	H	134	ASN
10	I	114	GLN
11	J	64	ASN
12	K	2	ASN
12	K	52	ASN
12	K	92	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	R	7/9 (77%)	3 (42%)	0

All (3) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	R	2	U
1	R	5	A
1	R	8	G

There are no RNA pucker outliers to report.

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

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	3.63	7 (36%)	18,33,36	1.58	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	12.79	1.46	1.28
2	T	19	WVQ	C4-N9	4.65	1.45	1.35
2	T	19	WVQ	C2-N2	4.18	1.45	1.34
2	T	19	WVQ	C6-C5	-4.05	1.36	1.47
2	T	19	WVQ	C6-N1	-3.11	1.32	1.38
2	T	19	WVQ	O6-C6	-2.67	1.18	1.23
2	T	19	WVQ	C5-C4	-2.28	1.37	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	-4.45	119.39	126.44
2	T	19	WVQ	N2-C2-N3	2.34	120.30	116.57
2	T	19	WVQ	N9-C4-N3	-2.08	116.60	119.70
2	T	19	WVQ	N2-C2-N1	2.08	120.31	117.09

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	T	19	WVQ	C3'-C4'-C5'-O5'
2	T	19	WVQ	O4'-C4'-C5'-O5'
2	T	19	WVQ	O4'-C1'-N9-C4
2	T	19	WVQ	C4'-C5'-O5'-P

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	T	19	WVQ	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	ATP	B	1302	-	32,33,33	0.28	0	48,52,52	0.37	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	ATP	B	1302	-	-	6/22/38/38	0/3/3/3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (6) torsion outliers are listed below:

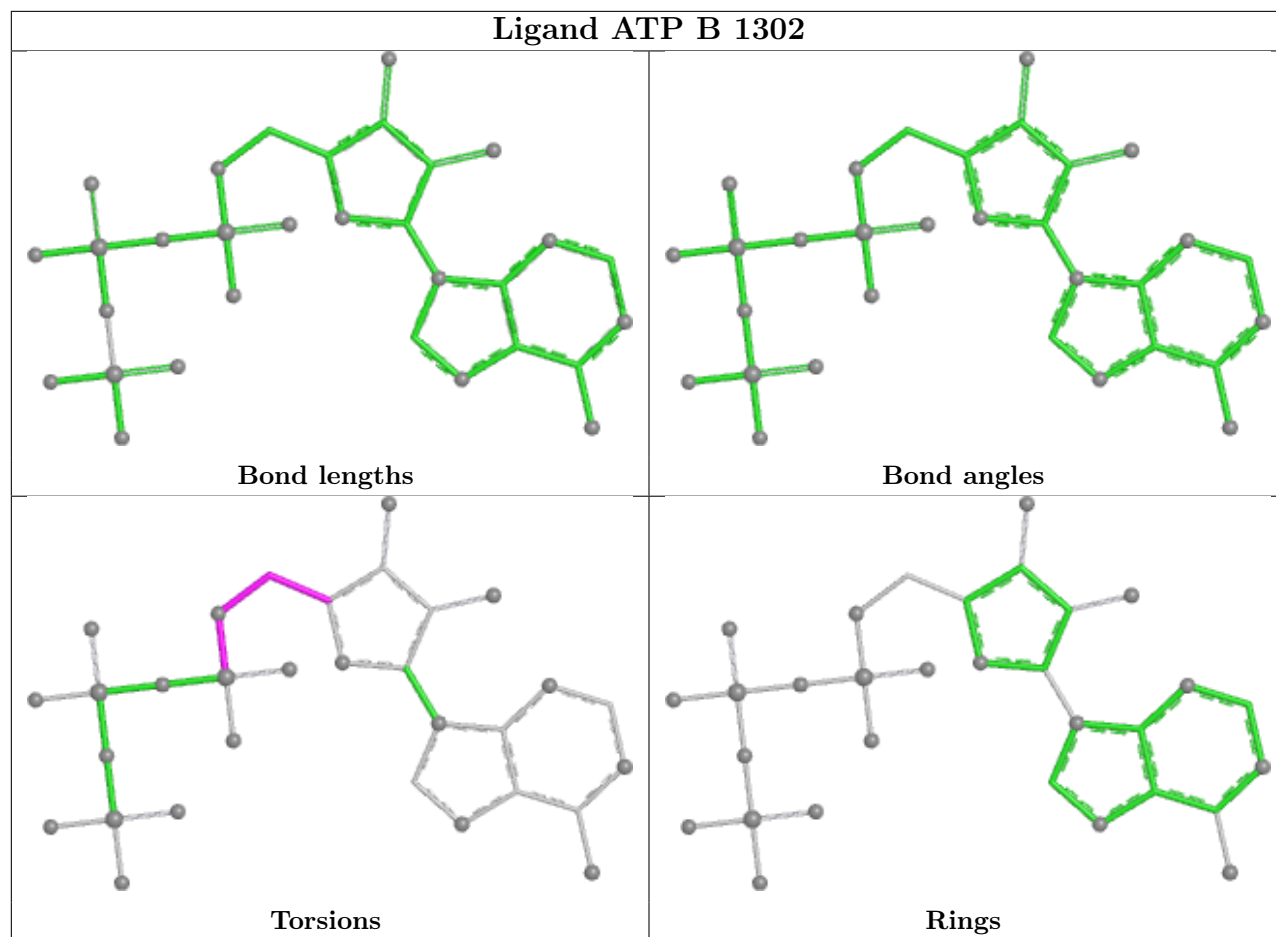
Mol	Chain	Res	Type	Atoms
16	B	1302	ATP	C5'-O5'-PA-O1A
16	B	1302	ATP	C5'-O5'-PA-O2A
16	B	1302	ATP	C5'-O5'-PA-O3A
16	B	1302	ATP	O4'-C4'-C5'-O5'
16	B	1302	ATP	C4'-C5'-O5'-PA
16	B	1302	ATP	C3'-C4'-C5'-O5'

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	B	1302	ATP	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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	9/9 (100%)	-0.11	0	100	100	111, 134, 207, 245	0
2	T	23/29 (79%)	0.20	0	100	100	113, 216, 300, 320	0
3	N	13/18 (72%)	0.19	0	100	100	215, 252, 297, 312	0
4	A	1384/1733 (79%)	0.25	51 (3%)	45	31	81, 142, 221, 332	0
5	B	1123/1224 (91%)	0.34	54 (4%)	35	26	61, 131, 197, 288	0
6	C	267/318 (83%)	0.31	11 (4%)	41	29	58, 119, 186, 246	0
7	E	212/215 (98%)	0.10	7 (3%)	49	33	126, 174, 259, 319	0
8	F	86/155 (55%)	0.02	3 (3%)	47	32	90, 134, 191, 258	0
9	H	133/146 (91%)	0.06	0	100	100	96, 162, 229, 346	0
10	I	118/122 (96%)	0.14	0	100	100	114, 171, 225, 258	0
11	J	65/70 (92%)	0.38	2 (3%)	51	34	68, 118, 167, 225	0
12	K	114/120 (95%)	0.10	7 (6%)	27	22	72, 122, 173, 199	0
13	L	43/70 (61%)	0.52	2 (4%)	36	26	112, 255, 330, 400	0
All	All	3590/4229 (84%)	0.26	137 (3%)	44	31	58, 139, 227, 400	0

All (137) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	B	543	SER	6.3
5	B	779	GLY	6.2
5	B	775	LYS	5.8
4	A	1010	ALA	4.9
7	E	93	MET	4.7
4	A	642	CYS	4.7
5	B	681	TRP	4.5
5	B	310	MET	4.4
4	A	328	ARG	4.4

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Mol	Chain	Res	Type	RSRZ
5	B	1140	ALA	4.2
4	A	355	GLY	4.2
6	C	33	LEU	4.1
5	B	533	CYS	4.0
5	B	658	ILE	4.0
6	C	29	MET	4.0
4	A	1195	LEU	3.9
5	B	386	LEU	3.8
5	B	700	SER	3.8
5	B	381	MET	3.8
4	A	1371	LEU	3.7
5	B	819	ALA	3.6
12	K	42	LEU	3.6
7	E	111	VAL	3.5
5	B	778	MET	3.4
5	B	1093	GLN	3.4
5	B	780	VAL	3.4
4	A	1390	ASN	3.4
4	A	96	ILE	3.3
5	B	1204	PHE	3.3
5	B	489	SER	3.2
4	A	997	LEU	3.2
4	A	1429	ILE	3.2
5	B	638	PHE	3.2
4	A	669	THR	3.1
4	A	873	MET	3.1
6	C	159	ALA	3.1
5	B	43	LEU	3.1
4	A	488	ASN	3.0
11	J	44	TYR	3.0
5	B	167	ILE	3.0
6	C	31	ASN	3.0
4	A	466	SER	3.0
4	A	1020	CYS	2.9
5	B	1214	PRO	2.9
4	A	815	PHE	2.9
4	A	1328	TYR	2.9
5	B	488	TYR	2.9
4	A	55	ASP	2.8
4	A	1396	ALA	2.8
5	B	51	PHE	2.8
5	B	822	ASN	2.8

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Mol	Chain	Res	Type	RSRZ
4	A	834	THR	2.8
4	A	722	LEU	2.8
4	A	303	TYR	2.7
5	B	750	GLY	2.7
12	K	44	ASN	2.7
5	B	751	VAL	2.7
4	A	1197	LEU	2.7
7	E	112	TYR	2.7
4	A	448	PRO	2.7
5	B	1211	ASN	2.7
5	B	1006	ILE	2.6
13	L	28	LYS	2.6
5	B	446	LEU	2.6
6	C	97	VAL	2.6
4	A	1267	MET	2.6
6	C	251	LEU	2.6
7	E	209	ALA	2.6
4	A	646	PHE	2.6
4	A	1149	ALA	2.5
5	B	802	PRO	2.5
5	B	1021	MET	2.5
5	B	532	ALA	2.5
4	A	98	LYS	2.5
4	A	336	ILE	2.5
8	F	84	TYR	2.5
5	B	823	ALA	2.5
5	B	849	GLY	2.5
13	L	67	PHE	2.5
4	A	1073	GLY	2.5
6	C	8	VAL	2.5
7	E	97	VAL	2.4
12	K	65	HIS	2.4
5	B	25	ILE	2.4
7	E	23	VAL	2.4
8	F	93	ILE	2.4
4	A	62	ASP	2.4
4	A	1306	LEU	2.4
5	B	420	LEU	2.4
4	A	960	ILE	2.3
12	K	71	PHE	2.3
4	A	161	LEU	2.3
7	E	82	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
5	B	690	VAL	2.3
4	A	656	TRP	2.3
5	B	851	PHE	2.3
5	B	1212	ILE	2.3
5	B	1072	MET	2.3
5	B	714	GLU	2.2
8	F	85	MET	2.2
5	B	1123	SER	2.2
4	A	350	ARG	2.2
5	B	939	THR	2.2
4	A	862	ASN	2.2
4	A	314	ALA	2.2
4	A	504	LEU	2.2
5	B	55	VAL	2.2
5	B	850	LEU	2.2
12	K	101	LEU	2.2
4	A	658	LEU	2.2
12	K	40	HIS	2.1
5	B	611	PRO	2.1
4	A	1076	ALA	2.1
12	K	39	ASP	2.1
4	A	1240	CYS	2.1
4	A	630	ILE	2.1
5	B	33	VAL	2.1
6	C	57	VAL	2.1
5	B	413	LEU	2.1
11	J	35	ALA	2.1
4	A	798	GLY	2.1
5	B	988	GLY	2.1
5	B	983	ARG	2.1
5	B	538	ASN	2.1
6	C	22	LEU	2.1
4	A	108	MET	2.1
6	C	202	PRO	2.1
4	A	776	ALA	2.1
6	C	74	SER	2.1
4	A	341	MET	2.1
4	A	683	ILE	2.0
5	B	813	LYS	2.0
4	A	92	HIS	2.0
4	A	649	ILE	2.0
5	B	620	ARG	2.0

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Mol	Chain	Res	Type	RSRZ
5	B	1077	THR	2.0
4	A	33	ALA	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	0.84	0.11	171,184,201,215	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

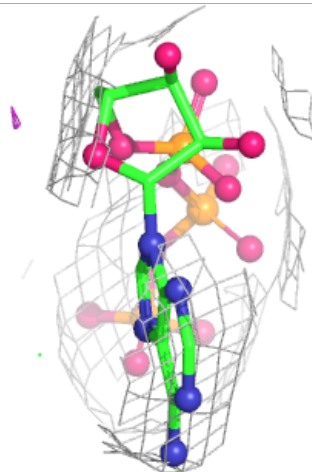
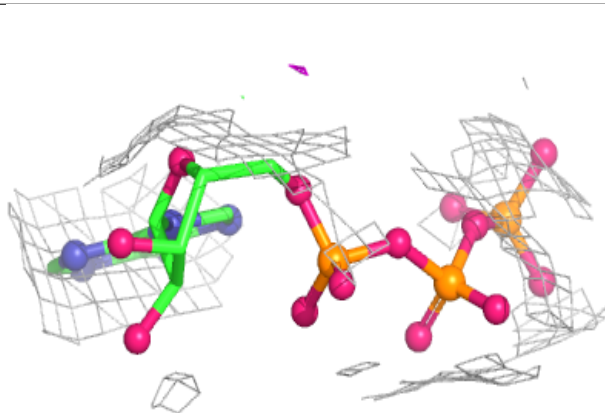
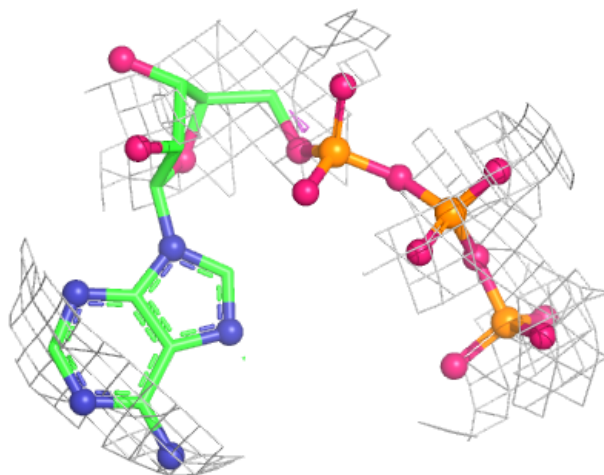
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists 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	ATP	B	1302	31/31	0.72	0.10	140,168,215,232	0
15	MG	A	1803	1/1	0.88	0.05	107,107,107,107	0
14	ZN	L	101	1/1	0.88	0.09	369,369,369,369	0
14	ZN	A	1801	1/1	0.89	0.05	342,342,342,342	0
14	ZN	I	202	1/1	0.90	0.08	287,287,287,287	0
14	ZN	I	201	1/1	0.93	0.06	216,216,216,216	0
14	ZN	B	1301	1/1	0.96	0.04	216,216,216,216	0
14	ZN	A	1802	1/1	0.96	0.04	208,208,208,208	0
14	ZN	C	401	1/1	0.97	0.05	158,158,158,158	0
14	ZN	J	101	1/1	0.99	0.05	115,115,115,115	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around ATP B 1302:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.