



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 01:15 AM UTC

PDB ID : 3GTO / pdb_00003gto
Title : Backtracked RNA polymerase II complex with 15mer RNA
Authors : Wang, D.; Bushnell, D.A.; Huang, X.; Westover, K.D.; Levitt, M.; Kornberg, R.D.
Deposited on : 2009-03-27
Resolution : 4.00 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
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

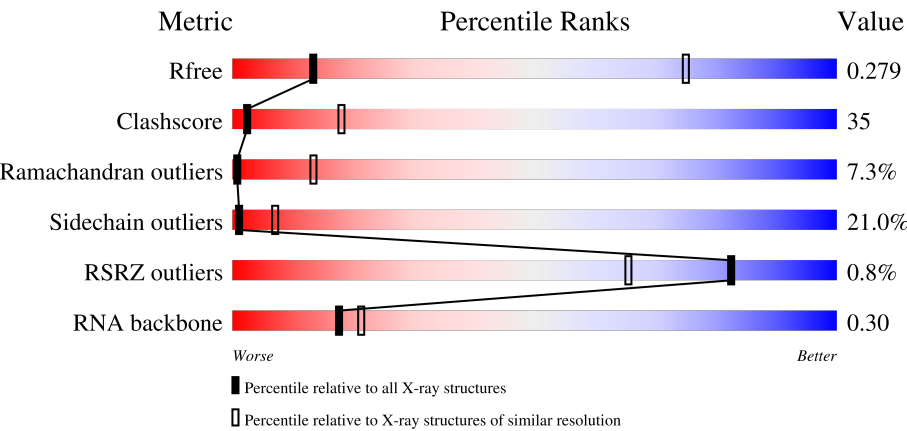
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.00 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	1082 (4.20-3.80)
Clashscore	190562	1129 (4.20-3.80)
Ramachandran outliers	187476	1064 (4.20-3.80)
Sidechain outliers	187428	1055 (4.20-3.80)
RSRZ outliers	180081	1082 (4.20-3.80)
RNA backbone	3983	1017 (4.84-3.10)

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	A	1733	29% 36% 13% • 20%
2	B	1224	33% 41% 14% • 10%
3	C	318	33% 38% 10% • 16%
4	E	215	44% 42% 12% •

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Mol	Chain	Length	Quality of chain
5	F	155	23%22%8%•46%
6	H	146	% 36%37%18%9%
7	I	122	% 38%45%15%•
8	J	70	23%50%16%•7%
9	K	120	38%44%12%•5%
10	L	70	% 19%29%16%•34%
11	R	15	13%33%27%7%20%
12	T	28	36%64%
13	N	14	7% 79%21%

2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 29259 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 protein called DNA-directed RNA polymerase II subunit RPB1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1395	Total	C	N	O	S	0	0	0
			10969	6917	1923	2068	61			

- Molecule 2 is a protein called DNA-directed RNA polymerase II subunit RPB2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	1106	Total	C	N	O	S	0	0	0
			8792	5568	1538	1631	55			

- Molecule 3 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	266	Total	C	N	O	S	0	0	0
			2095	1317	348	417	13			

- Molecule 4 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	214	Total	C	N	O	S	0	0	0
			1752	1111	309	321	11			

- Molecule 5 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	84	Total	C	N	O	S	0	0	0
			679	434	115	127	3			

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	H	133	Total	C	N	O	S	0	0	0
			1068	673	180	211	4			

- Molecule 7 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	I	119	Total	C	N	O	S	0	0	0
			971	596	179	186	10			

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

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

- Molecule 9 is a protein called DNA-directed RNA polymerase II subunit RPB11.

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

- Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	L	46	Total	C	N	O	S	0	0	0
			363	224	72	63	4			

- Molecule 11 is a RNA chain called RNA (5'-R(*AP*UP*CP*GP*AP*GP*AP*GP*GP*AP*UP*GP*CP*AP*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	R	12	Total	C	N	O	P	0	0	0
			260	117	52	80	11			

- Molecule 12 is a DNA chain called DNA (28-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	T	28	Total	C	N	O	P	0	0	0
			566	271	104	164	27			

- Molecule 13 is a DNA chain called DNA (5'-D(*CP*TP*GP*CP*TP*TP*AP*TP*CP*GP*GP*TP*AP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	N	14	Total	C	N	O	P	0	0	0
			284	137	49	85	13			

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

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

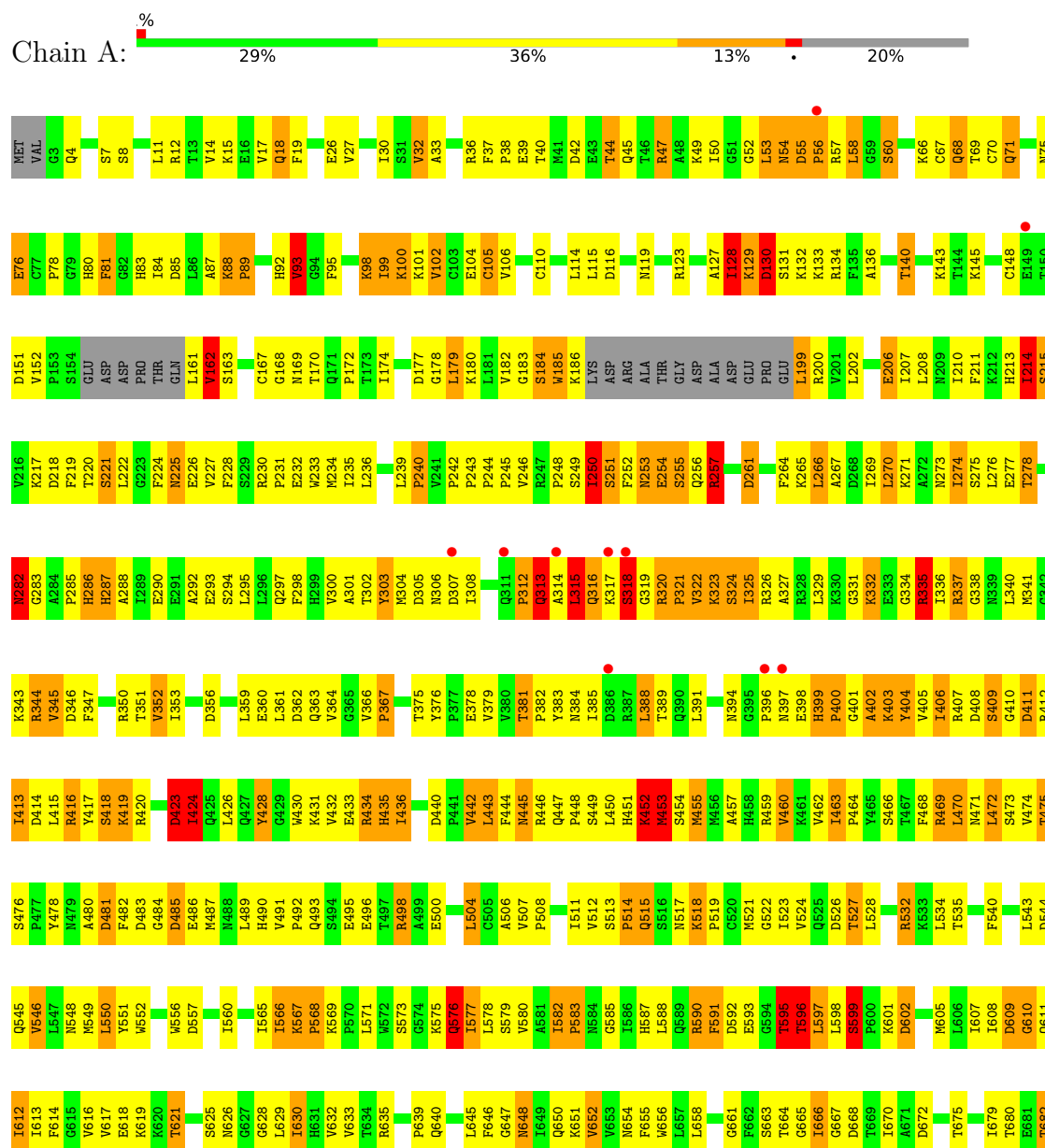
- Molecule 15 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

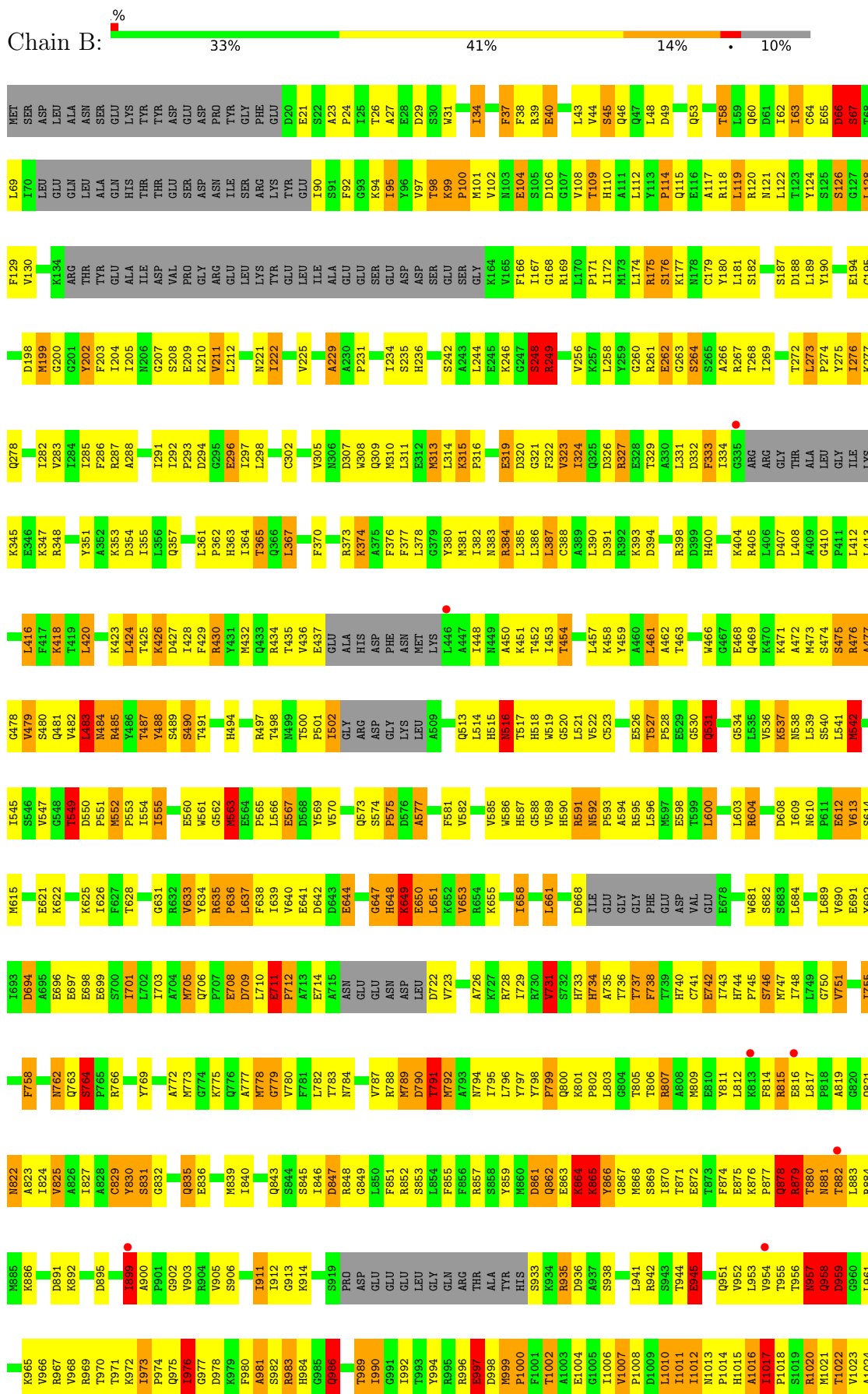
3 Residue-property plots

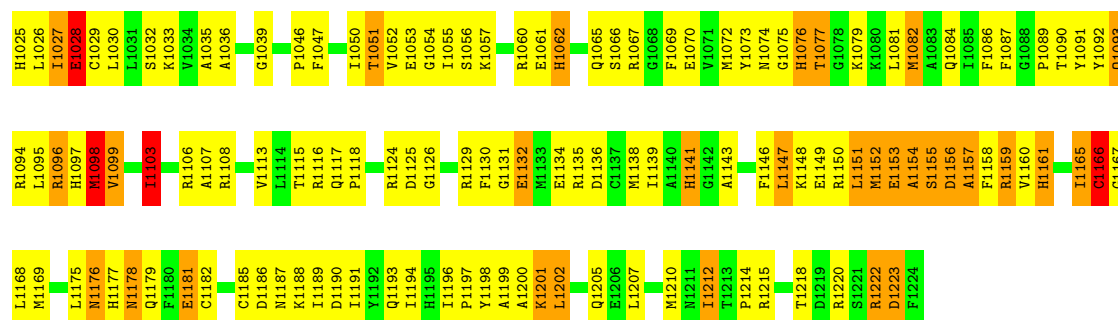
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: DNA-directed RNA polymerase II subunit RPB1



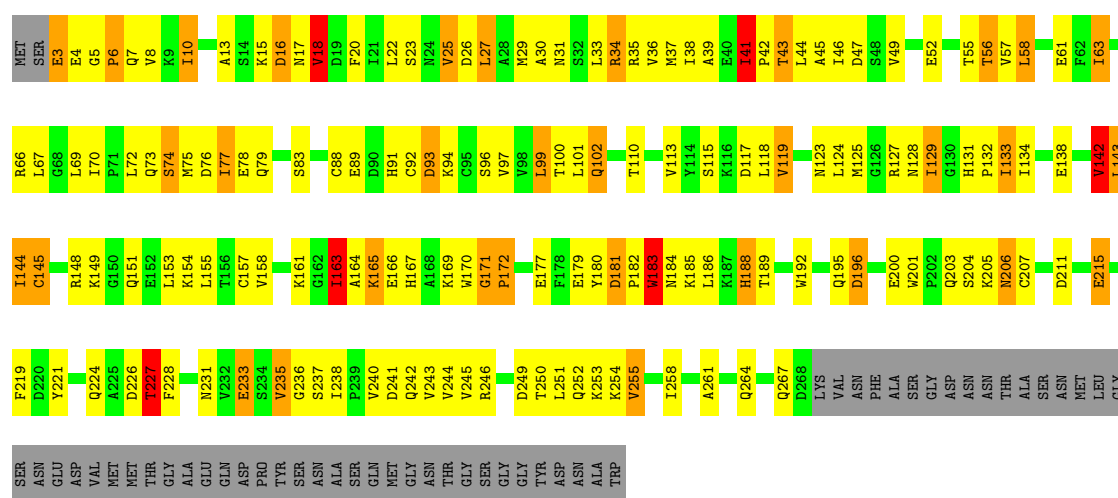
- Molecule 2: DNA-directed RNA polymerase II subunit RPB2





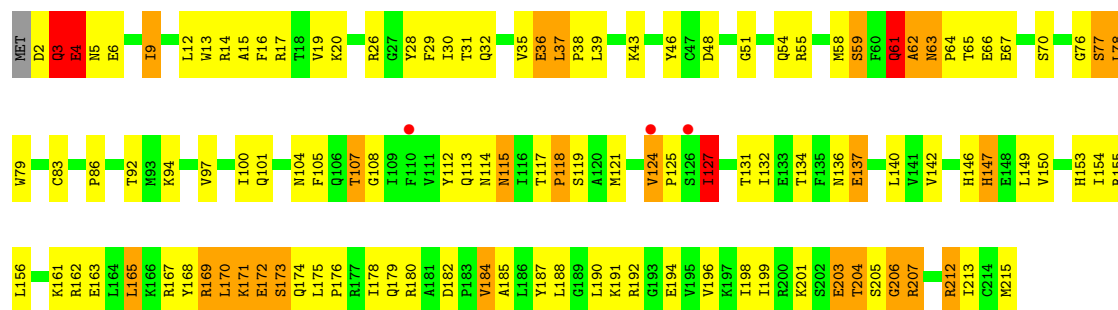
• Molecule 3: DNA-directed RNA polymerase II subunit RPB3

Chain C: 33% 38% 10% 16%



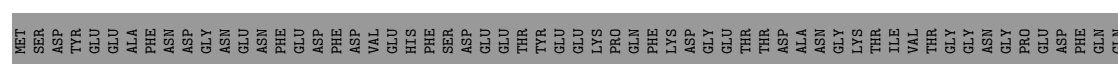
• Molecule 4: DNA-directed RNA polymerases I, II, and III subunit RPABC1

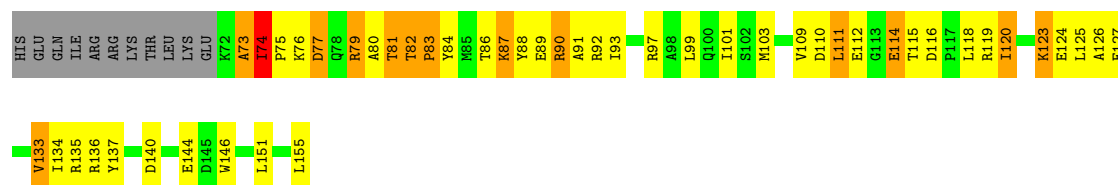
Chain E: 44% 42% 12%



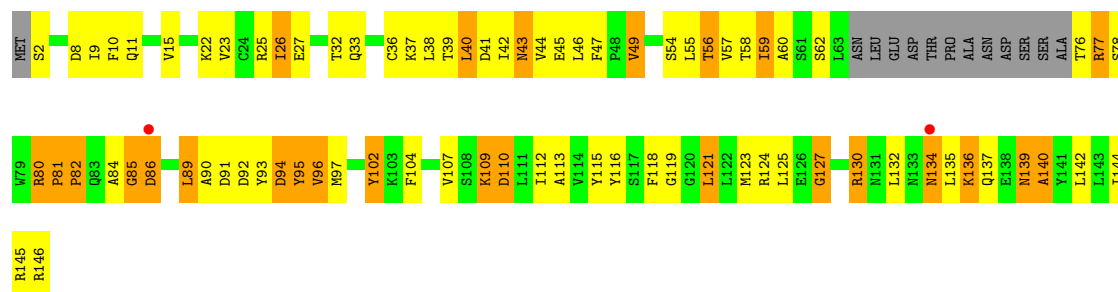
• Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC2

Chain F: 23% 22% 8% 46%

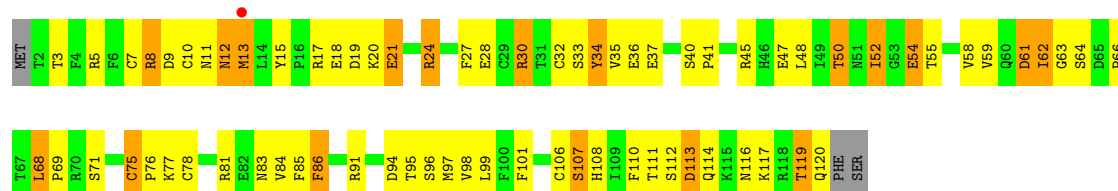




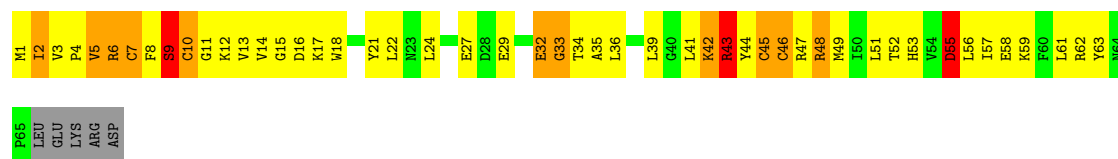
- Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC3



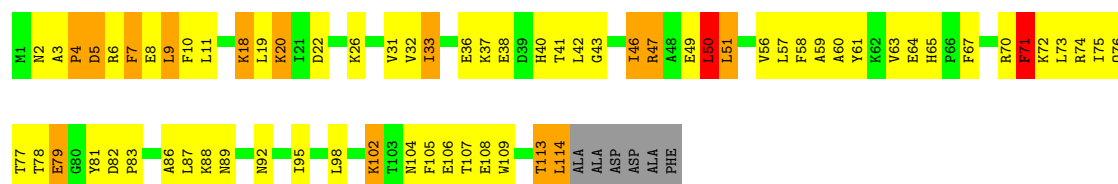
- Molecule 7: DNA-directed RNA polymerase II subunit RPB9



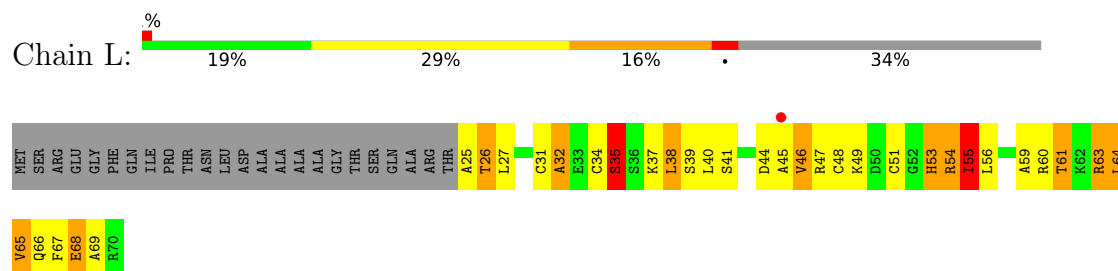
- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC5



- Molecule 9: DNA-directed RNA polymerase II subunit RPB11



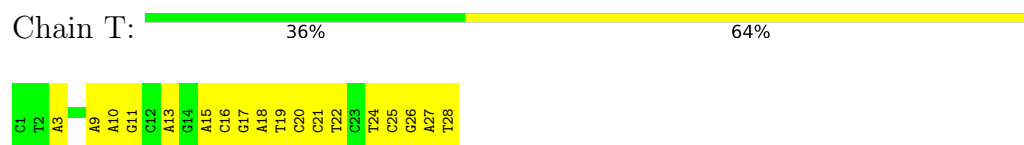
- Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC4



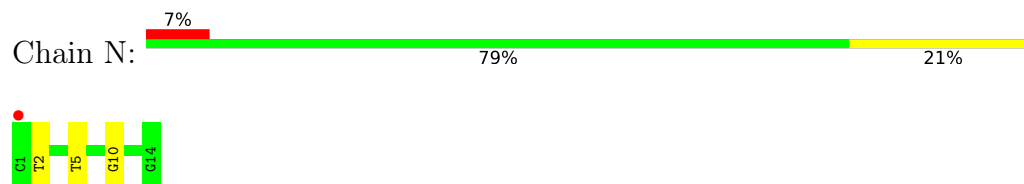
- Molecule 11: RNA (5'-R(*AP*UP*CP*GP*AP*GP*AP*GP*GP*AP*UP*GP*CP*AP*C)-3')



- Molecule 12: DNA (28-MER)



- Molecule 13: DNA (5'-D(*CP*TP*GP*CP*TP*TP*AP*TP*CP*GP*GP*TP*AP*G)-3')



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	170.85Å 222.80Å 194.98Å 90.00° 101.98° 90.00°	Depositor
Resolution (Å)	50.00 – 4.00 50.00 – 4.00	Depositor EDS
% Data completeness (in resolution range)	93.6 (50.00-4.00) 93.6 (50.00-4.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.52 (at 4.00Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.269 , 0.290 0.263 , 0.279	Depositor DCC
R_{free} test set	2847 reflections (4.74%)	wwPDB-VP
Wilson B-factor (Å ²)	109.1	Xtriage
Anisotropy	0.101	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 86.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	29259	wwPDB-VP
Average B, all atoms (Å ²)	125.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.71% 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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.13	46/11163 (0.4%)	1.13	50/15091 (0.3%)
2	B	1.25	48/8963 (0.5%)	1.15	43/12086 (0.4%)
3	C	1.24	9/2133 (0.4%)	1.16	10/2891 (0.3%)
4	E	1.19	12/1788 (0.7%)	1.02	4/2406 (0.2%)
5	F	1.18	3/691 (0.4%)	1.08	1/933 (0.1%)
6	H	1.14	3/1086 (0.3%)	1.07	8/1470 (0.5%)
7	I	1.25	7/989 (0.7%)	1.12	5/1331 (0.4%)
8	J	1.25	7/541 (1.3%)	1.16	3/727 (0.4%)
9	K	1.11	2/937 (0.2%)	1.01	0/1265
10	L	1.37	2/365 (0.5%)	1.20	2/485 (0.4%)
11	R	0.90	1/292 (0.3%)	1.32	5/455 (1.1%)
12	T	0.67	1/634 (0.2%)	1.20	4/975 (0.4%)
13	N	0.85	0/317	0.96	1/488 (0.2%)
All	All	1.18	141/29899 (0.5%)	1.13	136/40603 (0.3%)

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
3	C	0	1
6	H	0	1
7	I	0	1
All	All	0	3

All (141) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	731	VAL	C-O	9.47	1.35	1.24
2	B	823	ALA	C-O	8.81	1.34	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	J	33	GLY	C-O	8.61	1.35	1.23
2	B	574	SER	CB-OG	8.43	1.59	1.42
4	E	155	ARG	CZ-NH1	8.18	1.44	1.32
1	A	870	GLU	C-O	8.06	1.34	1.24
1	A	1194	ARG	CZ-NH1	8.02	1.44	1.32
1	A	900	ASP	C-O	7.85	1.32	1.24
1	A	179	LEU	C-O	7.79	1.33	1.23
1	A	682	THR	C-O	7.72	1.34	1.24
1	A	1270	ASN	C-N	7.61	1.40	1.33
4	E	121	MET	SD-CE	7.58	1.98	1.79
1	A	1433	MET	SD-CE	7.49	1.98	1.79
1	A	1117	THR	CB-OG1	7.37	1.55	1.43
1	A	1173	HIS	CE1-NE2	7.20	1.39	1.32
6	H	49	VAL	C-O	6.99	1.32	1.23
4	E	137	GLU	CD-OE1	6.94	1.38	1.25
8	J	46	CYS	C-O	6.86	1.32	1.24
7	I	61	ASP	CG-OD1	6.69	1.38	1.25
3	C	170	TRP	C-O	6.67	1.32	1.24
7	I	54	GLU	CD-OE1	6.62	1.38	1.25
2	B	1117	GLN	CD-NE2	6.60	1.47	1.33
10	L	35	SER	C-O	6.59	1.32	1.24
3	C	18	VAL	C-O	6.56	1.31	1.24
4	E	62	ALA	C-O	6.54	1.31	1.23
2	B	935	ARG	CZ-NH1	6.50	1.41	1.32
1	A	732	LEU	C-O	6.50	1.32	1.24
4	E	94	LYS	C-O	6.44	1.32	1.24
1	A	85	ASP	CG-OD1	6.41	1.37	1.25
4	E	201	LYS	C-O	6.30	1.31	1.23
1	A	1426	GLU	CD-OE1	6.30	1.37	1.25
5	F	103	MET	SD-CE	6.29	1.95	1.79
2	B	731	VAL	C-N	6.29	1.41	1.33
2	B	327	ARG	CZ-NH2	6.25	1.41	1.33
4	E	207	ARG	CZ-NH1	6.24	1.41	1.32
1	A	871	ASP	N-CA	6.22	1.51	1.46
2	B	39	ARG	CZ-NH1	6.21	1.41	1.32
2	B	598	GLU	CD-OE2	6.21	1.37	1.25
3	C	41	ILE	CA-CB	6.20	1.62	1.54
1	A	1423	GLY	C-O	6.19	1.32	1.23
2	B	1161	HIS	CE1-NE2	6.17	1.38	1.32
1	A	1426	GLU	CD-OE2	6.14	1.37	1.25
2	B	661	LEU	C-O	6.09	1.32	1.24
2	B	114	PRO	C-N	6.09	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	L	67	PHE	C-N	6.09	1.42	1.33
3	C	74	SER	CB-OG	6.08	1.54	1.42
1	A	177	ASP	CG-OD1	6.08	1.36	1.25
2	B	635	ARG	CZ-NH1	6.08	1.41	1.32
2	B	990	ILE	CA-CB	6.07	1.60	1.54
1	A	449	SER	C-O	6.06	1.31	1.24
1	A	665	GLY	C-O	6.06	1.29	1.23
2	B	957	ASN	CG-OD1	6.04	1.35	1.23
1	A	700	ASN	CG-OD1	6.02	1.34	1.23
1	A	1173	HIS	CG-ND1	6.00	1.44	1.38
4	E	63	ASN	CG-OD1	5.96	1.34	1.23
2	B	384	ARG	CZ-NH1	5.95	1.41	1.32
2	B	110	HIS	CE1-NE2	5.92	1.38	1.32
1	A	1025	ARG	NE-CZ	5.92	1.39	1.33
2	B	989	THR	CA-CB	5.90	1.63	1.53
2	B	967	ARG	CZ-NH1	5.87	1.41	1.32
2	B	1199	ALA	C-O	5.87	1.31	1.24
2	B	549	THR	CB-OG1	5.85	1.53	1.43
2	B	722	ASP	CG-OD2	5.83	1.36	1.25
2	B	531	GLN	CD-NE2	5.82	1.45	1.33
1	A	930	ASP	CG-OD2	5.81	1.36	1.25
2	B	327	ARG	CD-NE	5.80	1.54	1.46
4	E	61	GLN	CD-NE2	5.79	1.45	1.33
3	C	250	THR	CB-OG1	5.79	1.53	1.43
7	I	12	ASN	CG-ND2	5.79	1.45	1.33
7	I	113	ASP	CG-OD1	5.78	1.36	1.25
6	H	127	GLY	C-O	5.77	1.31	1.23
1	A	36	ARG	NE-CZ	5.76	1.39	1.33
2	B	542	MET	SD-CE	5.76	1.94	1.79
2	B	307	ASP	CG-OD1	5.75	1.36	1.25
6	H	130	ARG	C-O	5.73	1.31	1.24
2	B	742	GLU	CD-OE1	5.72	1.36	1.25
3	C	58	LEU	C-O	5.71	1.30	1.23
2	B	407	ASP	C-O	5.70	1.30	1.24
1	A	278	THR	C-O	5.69	1.31	1.24
2	B	750	GLY	N-CA	5.69	1.51	1.45
2	B	307	ASP	CG-OD2	5.65	1.36	1.25
2	B	262	GLU	C-O	5.65	1.30	1.23
12	T	3	DA	O5'-C5'	5.63	1.59	1.42
1	A	36	ARG	CZ-NH1	5.63	1.40	1.32
1	A	350	ARG	CZ-NH1	5.62	1.40	1.32
2	B	986	GLN	CG-CD	5.61	1.66	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	980	ASP	CG-OD1	5.59	1.35	1.25
2	B	353	LYS	CG-CD	5.58	1.69	1.52
2	B	1070	GLU	CB-CG	5.58	1.69	1.52
4	E	127	ILE	CA-CB	5.56	1.61	1.54
4	E	4	GLU	CD-OE1	5.54	1.35	1.25
8	J	43	ARG	CZ-NH1	5.53	1.40	1.32
5	F	82	THR	CB-OG1	-5.52	1.34	1.43
2	B	1035	ALA	C-O	5.50	1.31	1.24
2	B	1155	SER	CA-C	5.46	1.58	1.53
9	K	38	GLU	CD-OE1	5.46	1.35	1.25
2	B	549	THR	CA-CB	5.45	1.60	1.53
8	J	9	SER	CB-OG	5.44	1.53	1.42
1	A	1108	ALA	C-O	5.43	1.30	1.24
2	B	430	ARG	CZ-NH1	5.42	1.40	1.32
8	J	29	GLU	CD-OE2	5.42	1.35	1.25
3	C	206	ASN	CG-OD1	5.41	1.33	1.23
3	C	224	GLN	CD-OE1	5.39	1.33	1.23
11	R	10	A	P-O5'	5.35	1.67	1.59
1	A	1372	VAL	CA-CB	5.34	1.59	1.54
2	B	110	HIS	CG-ND1	5.33	1.44	1.38
1	A	870	GLU	C-N	5.30	1.44	1.34
2	B	959	ASP	C-O	5.29	1.30	1.24
1	A	1154	TYR	C-O	5.29	1.30	1.23
7	I	24	ARG	CZ-NH1	5.29	1.40	1.32
8	J	55	ASP	CG-OD2	5.29	1.35	1.25
1	A	220	THR	C-O	5.28	1.30	1.24
1	A	217	LYS	C-O	5.26	1.30	1.24
1	A	609	ASP	C-N	5.22	1.41	1.33
1	A	787	PHE	C-O	5.22	1.30	1.23
5	F	87	LYS	CG-CD	5.22	1.68	1.52
1	A	1394	THR	CA-CB	5.20	1.60	1.53
7	I	45	ARG	CZ-NH1	5.20	1.40	1.32
1	A	1030	ARG	NE-CZ	5.19	1.38	1.33
1	A	1165	GLU	CD-OE1	5.18	1.35	1.25
1	A	240	PRO	C-N	5.18	1.37	1.33
1	A	435	HIS	CE1-NE2	5.14	1.37	1.32
2	B	722	ASP	CG-OD1	5.13	1.35	1.25
1	A	1187	GLN	CD-NE2	5.13	1.44	1.33
7	I	81	ARG	CZ-NH1	5.13	1.40	1.32
3	C	118	LEU	C-O	5.12	1.30	1.23
1	A	847	ASP	C-O	5.12	1.31	1.24
9	K	5	ASP	CG-OD2	5.12	1.35	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	522	GLY	N-CA	5.12	1.52	1.45
4	E	137	GLU	CD-OE2	5.11	1.35	1.25
2	B	789	MET	SD-CE	5.09	1.92	1.79
1	A	992	ASP	CG-OD2	5.08	1.35	1.25
2	B	990	ILE	C-O	5.08	1.29	1.24
2	B	779	GLY	C-N	5.06	1.38	1.33
2	B	454	THR	CB-OG1	5.05	1.51	1.43
2	B	374	LYS	C-O	5.03	1.30	1.24
2	B	577	ALA	C-O	5.03	1.30	1.24
2	B	1025	HIS	CE1-NE2	5.03	1.37	1.32
8	J	29	GLU	CD-OE1	5.02	1.34	1.25
1	A	609	ASP	C-O	5.01	1.30	1.24
1	A	47	ARG	NE-CZ	5.01	1.38	1.33

All (136) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1172	LEU	N-CA-C	21.07	136.75	112.72
1	A	1173	HIS	N-CA-C	12.70	137.86	110.80
2	B	323	VAL	N-CA-C	-9.33	103.27	113.43
1	A	1172	LEU	CB-CA-C	-8.67	96.63	110.94
1	A	88	LYS	CA-C-N	8.20	130.09	119.84
1	A	88	LYS	C-N-CA	8.20	130.09	119.84
8	J	5	VAL	N-CA-C	-8.03	101.30	110.05
2	B	976	ILE	N-CA-C	7.85	117.91	110.30
2	B	469	GLN	N-CA-C	7.83	120.91	111.82
2	B	764	SER	CA-C-N	-7.67	112.30	119.82
2	B	764	SER	C-N-CA	-7.67	112.30	119.82
2	B	723	VAL	N-CA-C	7.56	118.75	108.17
6	H	92	ASP	N-CA-C	-7.37	104.29	113.28
1	A	1173	HIS	N-CA-CB	-7.29	98.17	110.49
2	B	1154	ALA	N-CA-C	-7.22	101.53	110.41
2	B	1011	ILE	CB-CA-C	-7.18	101.08	110.84
2	B	69	LEU	N-CA-C	7.08	118.84	108.86
1	A	714	PHE	N-CA-C	-7.03	104.58	113.43
2	B	758	PHE	CA-C-N	-7.00	111.77	119.19
2	B	758	PHE	C-N-CA	-7.00	111.77	119.19
12	T	3	DA	C5'-C4'-C3'	6.90	125.25	114.90
3	C	41	ILE	CA-C-N	6.86	126.89	119.89
3	C	41	ILE	C-N-CA	6.86	126.89	119.89
2	B	861	ASP	N-CA-C	6.78	118.50	108.60
2	B	222	ILE	N-CA-C	6.60	117.35	108.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	H	109	LYS	CA-C-N	6.59	133.57	121.70
6	H	109	LYS	C-N-CA	6.59	133.57	121.70
1	A	595	THR	N-CA-C	6.50	119.32	108.20
1	A	345	VAL	N-CA-C	6.49	118.50	108.44
3	C	171	GLY	CA-C-N	6.49	127.95	119.84
3	C	171	GLY	C-N-CA	6.49	127.95	119.84
2	B	479	VAL	N-CA-C	-6.46	99.58	109.78
2	B	903	VAL	N-CA-C	6.43	117.87	109.58
6	H	137	GLN	N-CA-C	6.42	119.96	110.46
1	A	1393	ASN	N-CA-C	6.37	124.36	110.80
1	A	886	ILE	N-CA-C	6.34	117.91	111.00
12	T	21	DC	O3'-P-O5'	-6.33	94.51	104.00
3	C	255	VAL	N-CA-C	-6.26	104.65	110.53
4	E	149	LEU	CA-C-N	-6.26	117.28	123.04
4	E	149	LEU	C-N-CA	-6.26	117.28	123.04
2	B	66	ASP	N-CA-C	-6.25	105.30	113.17
1	A	596	THR	N-CA-C	6.24	117.93	110.44
1	A	977	LYS	CA-C-N	6.22	126.19	120.03
1	A	977	LYS	C-N-CA	6.22	126.19	120.03
2	B	99	LYS	CA-C-N	6.18	127.56	119.84
2	B	99	LYS	C-N-CA	6.18	127.56	119.84
1	A	388	LEU	N-CA-C	6.08	117.78	111.03
10	L	32	ALA	N-CA-C	6.06	119.14	111.69
2	B	476	ARG	N-CA-C	-6.05	104.47	112.34
2	B	899	ILE	CB-CA-C	-5.95	105.04	111.59
2	B	900	ALA	CA-C-N	5.94	127.26	119.84
2	B	900	ALA	C-N-CA	5.94	127.26	119.84
1	A	964	ILE	N-CA-C	5.89	115.95	110.42
10	L	67	PHE	N-CA-C	5.88	118.10	108.52
1	A	1279	ILE	N-CA-C	5.87	114.80	106.53
3	C	163	ILE	N-CA-C	5.86	118.42	108.86
1	A	973	ILE	N-CA-C	5.85	117.01	108.53
1	A	1319	VAL	CA-C-N	5.83	125.74	119.85
1	A	1319	VAL	C-N-CA	5.83	125.74	119.85
1	A	93	VAL	N-CA-C	5.79	121.39	109.34
1	A	423	ASP	CB-CA-C	-5.76	108.12	116.54
7	I	48	LEU	N-CA-C	-5.75	105.36	112.72
1	A	1163	ILE	CA-C-N	5.72	125.25	119.19
1	A	1163	ILE	C-N-CA	5.72	125.25	119.19
11	R	9	G	C4'-C3'-O3'	-5.72	104.43	113.00
1	A	452	LYS	N-CA-C	-5.66	105.19	111.36
1	A	993	LEU	N-CA-C	-5.65	105.04	111.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	273	LEU	CA-C-N	5.62	126.87	119.84
2	B	273	LEU	C-N-CA	5.62	126.87	119.84
2	B	320	ASP	N-CA-C	-5.62	106.46	113.15
11	R	10	A	C4'-C3'-O3'	-5.62	104.58	113.00
1	A	1299	VAL	N-CA-C	5.61	115.67	108.82
1	A	1222	ASN	N-CA-C	5.61	116.45	108.54
3	C	181	ASP	CA-C-N	5.60	126.84	119.84
3	C	181	ASP	C-N-CA	5.60	126.84	119.84
1	A	890	ASP	N-CA-C	-5.57	105.58	112.38
13	N	10	DG	P-O3'-C3'	5.55	128.53	120.20
1	A	71	GLN	CB-CA-C	-5.54	109.20	115.79
2	B	1016	ALA	N-CA-C	-5.54	107.10	112.97
6	H	26	ILE	N-CA-C	5.52	115.94	107.77
1	A	242	PRO	CA-C-N	5.52	126.06	120.38
1	A	242	PRO	C-N-CA	5.52	126.06	120.38
1	A	582	ILE	CA-C-N	5.51	126.73	119.84
1	A	582	ILE	C-N-CA	5.51	126.73	119.84
2	B	211	VAL	CB-CA-C	-5.51	102.99	111.31
12	T	3	DA	C5'-C4'-O4'	5.51	117.66	109.40
1	A	652	VAL	CB-CA-C	-5.47	104.71	111.94
1	A	532	ARG	N-CA-C	-5.47	104.96	111.03
1	A	999	VAL	N-CA-C	-5.47	107.30	111.62
4	E	115	ASN	N-CA-C	5.47	116.76	108.07
3	C	188	HIS	N-CA-C	-5.46	106.57	113.18
2	B	296	GLU	N-CA-C	-5.45	104.87	112.45
1	A	543	LEU	N-CA-C	5.45	117.65	111.11
2	B	734	HIS	N-CA-C	5.45	122.41	110.80
1	A	870	GLU	CA-C-N	-5.43	111.81	120.17
1	A	870	GLU	C-N-CA	-5.43	111.81	120.17
2	B	523	CYS	CA-C-N	5.41	124.93	119.19
2	B	523	CYS	C-N-CA	5.41	124.93	119.19
2	B	1125	ASP	N-CA-C	-5.41	103.92	111.39
4	E	147	HIS	N-CA-C	5.41	117.87	110.24
2	B	1222	ARG	NE-CZ-NH2	5.40	124.06	119.20
2	B	1076	HIS	N-CA-C	-5.39	105.56	111.82
1	A	453	MET	N-CA-C	5.39	119.34	112.87
1	A	1428	VAL	N-CA-C	-5.37	105.48	110.53
11	R	10	A	O3'-P-O5'	-5.33	96.00	104.00
2	B	37	PHE	N-CA-C	-5.28	103.51	110.43
1	A	1323	ASP	CA-C-N	5.28	126.44	119.84
1	A	1323	ASP	C-N-CA	5.28	126.44	119.84
11	R	12	G	C3'-C2'-C1'	5.20	106.70	101.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	H	96	VAL	N-CA-C	5.20	115.39	108.27
2	B	410	GLY	CA-C-N	5.19	124.91	119.82
2	B	410	GLY	C-N-CA	5.19	124.91	119.82
3	C	183	TRP	N-CA-C	-5.19	103.67	110.53
6	H	40	LEU	N-CA-C	5.18	117.81	108.48
2	B	1000	PRO	N-CA-C	-5.18	103.97	111.22
8	J	45	CYS	N-CA-C	-5.18	105.55	111.14
7	I	68	LEU	CA-C-N	5.18	125.18	120.21
7	I	68	LEU	C-N-CA	5.18	125.18	120.21
2	B	711	GLU	CA-C-N	-5.14	113.41	119.84
2	B	711	GLU	C-N-CA	-5.14	113.41	119.84
2	B	945	GLU	N-CA-C	5.13	118.31	110.36
8	J	10	CYS	CA-CB-SG	5.13	126.20	114.40
1	A	261	ASP	N-CA-C	5.12	119.38	113.18
2	B	1098	MET	CB-CG-SD	-5.12	97.36	112.70
1	A	924	LYS	N-CA-C	-5.11	107.02	114.12
5	F	83	PRO	N-CA-C	-5.10	106.89	113.57
11	R	11	U	N1-C1'-C2'	5.10	119.65	112.00
1	A	776	ALA	N-CA-C	5.08	116.89	110.33
12	T	22	DT	O3'-P-O5'	-5.08	96.39	104.00
1	A	1405	THR	N-CA-C	5.05	116.48	110.97
1	A	352	VAL	CB-CA-C	-5.04	104.72	111.13
6	H	36	CYS	N-CA-C	5.03	117.53	108.48
7	I	75	CYS	CA-C-N	5.02	126.12	119.84
7	I	75	CYS	C-N-CA	5.02	126.12	119.84
2	B	114	PRO	O-C-N	5.02	127.60	122.18
1	A	746	MET	N-CA-C	-5.00	105.91	111.36

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	172	PRO	Peptide
6	H	136	LYS	Peptide
7	I	77	LYS	Peptide

5.2 Too-close contacts

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

the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	10969	0	11071	970	0
2	B	8792	0	8824	662	0
3	C	2095	0	2052	139	0
4	E	1752	0	1776	95	0
5	F	679	0	701	47	0
6	H	1068	0	1040	68	0
7	I	971	0	928	48	0
8	J	532	0	544	71	0
9	K	919	0	929	67	0
10	L	363	0	387	21	0
11	R	260	0	132	15	0
12	T	566	0	316	22	0
13	N	284	0	161	5	0
14	A	2	0	0	0	0
14	B	1	0	0	0	0
14	C	1	0	0	1	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
All	All	29259	0	28861	2038	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 35.

All (2038) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:399:HIS:CG	1:A:400:PRO:HD3	1.44	1.48
1:A:315:LEU:HB2	1:A:316:GLN:C	1.39	1.47
1:A:315:LEU:HB2	1:A:316:GLN:CA	1.51	1.38
1:A:256:GLN:CA	1:A:257:ARG:HB3	1.59	1.30
1:A:1111:MET:CG	1:A:1114:PRO:HG3	1.64	1.27
1:A:1116:LEU:HD23	1:A:1329:THR:CG2	1.68	1.22
1:A:256:GLN:HA	1:A:257:ARG:CB	1.60	1.21
1:A:868:TYR:CE1	1:A:1064:VAL:HG11	1.76	1.21
1:A:320:ARG:N	1:A:320:ARG:HD2	1.45	1.19
2:B:864:LYS:HG3	2:B:865:LYS:N	1.59	1.18
1:A:399:HIS:CG	1:A:400:PRO:CD	2.29	1.16
1:A:399:HIS:CD2	1:A:400:PRO:HD3	1.81	1.16

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:J:44:TYR:HA	8:J:47:ARG:HB2	1.26	1.15
1:A:399:HIS:CB	1:A:400:PRO:HD3	1.75	1.15
1:A:315:LEU:CD2	1:A:316:GLN:HA	1.77	1.14
1:A:323:LYS:HD3	1:A:323:LYS:N	1.50	1.14
2:B:635:ARG:HB2	2:B:636:PRO:HD2	1.29	1.14
2:B:865:LYS:CG	2:B:866:TYR:H	1.61	1.14
1:A:1116:LEU:HD23	1:A:1329:THR:HG22	1.30	1.12
1:A:129:LYS:O	1:A:130:ASP:HB2	1.45	1.12
1:A:253:ASN:HA	1:A:256:GLN:O	1.48	1.11
1:A:590:ARG:HG3	1:A:590:ARG:HH11	0.99	1.11
1:A:351:THR:HG23	2:B:1103:ILE:HD12	1.12	1.11
2:B:796:LEU:HB3	2:B:799:PRO:HD3	1.29	1.11
1:A:399:HIS:CB	1:A:400:PRO:CD	2.29	1.10
1:A:567:LYS:HB2	1:A:568:PRO:HD2	1.12	1.10
1:A:399:HIS:HB3	1:A:400:PRO:CD	1.83	1.08
2:B:882:THR:HG21	2:B:935:ARG:HA	1.30	1.08
3:C:70:ILE:HD11	3:C:144:ILE:HD11	1.27	1.08
2:B:1099:VAL:HG12	2:B:1103:ILE:HD11	1.31	1.07
1:A:315:LEU:H	1:A:315:LEU:HD13	1.20	1.07
1:A:573:SER:O	1:A:576:GLN:HB2	1.52	1.07
1:A:315:LEU:HB2	1:A:317:LYS:N	1.68	1.07
11:R:4:G:H2'	11:R:5:A:H8	1.07	1.07
1:A:315:LEU:CB	1:A:316:GLN:CA	2.30	1.06
1:A:765:VAL:CG2	1:A:800:VAL:HB	1.84	1.06
2:B:976:ILE:O	2:B:990:ILE:HB	1.56	1.06
11:R:4:G:H2'	11:R:5:A:C8	1.89	1.06
1:A:213:HIS:O	1:A:214:ILE:O	1.72	1.06
1:A:805:LEU:C	1:A:805:LEU:HD13	1.78	1.06
2:B:865:LYS:HG2	2:B:866:TYR:N	1.44	1.06
2:B:642:ASP:HB3	2:B:649:LYS:HG3	1.32	1.06
1:A:49:LYS:HD3	1:A:55:ASP:OD1	1.54	1.05
1:A:315:LEU:CB	1:A:316:GLN:HA	1.84	1.05
1:A:567:LYS:CB	1:A:568:PRO:HD2	1.87	1.05
1:A:868:TYR:HE1	1:A:1064:VAL:CG1	1.71	1.04
1:A:315:LEU:HB3	1:A:318:SER:N	1.71	1.04
1:A:855:THR:HG21	1:A:857:ARG:HE	1.23	1.04
2:B:634:TYR:HE1	2:B:692:TYR:CD1	1.75	1.03
8:J:5:VAL:HG12	8:J:6:ARG:HG3	1.36	1.03
3:C:102:GLN:HG2	3:C:154:LYS:HD3	1.39	1.03
1:A:630:ILE:H	1:A:630:ILE:HD12	1.19	1.03
1:A:67:CYS:HB3	1:A:70:CYS:SG	1.97	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:320:ARG:H	1:A:320:ARG:CD	1.62	1.02
1:A:567:LYS:HB2	1:A:568:PRO:CD	1.88	1.02
1:A:315:LEU:CB	1:A:316:GLN:C	2.33	1.01
1:A:322:VAL:C	1:A:323:LYS:HD3	1.85	1.01
1:A:805:LEU:HD13	1:A:805:LEU:O	1.60	1.01
1:A:315:LEU:HB3	1:A:318:SER:H	0.85	1.01
1:A:868:TYR:HE1	1:A:1064:VAL:HG11	0.85	1.01
1:A:351:THR:CG2	2:B:1103:ILE:HD12	1.89	1.00
1:A:344:ARG:HG3	1:A:344:ARG:HH11	1.25	1.00
1:A:319:GLY:CA	1:A:320:ARG:HH11	1.75	1.00
2:B:913:GLY:HA2	2:B:938:SER:HB3	1.40	1.00
1:A:446:ARG:NE	1:A:480:ALA:HB2	1.77	0.99
1:A:1342:GLU:HG2	4:E:212:ARG:NH1	1.77	0.99
1:A:253:ASN:HB3	1:A:257:ARG:N	1.77	0.99
1:A:1364:ASN:ND2	1:A:1366:ARG:HG2	1.78	0.99
1:A:351:THR:HG23	2:B:1103:ILE:CD1	1.93	0.98
1:A:1111:MET:SD	1:A:1114:PRO:HG3	2.02	0.98
2:B:636:PRO:HB3	2:B:743:ILE:HG13	1.41	0.98
1:A:320:ARG:HD2	1:A:320:ARG:H	0.84	0.98
1:A:256:GLN:HA	1:A:257:ARG:HB3	1.05	0.98
6:H:47:PHE:HB3	6:H:95:TYR:HD1	1.28	0.98
1:A:573:SER:H	1:A:576:GLN:HG3	1.23	0.97
2:B:1149:GLU:HG3	2:B:1153:GLU:HG2	1.47	0.96
4:E:86:PRO:CB	4:E:114:ASN:HD22	1.77	0.96
2:B:1096:ARG:HG2	2:B:1096:ARG:HH11	1.26	0.96
1:A:590:ARG:HG3	1:A:590:ARG:NH1	1.79	0.96
2:B:864:LYS:HG3	2:B:865:LYS:H	1.27	0.95
1:A:765:VAL:HG23	1:A:800:VAL:HB	1.48	0.95
8:J:3:VAL:HG21	8:J:18:TRP:HB2	1.46	0.95
2:B:363:HIS:O	2:B:364:ILE:HB	1.67	0.94
1:A:567:LYS:HB3	6:H:96:VAL:H	1.32	0.94
1:A:253:ASN:CB	1:A:257:ARG:N	2.30	0.94
1:A:401:GLY:N	1:A:435:HIS:HD2	1.65	0.93
2:B:1076:HIS:ND1	9:K:40:HIS:CD2	2.35	0.93
1:A:805:LEU:C	1:A:805:LEU:CD1	2.39	0.93
1:A:315:LEU:HD12	1:A:319:GLY:HA2	1.49	0.93
2:B:174:LEU:HD22	2:B:204:ILE:HD11	1.51	0.93
2:B:955:THR:HG22	2:B:956:THR:H	1.34	0.92
1:A:315:LEU:CB	1:A:318:SER:H	1.81	0.92
1:A:315:LEU:HD23	1:A:316:GLN:HA	1.49	0.92
2:B:98:THR:O	2:B:126:SER:HB3	1.70	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:56:THR:HG21	3:C:145:CYS:SG	2.10	0.91
8:J:48:ARG:HH21	8:J:49:MET:HE1	1.35	0.91
1:A:256:GLN:CB	1:A:257:ARG:HB3	2.00	0.91
2:B:986:GLN:OE1	2:B:986:GLN:HA	1.68	0.91
1:A:446:ARG:CD	1:A:480:ALA:HB2	2.00	0.91
1:A:741:ASN:HD22	1:A:744:LYS:H	1.13	0.91
1:A:630:ILE:HD12	1:A:630:ILE:N	1.85	0.91
1:A:1254:ALA:O	1:A:1255:GLU:HB2	1.69	0.91
2:B:864:LYS:CG	2:B:865:LYS:H	1.83	0.91
1:A:1111:MET:HG2	1:A:1114:PRO:HG3	1.53	0.90
1:A:315:LEU:CB	1:A:317:LYS:N	2.33	0.90
1:A:319:GLY:CA	1:A:320:ARG:NH1	2.33	0.90
1:A:401:GLY:H	1:A:435:HIS:HD2	1.19	0.90
1:A:855:THR:CG2	1:A:857:ARG:HE	1.85	0.90
2:B:913:GLY:HA2	2:B:938:SER:CB	2.01	0.90
3:C:70:ILE:HD11	3:C:144:ILE:CD1	2.01	0.90
1:A:315:LEU:CD1	1:A:319:GLY:HA2	2.02	0.90
2:B:992:ILE:HD11	9:K:67:PHE:HE2	1.35	0.90
1:A:239:LEU:HD12	1:A:240:PRO:HD2	1.50	0.89
1:A:1015:VAL:HG12	1:A:1019:CYS:SG	2.13	0.89
5:F:109:VAL:HG12	5:F:110:ASP:H	1.37	0.88
1:A:253:ASN:CB	1:A:256:GLN:C	2.46	0.88
1:A:351:THR:HG22	1:A:352:VAL:N	1.88	0.88
4:E:28:TYR:CE1	4:E:78:LEU:HD13	2.09	0.88
1:A:1118:VAL:HG23	1:A:1306:LEU:HB2	1.56	0.87
3:C:142:VAL:HG13	3:C:143:LEU:N	1.89	0.87
8:J:7:CYS:SG	8:J:10:CYS:N	2.46	0.87
2:B:634:TYR:CE1	2:B:692:TYR:CD1	2.61	0.87
1:A:1404:GLU:O	1:A:1408:ILE:HG12	1.75	0.87
1:A:265:LYS:C	1:A:267:ALA:H	1.83	0.87
2:B:955:THR:HG22	2:B:956:THR:N	1.88	0.86
7:I:111:THR:HG22	7:I:113:ASP:H	1.37	0.86
1:A:406:ILE:HD12	1:A:406:ILE:N	1.91	0.86
1:A:751:SER:HB2	2:B:1015:HIS:HE1	1.39	0.86
1:A:253:ASN:HB2	1:A:256:GLN:C	2.01	0.85
1:A:1364:ASN:ND2	1:A:1366:ARG:H	1.74	0.85
1:A:315:LEU:HD12	1:A:319:GLY:CA	2.05	0.85
2:B:635:ARG:O	2:B:636:PRO:O	1.93	0.85
2:B:864:LYS:HE2	2:B:870:ILE:O	1.76	0.85
1:A:630:ILE:H	1:A:630:ILE:CD1	1.89	0.85
2:B:293:PRO:O	2:B:297:ILE:HG12	1.75	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:23:ALA:HB1	2:B:24:PRO:HD2	1.59	0.84
2:B:807:ARG:HG3	2:B:807:ARG:HH11	1.40	0.84
8:J:42:LYS:O	8:J:47:ARG:HD2	1.78	0.84
1:A:320:ARG:N	1:A:320:ARG:CD	2.30	0.84
1:A:323:LYS:O	1:A:324:SER:HB3	1.76	0.84
2:B:899:ILE:HD11	2:B:911:ILE:HG12	1.58	0.84
7:I:17:ARG:HG2	7:I:18:GLU:H	1.43	0.84
1:A:399:HIS:HB3	1:A:400:PRO:HD2	1.57	0.84
1:A:830:LYS:HD3	1:A:1079:MET:O	1.78	0.84
1:A:315:LEU:HD13	1:A:315:LEU:N	1.91	0.83
2:B:567:GLU:H	2:B:567:GLU:CD	1.86	0.83
2:B:975:GLN:HG2	2:B:976:ILE:H	1.43	0.83
1:A:590:ARG:HH11	1:A:590:ARG:CG	1.85	0.83
2:B:542:MET:HB3	2:B:636:PRO:HD3	1.60	0.83
2:B:880:THR:O	2:B:881:ASN:HB2	1.75	0.83
2:B:37:PHE:O	2:B:38:PHE:HB2	1.75	0.83
1:A:319:GLY:HA3	1:A:320:ARG:NH1	1.93	0.83
1:A:257:ARG:O	1:A:257:ARG:HG2	1.78	0.83
9:K:113:THR:O	9:K:114:LEU:HB2	1.78	0.83
6:H:47:PHE:HB3	6:H:95:TYR:CD1	2.13	0.83
7:I:7:CYS:SG	7:I:8:ARG:O	2.36	0.83
1:A:590:ARG:O	1:A:591:PHE:CD1	2.31	0.82
3:C:70:ILE:CD1	3:C:144:ILE:HD11	2.08	0.82
9:K:65:HIS:HD2	9:K:67:PHE:H	1.23	0.82
1:A:518:LYS:HG3	1:A:519:PRO:HD2	1.61	0.82
1:A:1111:MET:SD	1:A:1114:PRO:CG	2.68	0.82
1:A:889:SER:HB2	1:A:892:ALA:H	1.42	0.82
1:A:777:PHE:CE2	1:A:781:ASP:O	2.33	0.82
4:E:61:GLN:HB3	4:E:79:TRP:HE3	1.45	0.81
1:A:1111:MET:HG3	1:A:1114:PRO:HG3	1.60	0.81
8:J:3:VAL:HG21	8:J:18:TRP:CB	2.09	0.81
1:A:55:ASP:H	1:A:56:PRO:HD2	1.44	0.81
1:A:1215:ARG:HH12	1:A:1272:THR:HG22	1.45	0.81
2:B:653:VAL:HG22	2:B:689:LEU:HB3	1.63	0.81
11:R:3:C:H42	12:T:26:DG:H1	1.29	0.81
1:A:239:LEU:HD12	1:A:240:PRO:CD	2.08	0.81
2:B:803:LEU:N	2:B:822:ASN:HD21	1.78	0.81
1:A:276:LEU:HD11	1:A:292:ALA:HB3	1.61	0.81
2:B:1002:THR:HG23	2:B:1004:GLU:H	1.44	0.81
1:A:344:ARG:HG3	1:A:344:ARG:NH1	1.93	0.80
2:B:875:GLU:O	2:B:877:PRO:HD3	1.81	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:K:70:ARG:O	9:K:71:PHE:HB3	1.81	0.80
2:B:351:TYR:O	2:B:355:ILE:HG13	1.82	0.80
1:A:67:CYS:CB	1:A:70:CYS:SG	2.70	0.80
1:A:765:VAL:HG21	1:A:800:VAL:HB	1.63	0.80
2:B:636:PRO:HB3	2:B:743:ILE:CG1	2.10	0.80
2:B:1076:HIS:ND1	9:K:40:HIS:HD2	1.80	0.80
1:A:351:THR:HG22	1:A:352:VAL:H	1.47	0.80
2:B:635:ARG:CB	2:B:636:PRO:HD2	2.12	0.80
2:B:1147:LEU:HD22	2:B:1151:LEU:HD22	1.63	0.80
1:A:666:ILE:HD11	2:B:1030:LEU:HD13	1.64	0.80
3:C:102:GLN:HG2	3:C:154:LYS:CD	2.13	0.79
1:A:1101:LEU:HD13	1:A:1355:VAL:HG11	1.63	0.79
2:B:992:ILE:HD11	9:K:67:PHE:CE2	2.17	0.79
1:A:315:LEU:HD12	1:A:318:SER:C	2.08	0.79
1:A:840:ARG:HG2	1:A:1402:PHE:HZ	1.48	0.79
1:A:1394:THR:HG21	1:A:1398:MET:HE3	1.65	0.79
2:B:783:THR:HG22	8:J:63:TYR:HE1	1.46	0.79
1:A:255:SER:C	1:A:256:GLN:HG3	2.08	0.79
1:A:1441:PHE:CZ	5:F:89:GLU:HA	2.17	0.79
1:A:249:SER:O	1:A:250:ILE:CG1	2.30	0.79
1:A:346:ASP:H	2:B:1154:ALA:HB1	1.47	0.79
2:B:706:GLN:O	2:B:710:LEU:HB2	1.82	0.79
1:A:151:ASP:CG	1:A:163:SER:HA	2.08	0.79
1:A:316:GLN:O	1:A:316:GLN:CG	2.31	0.78
1:A:319:GLY:HA2	1:A:320:ARG:NH1	1.97	0.78
2:B:708:GLU:HG3	2:B:709:ASP:H	1.48	0.78
2:B:864:LYS:HE3	2:B:871:THR:HG23	1.66	0.78
1:A:283:GLY:O	1:A:285:PRO:HD3	1.84	0.78
1:A:913:LEU:HD11	1:A:981:LEU:O	1.84	0.78
1:A:261:ASP:HB3	1:A:323:LYS:HE3	1.64	0.78
2:B:64:CYS:HA	2:B:67:SER:HB2	1.65	0.78
1:A:401:GLY:H	1:A:435:HIS:CD2	2.01	0.78
2:B:552:MET:HG3	2:B:553:PRO:HD3	1.65	0.78
2:B:726:ALA:HB1	2:B:1051:THR:HG21	1.66	0.77
1:A:315:LEU:HD23	1:A:316:GLN:CA	2.14	0.77
1:A:319:GLY:HA3	1:A:320:ARG:HH11	1.49	0.77
1:A:182:VAL:HG12	1:A:183:GLY:H	1.48	0.77
1:A:323:LYS:O	1:A:324:SER:CB	2.32	0.77
2:B:778:MET:HE1	2:B:1094:ARG:HH11	1.48	0.77
12:T:15:DA:H2''	12:T:16:DC:O5'	1.85	0.77
1:A:507:VAL:HG13	1:A:521:MET:HE1	1.66	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:344:ARG:HH11	1:A:344:ARG:CG	1.95	0.77
1:A:1407:GLU:CD	1:A:1407:GLU:H	1.93	0.77
3:C:91:HIS:HB2	3:C:96:SER:OG	1.84	0.77
1:A:323:LYS:N	1:A:323:LYS:CD	2.34	0.76
2:B:980:PHE:O	2:B:981:ALA:HB2	1.85	0.76
2:B:639:ILE:HD11	2:B:691:GLU:HG3	1.68	0.76
4:E:86:PRO:HB3	4:E:114:ASN:ND2	2.00	0.76
1:A:1111:MET:CG	1:A:1114:PRO:CG	2.57	0.76
1:A:315:LEU:HB2	1:A:316:GLN:HA	1.41	0.76
1:A:711:ARG:HG2	7:I:97:MET:HE3	1.68	0.76
1:A:182:VAL:HG12	1:A:183:GLY:N	1.99	0.76
1:A:249:SER:C	1:A:250:ILE:HG23	2.09	0.76
3:C:45:ALA:HA	3:C:72:LEU:HD12	1.67	0.76
1:A:590:ARG:O	1:A:591:PHE:HB2	1.84	0.76
2:B:101:MET:HE3	2:B:169:ARG:HH12	1.51	0.76
3:C:101:LEU:HD12	3:C:117:ASP:O	1.84	0.76
1:A:590:ARG:O	1:A:591:PHE:CB	2.32	0.76
3:C:133:ILE:HD13	3:C:236:GLY:O	1.86	0.76
1:A:315:LEU:CG	1:A:316:GLN:HA	2.16	0.76
2:B:471:LYS:HG3	2:B:472:ALA:N	2.01	0.75
1:A:446:ARG:HD2	1:A:480:ALA:HB2	1.66	0.75
6:H:145:ARG:O	6:H:146:ARG:OXT	2.04	0.75
1:A:255:SER:O	1:A:256:GLN:HG3	1.87	0.75
1:A:399:HIS:NE2	1:A:462:VAL:HG21	2.02	0.75
2:B:1096:ARG:HG3	2:B:1097:HIS:CD2	2.20	0.75
2:B:1148:LYS:O	2:B:1152:MET:HB2	1.87	0.75
5:F:82:THR:HG22	5:F:84:TYR:HB2	1.67	0.75
2:B:789:MET:HE1	2:B:965:LYS:HB3	1.69	0.75
9:K:92:ASN:HA	9:K:95:ILE:HD12	1.68	0.75
3:C:67:LEU:HD11	3:C:155:LEU:HD13	1.68	0.74
2:B:1166:CYS:SG	2:B:1166:CYS:O	2.45	0.74
2:B:744:HIS:HD2	2:B:746:SER:OG	1.71	0.74
1:A:1291:VAL:HG22	1:A:1292:PRO:HD2	1.70	0.74
4:E:86:PRO:CB	4:E:114:ASN:ND2	2.50	0.74
1:A:668:ASP:HB3	1:A:743:VAL:HG23	1.68	0.74
1:A:875:ALA:HA	1:A:878:ILE:HD12	1.69	0.74
2:B:64:CYS:HA	2:B:67:SER:CB	2.18	0.74
2:B:1136:ASP:HA	2:B:1139:ILE:HD12	1.68	0.74
2:B:1159:ARG:HD3	2:B:1193:GLN:HG3	1.69	0.74
1:A:532:ARG:HH22	1:A:745:GLN:HE21	1.36	0.74
1:A:1111:MET:SD	1:A:1114:PRO:CB	2.75	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:635:ARG:HB2	2:B:636:PRO:CD	2.13	0.74
8:J:35:ALA:O	8:J:39:LEU:HD12	1.88	0.74
4:E:86:PRO:HB3	4:E:114:ASN:HD22	1.52	0.73
2:B:956:THR:HA	2:B:961:LEU:O	1.87	0.73
1:A:249:SER:O	1:A:250:ILE:HG12	1.87	0.73
4:E:15:ALA:HA	4:E:140:LEU:O	1.88	0.73
1:A:446:ARG:HE	1:A:480:ALA:HB2	1.51	0.73
2:B:494:HIS:HD2	2:B:497:ARG:NH1	1.86	0.73
1:A:1144:LYS:HA	1:A:1268:LEU:HD22	1.70	0.73
3:C:186:LEU:HB3	3:C:188:HIS:CD2	2.24	0.73
1:A:361:LEU:HD21	1:A:521:MET:HE3	1.71	0.73
2:B:973:ILE:HG22	2:B:974:PRO:HD2	1.70	0.73
2:B:95:ILE:HD12	2:B:130:VAL:HG22	1.71	0.72
1:A:253:ASN:CA	1:A:256:GLN:O	2.32	0.72
1:A:446:ARG:HD2	1:A:480:ALA:CB	2.19	0.72
2:B:373:ARG:HA	2:B:566:LEU:HD23	1.71	0.72
2:B:1004:GLU:O	3:C:177:GLU:HG2	1.88	0.72
11:R:4:G:C2'	11:R:5:A:H8	1.95	0.72
3:C:74:SER:O	3:C:77:ILE:HB	1.88	0.72
4:E:77:SER:HB2	4:E:105:PHE:HA	1.70	0.72
1:A:511:ILE:HG12	1:A:521:MET:HE2	1.69	0.72
2:B:840:ILE:HG12	2:B:992:ILE:HG22	1.71	0.72
8:J:45:CYS:SG	8:J:46:CYS:N	2.62	0.72
1:A:802:ASN:HD21	2:B:729:ILE:H	1.35	0.72
2:B:955:THR:CG2	2:B:956:THR:H	2.02	0.72
12:T:26:DG:N3	12:T:27:DA:H1'	2.04	0.72
1:A:1342:GLU:HG2	4:E:212:ARG:HH11	1.53	0.72
2:B:649:LYS:O	2:B:650:GLU:HB2	1.90	0.72
1:A:902:LEU:HG	1:A:926:GLN:HG3	1.70	0.72
2:B:31:TRP:CZ2	2:B:744:HIS:CD2	2.78	0.72
1:A:452:LYS:HB2	2:B:1141:HIS:CE1	2.24	0.72
1:A:1348:LEU:HD23	1:A:1372:VAL:HG22	1.71	0.72
1:A:151:ASP:OD1	1:A:163:SER:HB2	1.90	0.72
3:C:182:PRO:HB2	3:C:207:CYS:SG	2.30	0.72
1:A:414:ASP:OD1	1:A:416:ARG:HG2	1.89	0.71
1:A:679:ILE:HG23	1:A:729:ALA:HB1	1.72	0.71
2:B:591:ARG:O	2:B:592:ASN:HB3	1.89	0.71
1:A:485:ASP:OD1	1:A:485:ASP:N	2.21	0.71
2:B:980:PHE:O	2:B:981:ALA:CB	2.37	0.71
1:A:364:VAL:HG12	1:A:459:ARG:O	1.89	0.71
8:J:32:GLU:CD	8:J:32:GLU:H	1.96	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:873:MET:HG2	1:A:957:PRO:HG3	1.72	0.71
2:B:839:MET:HE3	2:B:1010:LEU:HD13	1.73	0.71
6:H:44:VAL:O	6:H:44:VAL:HG12	1.91	0.71
1:A:413:ILE:N	1:A:413:ILE:CD1	2.54	0.71
1:A:814:PHE:CE1	2:B:514:LEU:HD21	2.25	0.71
1:A:1342:GLU:HG2	4:E:212:ARG:HH12	1.54	0.71
2:B:636:PRO:CB	2:B:637:LEU:HA	2.21	0.71
1:A:1111:MET:SD	1:A:1114:PRO:CA	2.79	0.71
9:K:18:LYS:O	9:K:19:LEU:HD23	1.90	0.71
1:A:667:GLY:HA2	1:A:670:ILE:HG13	1.73	0.71
1:A:1116:LEU:H	1:A:1308:THR:HB	1.55	0.71
1:A:1324:PRO:HB2	4:E:142:VAL:HG11	1.73	0.71
2:B:1187:ASN:HD21	2:B:1190:ASP:HB2	1.54	0.71
1:A:315:LEU:HD12	1:A:319:GLY:N	2.04	0.70
2:B:969:ARG:NH1	3:C:61:GLU:OE1	2.23	0.70
1:A:276:LEU:CD1	1:A:292:ALA:HB3	2.20	0.70
1:A:315:LEU:H	1:A:315:LEU:CD1	1.93	0.70
1:A:896:ARG:HB3	1:A:897:TYR:CD1	2.27	0.70
2:B:474:SER:C	2:B:476:ARG:H	1.98	0.70
2:B:744:HIS:CD2	2:B:746:SER:OG	2.44	0.70
2:B:1094:ARG:HH22	2:B:1098:MET:HG2	1.53	0.70
12:T:13:DA:H61	13:N:2:DT:C7	2.04	0.70
2:B:485:ARG:HH11	2:B:485:ARG:HG2	1.56	0.70
2:B:634:TYR:CE1	2:B:692:TYR:HD1	2.08	0.70
2:B:881:ASN:HB2	2:B:933:SER:N	2.06	0.70
3:C:97:VAL:HG21	3:C:129:ILE:HG23	1.74	0.70
4:E:61:GLN:HB3	4:E:79:TRP:CE3	2.26	0.70
2:B:102:VAL:HG23	2:B:112:LEU:HB2	1.74	0.70
2:B:610:ASN:OD1	2:B:612:GLU:HB2	1.92	0.70
3:C:142:VAL:HG13	3:C:143:LEU:H	1.57	0.70
6:H:38:LEU:HD13	6:H:125:LEU:HD13	1.74	0.70
1:A:316:GLN:O	1:A:316:GLN:HG3	1.91	0.70
1:A:855:THR:HG21	1:A:857:ARG:NE	2.02	0.70
1:A:37:PHE:HB2	1:A:52:GLY:HA3	1.73	0.69
2:B:302:CYS:SG	2:B:310:MET:HG2	2.32	0.69
8:J:48:ARG:HH21	8:J:49:MET:CE	2.04	0.69
2:B:972:LYS:HD3	2:B:1098:MET:SD	2.32	0.69
1:A:250:ILE:O	1:A:251:SER:HB3	1.93	0.69
6:H:43:ASN:CG	6:H:46:LEU:HD12	2.17	0.69
3:C:219:PHE:CD2	6:H:45:GLU:HG2	2.27	0.69
10:L:40:LEU:HD22	10:L:44:ASP:OD2	1.93	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:636:PRO:HB2	2:B:637:LEU:HB3	1.75	0.69
1:A:413:ILE:N	1:A:413:ILE:HD13	2.06	0.69
1:A:925:LEU:O	1:A:929:LEU:HB2	1.93	0.69
1:A:1017:LEU:HB2	4:E:205:SER:HA	1.74	0.69
2:B:1099:VAL:HG12	2:B:1103:ILE:CD1	2.16	0.69
3:C:91:HIS:ND1	3:C:158:VAL:HG11	2.08	0.69
4:E:77:SER:CB	4:E:105:PHE:HA	2.23	0.69
8:J:6:ARG:HB3	8:J:11:GLY:O	1.92	0.69
1:A:304:MET:HG3	2:B:1210:MET:HG3	1.74	0.69
2:B:635:ARG:O	2:B:636:PRO:C	2.36	0.69
4:E:173:SER:O	4:E:174:GLN:HG2	1.92	0.69
1:A:445:ASN:HB2	1:A:454:SER:O	1.92	0.69
1:A:1194:ARG:NH2	1:A:1237:ILE:HD13	2.08	0.69
3:C:124:LEU:O	3:C:127:ARG:HG2	1.93	0.69
1:A:381:THR:HG22	1:A:384:ASN:ND2	2.09	0.68
1:A:457:ALA:HB3	1:A:506:ALA:HA	1.74	0.68
1:A:1132:LYS:O	1:A:1135:ARG:HB3	1.91	0.68
7:I:68:LEU:HB3	7:I:84:VAL:HG22	1.74	0.68
1:A:840:ARG:HG2	1:A:1402:PHE:CZ	2.28	0.68
1:A:901:LEU:H	1:A:926:GLN:NE2	1.91	0.68
2:B:859:TYR:OH	2:B:941:LEU:HD22	1.92	0.68
2:B:955:THR:HG23	10:L:54:ARG:O	1.93	0.68
2:B:1027:ILE:O	2:B:1029:CYS:N	2.26	0.68
1:A:256:GLN:HB3	1:A:257:ARG:HB3	1.75	0.68
1:A:401:GLY:O	1:A:402:ALA:HB2	1.91	0.68
1:A:128:ILE:HG22	1:A:134:ARG:HG3	1.75	0.68
1:A:152:VAL:O	1:A:162:VAL:HG23	1.94	0.68
3:C:142:VAL:CG1	3:C:143:LEU:N	2.57	0.68
6:H:127:GLY:HA3	6:H:130:ARG:CZ	2.23	0.68
1:A:27:VAL:O	1:A:30:ILE:HG22	1.94	0.68
3:C:3:GLU:HA	9:K:104:ASN:HD21	1.58	0.68
3:C:167:HIS:HD2	3:C:169:LYS:H	1.39	0.68
1:A:249:SER:O	1:A:250:ILE:HG23	1.94	0.68
1:A:1025:ARG:HG2	1:A:1025:ARG:HH11	1.59	0.68
1:A:1101:LEU:O	1:A:1105:LEU:HD12	1.94	0.68
1:A:302:THR:HG21	1:A:313:GLN:NE2	2.08	0.67
2:B:515:HIS:HD2	2:B:517:THR:OG1	1.76	0.67
4:E:199:ILE:O	4:E:199:ILE:HG22	1.94	0.67
9:K:65:HIS:CD2	9:K:67:PHE:HB2	2.28	0.67
1:A:265:LYS:HZ1	1:A:323:LYS:HE2	1.58	0.67
2:B:361:LEU:HD21	2:B:377:PHE:HD2	1.59	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:413:ILE:HD13	1:A:413:ILE:H	1.59	0.67
1:A:243:PRO:HB2	1:A:245:PRO:HD2	1.77	0.67
1:A:896:ARG:HB3	1:A:897:TYR:HD1	1.59	0.67
1:A:1254:ALA:O	1:A:1255:GLU:CB	2.42	0.67
2:B:975:GLN:HG2	2:B:976:ILE:N	2.10	0.67
5:F:109:VAL:HG12	5:F:110:ASP:N	2.09	0.67
1:A:899:VAL:HB	1:A:929:LEU:CD1	2.24	0.67
1:A:1116:LEU:CD2	1:A:1329:THR:HG22	2.18	0.67
2:B:589:VAL:HG12	2:B:590:HIS:N	2.08	0.67
2:B:628:THR:O	2:B:628:THR:HG22	1.95	0.67
1:A:590:ARG:O	1:A:591:PHE:CG	2.47	0.67
1:A:1015:VAL:CG1	1:A:1019:CYS:SG	2.82	0.67
1:A:324:SER:O	1:A:325:ILE:C	2.38	0.67
2:B:494:HIS:CD2	2:B:497:ARG:NH1	2.63	0.67
3:C:123:ASN:HD22	3:C:125:MET:HG2	1.60	0.67
4:E:46:TYR:CE2	4:E:58:MET:HA	2.30	0.67
1:A:1063:MET:CG	1:A:1436:ILE:HG23	2.25	0.67
2:B:824:ILE:HG12	8:J:48:ARG:NH1	2.10	0.67
1:A:629:LEU:HD23	1:A:633:VAL:HG23	1.77	0.67
2:B:549:THR:HG22	2:B:550:ASP:H	1.59	0.67
2:B:825:VAL:HG23	2:B:1010:LEU:HG	1.74	0.67
4:E:14:ARG:HH12	4:E:142:VAL:HG22	1.60	0.67
1:A:78:PRO:O	2:B:1205:GLN:NE2	2.26	0.66
1:A:253:ASN:HA	1:A:256:GLN:C	2.19	0.66
1:A:315:LEU:HD22	1:A:316:GLN:HA	1.76	0.66
1:A:58:LEU:HD22	1:A:244:PRO:HD2	1.75	0.66
1:A:285:PRO:HB2	1:A:288:ALA:HB3	1.76	0.66
1:A:1409:LEU:HD13	2:B:1207:LEU:HD21	1.77	0.66
2:B:364:ILE:HD13	2:B:585:VAL:HG13	1.76	0.66
2:B:560:GLU:O	2:B:561:TRP:CD1	2.48	0.66
2:B:865:LYS:CG	2:B:866:TYR:N	2.31	0.66
4:E:29:PHE:O	4:E:30:ILE:HG13	1.95	0.66
1:A:1398:MET:O	1:A:1400:CYS:N	2.29	0.66
2:B:108:VAL:HG12	2:B:109:THR:H	1.60	0.66
3:C:172:PRO:O	3:C:235:VAL:HG23	1.96	0.66
6:H:22:LYS:O	6:H:23:VAL:HG23	1.95	0.66
1:A:115:LEU:HD11	1:A:145:LYS:HE3	1.77	0.66
2:B:884:ARG:O	2:B:936:ASP:HB3	1.96	0.66
1:A:455:MET:HE1	2:B:1130:PHE:HE1	1.61	0.66
1:A:565:ILE:HD13	6:H:46:LEU:CD1	2.26	0.66
2:B:129:PHE:CE2	2:B:166:PHE:HB2	2.30	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:980:PHE:O	2:B:1095:LEU:HD12	1.93	0.66
3:C:35:ARG:NH1	9:K:41:THR:OG1	2.29	0.66
8:J:10:CYS:SG	8:J:43:ARG:HD2	2.34	0.66
1:A:332:LYS:C	1:A:334:GLY:H	2.04	0.66
1:A:899:VAL:HB	1:A:929:LEU:HD12	1.78	0.66
6:H:26:ILE:HG22	6:H:40:LEU:O	1.96	0.66
1:A:1072:ILE:HD11	1:A:1368:MET:HA	1.78	0.66
2:B:766:ARG:NH1	2:B:769:TYR:CE1	2.64	0.66
3:C:88:CYS:SG	14:C:319:ZN:ZN	1.84	0.66
1:A:401:GLY:N	1:A:435:HIS:CD2	2.57	0.66
1:A:590:ARG:NH1	1:A:590:ARG:CG	2.52	0.66
1:A:629:LEU:HD23	1:A:633:VAL:CG2	2.26	0.66
2:B:591:ARG:O	2:B:592:ASN:CB	2.42	0.66
6:H:47:PHE:CB	6:H:95:TYR:HD1	2.04	0.66
1:A:628:GLY:O	1:A:632:VAL:HG23	1.95	0.66
1:A:1400:CYS:O	1:A:1405:THR:HG23	1.96	0.66
1:A:53:LEU:O	1:A:56:PRO:CD	2.44	0.66
1:A:1364:ASN:HD22	1:A:1366:ARG:H	1.43	0.66
1:A:472:LEU:HD21	2:B:835:GLN:HB3	1.78	0.65
1:A:1215:ARG:NH1	1:A:1272:THR:HG22	2.10	0.65
2:B:475:SER:C	2:B:477:ALA:N	2.53	0.65
1:A:672:ASP:HB2	1:A:736:ASN:HD21	1.60	0.65
4:E:185:ALA:HA	4:E:190:LEU:HD23	1.79	0.65
6:H:89:LEU:O	6:H:91:ASP:N	2.27	0.65
2:B:1130:PHE:HZ	2:B:1138:MET:HG2	1.60	0.65
3:C:172:PRO:C	3:C:235:VAL:HG23	2.21	0.65
1:A:782:ARG:NH1	1:A:785:PRO:HA	2.12	0.65
1:A:836:TYR:CZ	1:A:840:ARG:HD2	2.32	0.65
2:B:899:ILE:CD1	2:B:911:ILE:HG12	2.25	0.65
1:A:408:ASP:O	1:A:410:GLY:N	2.30	0.65
1:A:901:LEU:HA	1:A:907:THR:HG23	1.79	0.65
2:B:649:LYS:O	2:B:650:GLU:CB	2.45	0.65
1:A:667:GLY:HA2	1:A:670:ILE:CG1	2.27	0.65
1:A:1386:ARG:HD3	1:A:1403:GLU:HG2	1.79	0.65
2:B:816:GLU:OE1	2:B:816:GLU:N	2.30	0.65
1:A:406:ILE:HD13	1:A:431:LYS:HB2	1.79	0.65
4:E:172:GLU:O	4:E:174:GLN:N	2.30	0.65
1:A:1004:ASN:ND2	4:E:167:ARG:HD2	2.11	0.65
2:B:1106:ARG:HD3	2:B:1126:GLY:O	1.97	0.65
1:A:213:HIS:O	1:A:214:ILE:C	2.40	0.64
1:A:326:ARG:HG2	1:A:1406:VAL:HG21	1.77	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:463:ILE:HB	1:A:464:PRO:HD2	1.79	0.64
1:A:751:SER:CB	2:B:1015:HIS:HE1	2.08	0.64
1:A:842:VAL:HG11	2:B:1136:ASP:OD2	1.96	0.64
2:B:345:LYS:O	2:B:348:ARG:HG2	1.96	0.64
2:B:711:GLU:H	2:B:712:PRO:HD3	1.62	0.64
2:B:864:LYS:HZ3	2:B:867:GLY:N	1.95	0.64
1:A:17:VAL:HB	1:A:1419:ASP:HB3	1.78	0.64
2:B:378:LEU:O	2:B:382:ILE:HG12	1.97	0.64
4:E:171:LYS:O	4:E:173:SER:N	2.30	0.64
6:H:58:THR:HG22	6:H:59:ILE:N	2.11	0.64
8:J:58:GLU:HA	8:J:61:LEU:HD12	1.80	0.64
1:A:675:THR:HG22	1:A:679:ILE:HD11	1.78	0.64
1:A:1118:VAL:CG2	1:A:1306:LEU:HB2	2.26	0.64
2:B:522:VAL:HG13	2:B:538:ASN:O	1.97	0.64
4:E:171:LYS:O	4:E:172:GLU:C	2.40	0.64
1:A:404:TYR:HA	1:A:413:ILE:O	1.98	0.64
1:A:672:ASP:CB	1:A:736:ASN:HD21	2.09	0.64
1:A:896:ARG:HD2	1:A:897:TYR:HE1	1.62	0.64
4:E:63:ASN:HB3	4:E:64:PRO:CD	2.27	0.64
1:A:388:LEU:HD22	1:A:432:VAL:HG11	1.79	0.64
1:A:406:ILE:HD12	1:A:406:ILE:H	1.62	0.64
2:B:108:VAL:HG12	2:B:109:THR:N	2.12	0.64
2:B:550:ASP:OD2	2:B:552:MET:CG	2.46	0.64
2:B:830:TYR:O	2:B:832:GLY:N	2.30	0.64
3:C:58:LEU:HD21	8:J:57:ILE:HD13	1.78	0.64
8:J:3:VAL:HG21	8:J:18:TRP:CG	2.33	0.64
1:A:253:ASN:CA	1:A:256:GLN:C	2.70	0.64
1:A:464:PRO:HG2	9:K:67:PHE:CD1	2.33	0.64
1:A:1312:ASN:O	1:A:1316:VAL:HG23	1.97	0.64
2:B:986:GLN:NE2	2:B:1016:ALA:HB1	2.13	0.64
3:C:77:ILE:HA	3:C:129:ILE:HD11	1.79	0.64
5:F:109:VAL:HG23	5:F:124:GLU:HG2	1.79	0.64
1:A:1127:ASP:HB3	1:A:1130:GLN:HB3	1.80	0.64
2:B:1103:ILE:HD13	2:B:1103:ILE:N	2.11	0.64
4:E:3:GLN:HG3	4:E:4:GLU:N	2.12	0.64
1:A:105:CYS:O	1:A:114:LEU:HG	1.98	0.64
2:B:451:LYS:HA	2:B:454:THR:HB	1.79	0.64
3:C:22:LEU:CD2	3:C:25:VAL:HG21	2.28	0.64
6:H:84:ALA:O	6:H:86:ASP:N	2.30	0.64
1:A:55:ASP:O	1:A:57:ARG:N	2.31	0.64
2:B:864:LYS:NZ	2:B:867:GLY:N	2.45	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:J:1:MET:N	8:J:56:LEU:H	1.96	0.64
1:A:777:PHE:CD2	1:A:781:ASP:O	2.52	0.63
2:B:952:VAL:HG13	2:B:966:VAL:HG22	1.80	0.63
7:I:35:VAL:HG12	7:I:36:GLU:N	2.13	0.63
2:B:276:ILE:HG22	2:B:278:GLN:H	1.63	0.63
2:B:830:TYR:O	2:B:831:SER:C	2.40	0.63
2:B:168:GLY:H	2:B:450:ALA:HB1	1.63	0.63
1:A:324:SER:O	1:A:326:ARG:N	2.32	0.63
1:A:472:LEU:O	1:A:475:THR:HB	1.98	0.63
1:A:802:ASN:ND2	2:B:729:ILE:H	1.95	0.63
1:A:1067:LEU:HD12	1:A:1067:LEU:O	1.99	0.63
2:B:999:MET:HG3	2:B:1000:PRO:HD2	1.79	0.63
1:A:265:LYS:O	1:A:267:ALA:N	2.31	0.63
1:A:440:ASP:H	1:A:460:VAL:HG23	1.63	0.63
1:A:1398:MET:C	1:A:1400:CYS:H	2.05	0.63
3:C:184:ASN:HD21	3:C:189:THR:H	1.46	0.63
1:A:351:THR:CG2	1:A:352:VAL:N	2.60	0.63
1:A:401:GLY:CA	1:A:435:HIS:HD2	2.11	0.63
1:A:955:PRO:O	1:A:956:LEU:HG	1.99	0.63
1:A:1402:PHE:CD2	1:A:1403:GLU:HB2	2.34	0.63
2:B:879:ARG:H	2:B:879:ARG:CZ	2.11	0.63
2:B:1148:LYS:O	2:B:1152:MET:N	2.31	0.63
3:C:47:ASP:HA	10:L:69:ALA:HB3	1.80	0.63
8:J:7:CYS:HG	8:J:10:CYS:H	1.43	0.63
1:A:264:PHE:CE1	1:A:317:LYS:HB3	2.34	0.63
1:A:1059:HIS:ND1	5:F:86:THR:HA	2.14	0.63
1:A:1154:TYR:CE2	1:A:1156:PRO:HG3	2.34	0.63
1:A:19:PHE:HB3	1:A:1413:GLY:HA2	1.81	0.62
1:A:269:ILE:HD11	1:A:300:VAL:HA	1.80	0.62
1:A:1116:LEU:HD23	1:A:1329:THR:HG21	1.72	0.62
2:B:168:GLY:HA2	2:B:454:THR:OG1	1.99	0.62
2:B:1084:GLN:HE21	3:C:192:TRP:HB2	1.64	0.62
2:B:420:LEU:O	2:B:423:LYS:HB3	1.99	0.62
4:E:28:TYR:HE1	4:E:78:LEU:HD13	1.63	0.62
6:H:113:ALA:HA	6:H:125:LEU:O	1.99	0.62
1:A:302:THR:HG21	1:A:313:GLN:HE22	1.63	0.62
1:A:475:THR:HG22	1:A:476:SER:N	2.13	0.62
1:A:577:ILE:O	1:A:580:VAL:HG23	2.00	0.62
1:A:821:ARG:O	1:A:825:ILE:HG12	2.00	0.62
2:B:474:SER:C	2:B:476:ARG:N	2.57	0.62
3:C:73:GLN:HE21	3:C:75:MET:H	1.47	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:100:THR:HB	3:C:119:VAL:HG12	1.81	0.62
2:B:552:MET:HG3	2:B:553:PRO:CD	2.29	0.62
2:B:803:LEU:H	2:B:822:ASN:HD21	1.47	0.62
1:A:1025:ARG:HG2	1:A:1025:ARG:NH1	2.14	0.62
2:B:865:LYS:HG2	2:B:866:TYR:H	0.66	0.62
4:E:180:ARG:HB2	4:E:215:MET:OXT	2.00	0.62
7:I:55:THR:HG23	7:I:58:VAL:HG21	1.81	0.62
1:A:55:ASP:N	1:A:56:PRO:CD	2.62	0.62
2:B:851:PHE:HB3	2:B:1094:ARG:HD2	1.82	0.62
1:A:518:LYS:CG	1:A:519:PRO:HD2	2.30	0.62
1:A:1436:ILE:O	1:A:1437:GLY:C	2.43	0.62
1:A:53:LEU:O	1:A:56:PRO:HD3	2.00	0.62
1:A:777:PHE:CD2	1:A:781:ASP:C	2.78	0.62
2:B:1187:ASN:ND2	2:B:1190:ASP:HB2	2.15	0.62
1:A:320:ARG:CB	1:A:321:PRO:HA	2.30	0.62
1:A:787:PHE:CZ	1:A:796:SER:HB2	2.35	0.62
1:A:845:LEU:O	1:A:848:ILE:HG12	1.99	0.62
2:B:1082:MET:HA	3:C:189:THR:HA	1.81	0.62
9:K:7:PHE:C	9:K:9:LEU:H	2.08	0.61
1:A:202:LEU:HB3	1:A:207:ILE:HD11	1.82	0.61
1:A:253:ASN:HB3	1:A:257:ARG:H	1.61	0.61
1:A:253:ASN:HB2	1:A:257:ARG:N	2.10	0.61
1:A:261:ASP:HB3	1:A:323:LYS:CE	2.30	0.61
1:A:567:LYS:HB2	6:H:95:TYR:HA	1.83	0.61
1:A:754:SER:H	1:A:757:ASN:HD22	1.46	0.61
1:A:901:LEU:HD22	1:A:919:ILE:HG22	1.82	0.61
2:B:211:VAL:O	2:B:480:SER:HA	2.00	0.61
1:A:338:GLY:HA2	2:B:1129:ARG:HH22	1.64	0.61
1:A:552:TRP:NE1	1:A:655:PHE:CD1	2.67	0.61
2:B:784:ASN:ND2	2:B:788:ARG:HD2	2.15	0.61
2:B:849:GLY:HA2	2:B:852:ARG:HD2	1.82	0.61
5:F:82:THR:CG2	5:F:84:TYR:HB2	2.30	0.61
2:B:211:VAL:HG23	2:B:483:LEU:HA	1.83	0.61
2:B:1166:CYS:HB3	2:B:1185:CYS:SG	2.40	0.61
5:F:111:LEU:HD13	5:F:111:LEU:H	1.65	0.61
1:A:408:ASP:O	1:A:409:SER:C	2.44	0.61
2:B:1096:ARG:HG2	2:B:1096:ARG:NH1	2.04	0.61
1:A:568:PRO:HB3	3:C:221:TYR:CZ	2.36	0.61
1:A:1025:ARG:HH11	1:A:1025:ARG:CG	2.14	0.61
2:B:29:ASP:HB3	2:B:658:ILE:HG12	1.83	0.61
8:J:44:TYR:CA	8:J:47:ARG:HB2	2.18	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:399:HIS:HB3	1:A:400:PRO:HD3	1.52	0.61
1:A:1111:MET:SD	1:A:1114:PRO:HA	2.41	0.61
2:B:1060:ARG:C	2:B:1062:HIS:H	2.07	0.61
9:K:33:ILE:HD13	9:K:87:LEU:HD22	1.83	0.61
1:A:98:LYS:O	1:A:101:LYS:N	2.33	0.61
1:A:765:VAL:HG21	1:A:800:VAL:CB	2.30	0.61
1:A:833:GLU:HG2	1:A:1102:LYS:HE3	1.83	0.61
1:A:265:LYS:C	1:A:267:ALA:N	2.53	0.60
2:B:589:VAL:CG1	2:B:590:HIS:N	2.64	0.60
1:A:7:SER:HB3	2:B:1193:GLN:OE1	2.01	0.60
2:B:322:PHE:CD1	2:B:322:PHE:O	2.55	0.60
2:B:766:ARG:HH21	2:B:1020:ARG:HB3	1.65	0.60
1:A:1063:MET:SD	1:A:1436:ILE:HG12	2.40	0.60
1:A:1161:THR:HG22	1:A:1162:VAL:H	1.66	0.60
2:B:622:LYS:HE2	7:I:59:VAL:HG22	1.82	0.60
2:B:863:GLU:O	2:B:864:LYS:C	2.43	0.60
1:A:648:ASN:O	1:A:652:VAL:HG23	2.02	0.60
1:A:1198:ASP:O	1:A:1202:MET:HG2	2.01	0.60
1:A:1319:VAL:HG12	1:A:1320:PRO:O	2.00	0.60
2:B:640:VAL:O	2:B:640:VAL:HG12	2.00	0.60
2:B:701:ILE:HD11	2:B:703:ILE:HD11	1.83	0.60
3:C:185:LYS:HE3	3:C:211:ASP:O	2.01	0.60
1:A:343:LYS:HZ1	2:B:1197:PRO:HB3	1.67	0.60
1:A:853:ASP:OD1	1:A:855:THR:HG22	2.02	0.60
1:A:672:ASP:H	1:A:736:ASN:ND2	1.99	0.60
1:A:791:ASP:C	1:A:791:ASP:OD1	2.44	0.60
2:B:1096:ARG:HG3	2:B:1097:HIS:CG	2.37	0.60
1:A:129:LYS:O	1:A:130:ASP:CB	2.32	0.60
1:A:442:VAL:HG11	1:A:489:LEU:HD21	1.83	0.60
1:A:596:THR:C	1:A:598:LEU:H	2.08	0.60
1:A:1227:ILE:HG22	1:A:1228:TRP:N	2.16	0.60
1:A:1394:THR:CG2	1:A:1398:MET:HE3	2.30	0.60
2:B:273:LEU:HD11	2:B:285:ILE:CD1	2.31	0.60
2:B:802:PRO:HA	2:B:1091:TYR:CD1	2.36	0.60
6:H:44:VAL:O	6:H:44:VAL:CG1	2.49	0.60
8:J:48:ARG:NH2	8:J:49:MET:HE1	2.13	0.60
1:A:55:ASP:H	1:A:56:PRO:CD	2.12	0.60
2:B:801:LYS:O	8:J:52:THR:CG2	2.50	0.60
2:B:1012:ILE:HD13	2:B:1092:TYR:OH	2.02	0.60
1:A:567:LYS:O	1:A:569:LYS:N	2.34	0.60
1:A:868:TYR:CE1	1:A:1064:VAL:CG1	2.60	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:883:LEU:HD11	1:A:1017:LEU:HD21	1.84	0.60
2:B:288:ALA:CB	2:B:331:LEU:HD12	2.32	0.60
2:B:1084:GLN:HG2	3:C:201:TRP:CZ2	2.36	0.60
10:L:41:SER:O	10:L:44:ASP:HB2	2.02	0.60
1:A:544:ASP:HB2	9:K:47:ARG:HH21	1.67	0.60
1:A:1364:ASN:ND2	1:A:1364:ASN:C	2.60	0.60
1:A:1437:GLY:HA3	5:F:88:TYR:CD2	2.36	0.60
9:K:20:LYS:HD3	9:K:22:ASP:OD2	2.02	0.60
1:A:376:TYR:C	1:A:376:TYR:CD2	2.80	0.59
2:B:322:PHE:HZ	7:I:30:ARG:HH11	1.48	0.59
2:B:1027:ILE:O	2:B:1028:GLU:C	2.45	0.59
1:A:754:SER:N	1:A:757:ASN:HD22	1.99	0.59
1:A:949:ASP:OD1	1:A:949:ASP:N	2.26	0.59
2:B:957:ASN:HD22	2:B:959:ASP:H	1.49	0.59
2:B:1153:GLU:OE2	2:B:1153:GLU:N	2.35	0.59
1:A:182:VAL:CG1	1:A:183:GLY:H	2.14	0.59
1:A:685:GLU:O	1:A:689:LYS:HB2	2.02	0.59
3:C:73:GLN:NE2	3:C:237:SER:O	2.35	0.59
4:E:2:ASP:O	4:E:3:GLN:HB3	2.02	0.59
1:A:675:THR:HG22	1:A:679:ILE:CD1	2.33	0.59
2:B:778:MET:HE3	2:B:853:SER:HB3	1.83	0.59
3:C:41:ILE:HG13	3:C:172:PRO:HG3	1.84	0.59
1:A:58:LEU:HD21	1:A:243:PRO:HB3	1.84	0.59
1:A:130:ASP:C	1:A:132:LYS:H	2.09	0.59
1:A:303:TYR:CG	1:A:303:TYR:O	2.56	0.59
1:A:557:ASP:HA	9:K:26:LYS:HE3	1.84	0.59
1:A:1140:HIS:HB2	1:A:1276:VAL:O	2.02	0.59
2:B:315:LYS:N	2:B:316:PRO:HD2	2.18	0.59
3:C:46:ILE:HG23	3:C:157:CYS:HB3	1.85	0.59
6:H:139:ASN:O	6:H:140:ALA:HB2	2.03	0.59
1:A:1017:LEU:HB2	4:E:206:GLY:H	1.68	0.59
2:B:501:PRO:O	2:B:502:ILE:HB	2.03	0.59
2:B:779:GLY:O	2:B:795:ILE:HG23	2.02	0.59
2:B:1027:ILE:O	2:B:1030:LEU:N	2.36	0.59
1:A:315:LEU:CD1	1:A:319:GLY:CA	2.72	0.59
3:C:186:LEU:HB3	3:C:188:HIS:HD2	1.68	0.59
9:K:49:GLU:C	9:K:51:LEU:H	2.09	0.59
1:A:996:ASN:HA	1:A:998:LEU:HD23	1.83	0.59
2:B:976:ILE:HD11	2:B:992:ILE:HD12	1.85	0.59
3:C:252:GLN:HG3	9:K:95:ILE:HG23	1.83	0.59
4:E:86:PRO:CA	4:E:114:ASN:HD22	2.14	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:399:HIS:CD2	1:A:400:PRO:CD	2.71	0.59
1:A:1428:VAL:HG21	2:B:1135:ARG:HD2	1.85	0.59
2:B:983:ARG:C	2:B:984:HIS:CG	2.80	0.59
2:B:1131:GLY:O	2:B:1134:GLU:N	2.34	0.59
3:C:13:ALA:HA	3:C:17:ASN:O	2.02	0.59
1:A:265:LYS:HD2	1:A:303:TYR:HB2	1.85	0.59
2:B:203:PHE:C	2:B:204:ILE:HD12	2.27	0.59
2:B:256:VAL:HG11	2:B:382:ILE:HD13	1.84	0.59
2:B:789:MET:CE	2:B:965:LYS:HB3	2.32	0.59
4:E:77:SER:HB2	4:E:105:PHE:CA	2.33	0.59
6:H:139:ASN:O	6:H:140:ALA:CB	2.51	0.59
1:A:470:LEU:HD21	1:A:487:MET:CE	2.32	0.58
1:A:567:LYS:CB	6:H:95:TYR:HA	2.33	0.58
1:A:787:PHE:CE1	1:A:796:SER:HB2	2.38	0.58
1:A:1063:MET:HG3	1:A:1436:ILE:HG23	1.85	0.58
1:A:1276:VAL:HB	1:A:1279:ILE:HD13	1.85	0.58
2:B:400:HIS:CE1	2:B:517:THR:HG21	2.38	0.58
2:B:1135:ARG:HG2	2:B:1139:ILE:HD11	1.85	0.58
4:E:100:ILE:HG23	4:E:105:PHE:HB2	1.84	0.58
1:A:1002:GLY:HA3	1:A:1007:ILE:HG21	1.85	0.58
2:B:550:ASP:OD2	2:B:552:MET:HG3	2.03	0.58
2:B:1103:ILE:HD13	2:B:1103:ILE:H	1.68	0.58
8:J:9:SER:OG	8:J:48:ARG:NH2	2.36	0.58
1:A:910:PRO:HA	1:A:916:GLY:HA3	1.85	0.58
3:C:93:ASP:O	3:C:127:ARG:NH2	2.36	0.58
2:B:986:GLN:OE1	2:B:986:GLN:CA	2.49	0.58
3:C:143:LEU:C	3:C:143:LEU:HD12	2.28	0.58
1:A:893:PHE:C	1:A:893:PHE:CD2	2.81	0.58
2:B:179:CYS:SG	2:B:180:TYR:N	2.76	0.58
2:B:269:ILE:HD11	2:B:386:LEU:HD21	1.85	0.58
8:J:7:CYS:HB3	8:J:46:CYS:SG	2.43	0.58
1:A:471:ASN:O	1:A:472:LEU:C	2.47	0.58
1:A:1105:LEU:HD23	1:A:1384:VAL:HG21	1.86	0.58
2:B:383:ASN:O	2:B:387:LEU:HB2	2.03	0.58
2:B:515:HIS:H	2:B:518:HIS:CD2	2.22	0.58
2:B:975:GLN:CG	2:B:976:ILE:H	2.16	0.58
2:B:1175:LEU:O	2:B:1176:ASN:CB	2.50	0.58
4:E:77:SER:HB3	4:E:105:PHE:HD2	1.69	0.58
6:H:127:GLY:HA3	6:H:130:ARG:NH2	2.19	0.58
1:A:95:PHE:O	1:A:99:ILE:HG13	2.03	0.58
1:A:399:HIS:CG	1:A:400:PRO:N	2.72	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:869:GLY:O	4:E:204:THR:HG21	2.03	0.58
1:A:1156:PRO:O	1:A:1158:PRO:HD3	2.03	0.58
2:B:98:THR:O	2:B:126:SER:CB	2.49	0.58
1:A:407:ARG:HD3	1:A:413:ILE:HD11	1.85	0.58
1:A:444:PHE:HE2	1:A:470:LEU:CD2	2.16	0.58
1:A:1224:LEU:HD12	1:A:1241:ARG:O	2.03	0.58
1:A:1398:MET:C	1:A:1400:CYS:N	2.61	0.58
2:B:128:LEU:HB2	2:B:167:ILE:O	2.04	0.58
2:B:705:MET:HA	2:B:705:MET:HE3	1.86	0.58
2:B:864:LYS:CE	2:B:870:ILE:O	2.51	0.58
1:A:599:SER:C	1:A:601:LYS:H	2.12	0.58
2:B:703:ILE:HA	2:B:740:HIS:O	2.04	0.58
2:B:766:ARG:HA	2:B:769:TYR:HD1	1.69	0.58
2:B:784:ASN:CG	2:B:788:ARG:HD2	2.29	0.58
1:A:151:ASP:OD2	1:A:163:SER:HA	2.04	0.58
1:A:352:VAL:CG2	2:B:1099:VAL:HG13	2.32	0.58
1:A:1433:MET:HE1	5:F:92:ARG:NH1	2.19	0.57
1:A:1436:ILE:HD13	2:B:1139:ILE:HG23	1.85	0.57
2:B:783:THR:HG22	8:J:63:TYR:CE1	2.34	0.57
1:A:845:LEU:HD12	1:A:1069:ALA:HB2	1.85	0.57
2:B:733:HIS:O	2:B:735:ALA:N	2.35	0.57
2:B:835:GLN:HA	2:B:1013:ASN:HD22	1.68	0.57
4:E:153:HIS:O	4:E:154:ILE:HD13	2.04	0.57
1:A:99:ILE:HA	1:A:102:VAL:HG23	1.87	0.57
1:A:182:VAL:CG1	1:A:183:GLY:N	2.67	0.57
1:A:256:GLN:HB3	1:A:257:ARG:CD	2.33	0.57
1:A:567:LYS:CG	1:A:568:PRO:HD2	2.33	0.57
3:C:43:THR:HG23	3:C:44:LEU:N	2.19	0.57
8:J:7:CYS:SG	8:J:9:SER:N	2.77	0.57
1:A:490:HIS:HB3	2:B:1150:ARG:CZ	2.34	0.57
1:A:807:GLY:O	2:B:728:ARG:HD3	2.04	0.57
2:B:596:LEU:O	2:B:600:LEU:HD23	2.05	0.57
2:B:980:PHE:HE1	2:B:990:ILE:HD11	1.68	0.57
3:C:144:ILE:HG22	3:C:145:CYS:HB3	1.87	0.57
5:F:74:ILE:HG21	5:F:144:GLU:HG2	1.86	0.57
1:A:49:LYS:HD3	1:A:55:ASP:CG	2.28	0.57
1:A:335:ARG:HH11	2:B:1202:LEU:HD12	1.68	0.57
1:A:890:ASP:H	1:A:1296:GLY:HA3	1.69	0.57
2:B:293:PRO:HG2	2:B:296:GLU:HB2	1.85	0.57
1:A:256:GLN:HA	1:A:257:ARG:HB2	1.74	0.57
1:A:323:LYS:HD3	1:A:323:LYS:H	1.60	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1342:GLU:CG	4:E:212:ARG:NH1	2.62	0.57
2:B:384:ARG:HH22	2:B:621:GLU:HG3	1.69	0.57
1:A:896:ARG:HD2	1:A:897:TYR:CE1	2.40	0.57
2:B:638:PHE:O	2:B:740:HIS:HB3	2.05	0.57
1:A:11:LEU:HA	2:B:1193:GLN:O	2.04	0.57
1:A:786:HIS:CE1	2:B:705:MET:HE1	2.40	0.57
1:A:858:ASN:C	1:A:858:ASN:HD22	2.12	0.57
1:A:894:GLU:C	1:A:896:ARG:H	2.13	0.57
2:B:515:HIS:CD2	2:B:517:THR:OG1	2.58	0.57
3:C:7:GLN:HB2	3:C:23:SER:HB2	1.86	0.57
11:R:9:G:O2'	11:R:10:A:H5'	2.04	0.57
1:A:119:ASN:O	1:A:123:ARG:HG3	2.04	0.57
1:A:635:ARG:HE	1:A:877:HIS:HA	1.70	0.57
1:A:1242:VAL:HG12	1:A:1243:VAL:N	2.20	0.57
2:B:636:PRO:CB	2:B:637:LEU:CA	2.83	0.57
2:B:736:THR:O	2:B:736:THR:HG22	2.05	0.57
9:K:58:PHE:HB3	9:K:76:GLN:HB3	1.87	0.57
2:B:315:LYS:HG2	7:I:13:MET:HE1	1.87	0.56
2:B:519:TRP:O	2:B:519:TRP:CD1	2.58	0.56
2:B:541:LEU:HB2	2:B:747:MET:HE3	1.86	0.56
2:B:1096:ARG:HH11	2:B:1096:ARG:CG	2.09	0.56
11:R:9:G:C2'	11:R:10:A:H5'	2.33	0.56
1:A:127:ALA:O	1:A:128:ILE:C	2.48	0.56
1:A:249:SER:O	1:A:250:ILE:HD13	2.04	0.56
1:A:814:PHE:O	1:A:817:ALA:HB3	2.06	0.56
1:A:1115:SER:HB3	1:A:1330:ASN:ND2	2.19	0.56
3:C:79:GLN:HE21	3:C:127:ARG:HB3	1.68	0.56
1:A:32:VAL:HB	1:A:57:ARG:CB	2.34	0.56
1:A:172:PRO:HB2	1:A:174:ILE:HG12	1.87	0.56
1:A:567:LYS:HB3	6:H:96:VAL:N	2.12	0.56
1:A:1364:ASN:HD22	1:A:1366:ARG:HG2	1.66	0.56
2:B:65:GLU:OE1	2:B:65:GLU:N	2.38	0.56
2:B:650:GLU:HG3	2:B:651:LEU:N	2.20	0.56
2:B:778:MET:CE	2:B:853:SER:HB3	2.34	0.56
3:C:39:ALA:O	3:C:164:ALA:HB3	2.05	0.56
3:C:69:LEU:O	8:J:6:ARG:NH1	2.32	0.56
12:T:27:DA:H2'	12:T:27:DA:N3	2.19	0.56
1:A:185:TRP:O	1:A:186:LYS:HB2	2.05	0.56
2:B:541:LEU:HB2	2:B:747:MET:CE	2.35	0.56
1:A:55:ASP:N	1:A:56:PRO:HD2	2.15	0.56
1:A:402:ALA:O	1:A:415:LEU:CD1	2.53	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:134:ILE:HG22	5:F:136:ARG:HG3	1.87	0.56
6:H:84:ALA:C	6:H:86:ASP:N	2.64	0.56
1:A:382:PRO:HD3	1:A:428:TYR:CE2	2.40	0.56
1:A:567:LYS:CB	1:A:568:PRO:CD	2.59	0.56
1:A:1277:GLU:O	1:A:1279:ILE:HD12	2.05	0.56
1:A:1295:THR:OG1	1:A:1297:GLU:OE1	2.24	0.56
2:B:636:PRO:HB2	2:B:637:LEU:CA	2.36	0.56
2:B:1074:ASN:OD1	2:B:1075:GLY:N	2.38	0.56
3:C:57:VAL:CG2	8:J:57:ILE:HD11	2.35	0.56
6:H:42:ILE:HG23	6:H:95:TYR:CE1	2.40	0.56
1:A:320:ARG:CB	1:A:321:PRO:CA	2.84	0.56
1:A:514:PRO:O	1:A:515:GLN:C	2.49	0.56
7:I:106:CYS:O	7:I:107:SER:C	2.49	0.56
1:A:962:ARG:O	1:A:964:ILE:N	2.39	0.56
9:K:33:ILE:CD1	9:K:87:LEU:HD22	2.36	0.56
1:A:809:THR:HB	1:A:810:PRO:HD2	1.87	0.56
12:T:26:DG:C2	12:T:27:DA:H1'	2.39	0.56
1:A:179:LEU:HD11	1:A:298:PHE:HD1	1.70	0.55
1:A:302:THR:HA	1:A:305:ASP:O	2.05	0.55
1:A:526:ASP:HB2	2:B:835:GLN:CD	2.31	0.55
1:A:705:LYS:HE3	1:A:713:SER:HB2	1.87	0.55
2:B:976:ILE:HG23	2:B:977:GLY:N	2.21	0.55
1:A:1342:GLU:HG3	4:E:198:ILE:HD13	1.87	0.55
6:H:130:ARG:HB3	6:H:134:ASN:HD22	1.72	0.55
7:I:85:PHE:HB3	7:I:101:PHE:CD2	2.40	0.55
1:A:1021:LEU:O	1:A:1022:LEU:C	2.48	0.55
2:B:814:PHE:C	2:B:816:GLU:H	2.14	0.55
2:B:1077:THR:CG2	2:B:1079:LYS:H	2.18	0.55
3:C:167:HIS:CD2	3:C:169:LYS:H	2.22	0.55
4:E:3:GLN:CG	4:E:5:ASN:H	2.18	0.55
4:E:171:LYS:H	4:E:174:GLN:HG3	1.70	0.55
2:B:114:PRO:HG3	2:B:181:LEU:HD11	1.88	0.55
2:B:175:ARG:HH11	2:B:175:ARG:CG	2.20	0.55
2:B:636:PRO:HB3	2:B:637:LEU:HA	1.87	0.55
1:A:378:GLU:HG2	1:A:388:LEU:HD11	1.89	0.55
1:A:463:ILE:CB	1:A:464:PRO:HD2	2.36	0.55
1:A:929:LEU:HD21	1:A:983:ILE:CG2	2.36	0.55
2:B:1017:ILE:H	2:B:1018:PRO:HD3	1.71	0.55
3:C:186:LEU:CB	3:C:188:HIS:HD2	2.20	0.55
1:A:249:SER:O	1:A:250:ILE:CD1	2.54	0.55
1:A:544:ASP:HB2	9:K:47:ARG:NH2	2.22	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:549:MET:HE1	1:A:656:TRP:HD1	1.72	0.55
1:A:661:GLY:N	2:B:1081:LEU:HD22	2.21	0.55
2:B:577:ALA:HB1	2:B:589:VAL:CG1	2.36	0.55
3:C:99:LEU:N	3:C:99:LEU:HD23	2.21	0.55
1:A:320:ARG:HB2	1:A:321:PRO:CA	2.36	0.55
1:A:352:VAL:HG12	1:A:353:ILE:N	2.22	0.55
1:A:406:ILE:N	1:A:406:ILE:CD1	2.62	0.55
1:A:765:VAL:CG2	1:A:800:VAL:CB	2.73	0.55
1:A:76:GLU:CD	2:B:1159:ARG:HH12	2.15	0.55
1:A:446:ARG:HG3	1:A:487:MET:HG2	1.89	0.55
2:B:169:ARG:O	2:B:171:PRO:HD3	2.07	0.55
3:C:91:HIS:HB2	3:C:96:SER:HG	1.71	0.55
5:F:101:ILE:HD13	5:F:120:ILE:HG22	1.88	0.55
7:I:85:PHE:O	7:I:86:PHE:HB3	2.07	0.55
1:A:33:ALA:HB3	1:A:83:HIS:H	1.72	0.55
1:A:315:LEU:HD12	1:A:318:SER:O	2.06	0.55
1:A:694:THR:HA	1:A:714:PHE:HE1	1.70	0.55
1:A:897:TYR:HD2	1:A:936:LEU:HD13	1.72	0.55
1:A:1061:GLY:O	1:A:1062:GLU:C	2.50	0.55
1:A:1166:ASP:CG	1:A:1194:ARG:HH21	2.15	0.55
2:B:95:ILE:CD1	2:B:130:VAL:HG22	2.36	0.55
11:R:5:A:C2	11:R:6:G:C5	2.95	0.55
1:A:472:LEU:HD21	2:B:835:GLN:CB	2.37	0.55
3:C:52:GLU:HB3	3:C:154:LYS:HB3	1.87	0.55
1:A:273:ASN:C	1:A:275:SER:H	2.15	0.54
1:A:344:ARG:O	2:B:1155:SER:HB2	2.06	0.54
1:A:1111:MET:HG3	1:A:1114:PRO:CG	2.30	0.54
2:B:426:LYS:HD2	2:B:430:ARG:HH22	1.71	0.54
2:B:475:SER:C	2:B:477:ALA:H	2.14	0.54
2:B:780:VAL:O	2:B:817:LEU:HD23	2.07	0.54
2:B:1182:CYS:SG	2:B:1185:CYS:HB2	2.46	0.54
3:C:251:LEU:O	3:C:255:VAL:HG23	2.06	0.54
7:I:71:SER:HB3	7:I:85:PHE:CE2	2.43	0.54
1:A:903:ASN:O	1:A:907:THR:OG1	2.26	0.54
2:B:364:ILE:O	2:B:365:THR:HB	2.07	0.54
6:H:109:LYS:HB3	6:H:110:ASP:C	2.31	0.54
1:A:704:ALA:HB2	1:A:710:LEU:HG	1.89	0.54
8:J:7:CYS:HA	8:J:49:MET:HG2	1.89	0.54
1:A:320:ARG:HB2	1:A:321:PRO:HB3	1.89	0.54
1:A:947:PHE:CD2	1:A:954:TRP:CE2	2.96	0.54
3:C:66:ARG:NH2	8:J:3:VAL:O	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:101:MET:CE	2:B:169:ARG:HH12	2.19	0.54
2:B:604:ARG:HA	2:B:609:ILE:O	2.07	0.54
2:B:992:ILE:CD1	9:K:67:PHE:HE2	2.12	0.54
5:F:86:THR:OG1	5:F:89:GLU:HG3	2.07	0.54
1:A:352:VAL:HG21	2:B:1099:VAL:HG13	1.89	0.54
1:A:568:PRO:HD3	6:H:94:ASP:O	2.06	0.54
2:B:1073:TYR:OH	3:C:179:GLU:HG3	2.07	0.54
2:B:1094:ARG:NH2	2:B:1098:MET:HG2	2.21	0.54
3:C:183:TRP:CD1	3:C:183:TRP:H	2.24	0.54
4:E:168:TYR:O	4:E:170:LEU:HG	2.06	0.54
5:F:76:LYS:O	5:F:79:ARG:HD2	2.07	0.54
7:I:27:PHE:O	7:I:35:VAL:HG13	2.08	0.54
3:C:165:LYS:O	9:K:6:ARG:NH1	2.40	0.54
4:E:36:GLU:O	4:E:38:PRO:HD3	2.07	0.54
4:E:168:TYR:HB3	4:E:170:LEU:HD11	1.90	0.54
6:H:93:TYR:HA	6:H:145:ARG:HB3	1.88	0.54
9:K:65:HIS:HD2	9:K:67:PHE:N	2.01	0.54
1:A:962:ARG:O	1:A:963:ILE:C	2.51	0.54
2:B:1060:ARG:C	2:B:1062:HIS:N	2.65	0.54
3:C:52:GLU:HA	10:L:64:LEU:HD22	1.89	0.54
5:F:109:VAL:HG11	5:F:123:LYS:HG2	1.90	0.54
9:K:51:LEU:HD13	9:K:59:ALA:HB3	1.90	0.54
1:A:383:TYR:HB3	5:F:115:THR:HB	1.89	0.54
1:A:419:LYS:HG3	1:A:420:ARG:HG3	1.88	0.54
1:A:444:PHE:CE2	1:A:470:LEU:HD23	2.43	0.54
1:A:805:LEU:CD2	2:B:1052:VAL:HG21	2.38	0.54
1:A:1193:LEU:HD21	1:A:1267:MET:HE2	1.90	0.54
4:E:191:LYS:H	4:E:194:GLU:HB2	1.72	0.54
1:A:1364:ASN:HD22	1:A:1364:ASN:C	2.15	0.54
1:A:1424:VAL:HG13	1:A:1436:ILE:HD11	1.89	0.54
2:B:273:LEU:HD11	2:B:285:ILE:HD11	1.90	0.54
1:A:252:PHE:CD1	1:A:252:PHE:C	2.85	0.53
1:A:332:LYS:H	1:A:337:ARG:HB3	1.71	0.53
1:A:402:ALA:O	1:A:415:LEU:HD12	2.08	0.53
1:A:709:THR:HG23	7:I:94:ASP:HA	1.90	0.53
3:C:63:ILE:HA	3:C:66:ARG:HG3	1.89	0.53
1:A:257:ARG:O	1:A:257:ARG:CG	2.51	0.53
2:B:329:THR:HA	2:B:332:ASP:CB	2.38	0.53
3:C:242:GLN:O	3:C:246:ARG:HG3	2.08	0.53
3:C:258:ILE:HD11	9:K:42:LEU:HD21	1.90	0.53
1:A:335:ARG:NH1	2:B:1202:LEU:HD12	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:351:THR:HG21	1:A:466:SER:O	2.08	0.53
2:B:1107:ALA:O	2:B:1108:ARG:HB3	2.08	0.53
5:F:80:ALA:O	5:F:81:THR:C	2.51	0.53
6:H:8:ASP:HB3	6:H:10:PHE:CE1	2.44	0.53
8:J:15:GLY:C	8:J:17:LYS:H	2.16	0.53
9:K:40:HIS:HE1	9:K:63:VAL:CG2	2.21	0.53
1:A:482:PHE:HD1	2:B:835:GLN:O	1.91	0.53
1:A:504:LEU:HD11	5:F:91:ALA:HB2	1.91	0.53
1:A:507:VAL:CG1	1:A:521:MET:HE1	2.38	0.53
1:A:526:ASP:OD2	2:B:829:CYS:CB	2.57	0.53
1:A:605:MET:HE3	1:A:614:PHE:O	2.09	0.53
1:A:822:GLU:O	1:A:826:ASP:CG	2.51	0.53
2:B:642:ASP:CB	2:B:649:LYS:HG3	2.23	0.53
3:C:57:VAL:HG23	8:J:57:ILE:HD11	1.90	0.53
9:K:65:HIS:CD2	9:K:67:PHE:H	2.14	0.53
1:A:367:PRO:HG3	1:A:466:SER:C	2.34	0.53
1:A:822:GLU:O	1:A:826:ASP:OD2	2.27	0.53
2:B:361:LEU:O	2:B:363:HIS:O	2.26	0.53
2:B:521:LEU:HD22	2:B:633:VAL:HB	1.89	0.53
2:B:824:ILE:HG12	8:J:48:ARG:HH12	1.72	0.53
3:C:92:CYS:SG	3:C:94:LYS:HB3	2.48	0.53
1:A:396:PRO:O	1:A:397:ASN:C	2.52	0.53
2:B:287:ARG:NH2	2:B:294:ASP:OD2	2.42	0.53
1:A:401:GLY:O	1:A:402:ALA:CB	2.56	0.53
4:E:15:ALA:O	4:E:19:VAL:HG23	2.08	0.53
9:K:46:ILE:O	9:K:50:LEU:HB2	2.08	0.53
1:A:528:LEU:HD23	1:A:751:SER:HA	1.91	0.53
1:A:590:ARG:HH21	1:A:621:THR:HA	1.74	0.53
1:A:1410:PHE:O	1:A:1413:GLY:N	2.41	0.53
2:B:913:GLY:HA2	2:B:938:SER:HB2	1.87	0.53
4:E:35:VAL:C	4:E:37:LEU:H	2.17	0.53
1:A:1400:CYS:SG	1:A:1409:LEU:HG	2.49	0.53
2:B:778:MET:O	2:B:819:ALA:HB1	2.08	0.53
3:C:5:GLY:O	3:C:7:GLN:HG2	2.09	0.53
3:C:43:THR:CG2	3:C:44:LEU:N	2.72	0.53
5:F:125:LEU:C	5:F:127:GLU:H	2.16	0.53
8:J:7:CYS:CB	8:J:46:CYS:SG	2.97	0.53
2:B:288:ALA:HB1	2:B:331:LEU:HD12	1.91	0.53
2:B:1002:THR:HG23	2:B:1004:GLU:N	2.17	0.53
8:J:2:ILE:HG23	8:J:2:ILE:O	2.09	0.53
1:A:545:GLN:O	1:A:546:VAL:C	2.52	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:650:GLN:HB3	1:A:654:ASN:HD21	1.74	0.52
1:A:1345:ARG:HD2	1:A:1373:ASP:OD1	2.09	0.52
2:B:124:TYR:HH	2:B:179:CYS:HG	1.56	0.52
2:B:592:ASN:N	2:B:593:PRO:CD	2.71	0.52
4:E:153:HIS:CD2	4:E:198:ILE:HG12	2.43	0.52
1:A:765:VAL:HG23	1:A:766:GLY:H	1.74	0.52
2:B:745:PRO:C	2:B:747:MET:N	2.64	0.52
2:B:954:VAL:O	10:L:55:ILE:O	2.27	0.52
2:B:1181:GLU:HG2	2:B:1188:LYS:HG2	1.91	0.52
1:A:252:PHE:HD1	1:A:252:PHE:O	1.91	0.52
1:A:880:LYS:CG	1:A:880:LYS:O	2.57	0.52
2:B:745:PRO:C	2:B:747:MET:H	2.16	0.52
3:C:66:ARG:HH21	8:J:4:PRO:HA	1.74	0.52
1:A:464:PRO:CG	9:K:67:PHE:CD1	2.92	0.52
2:B:983:ARG:O	2:B:984:HIS:CG	2.62	0.52
1:A:312:PRO:O	1:A:313:GLN:HB2	2.10	0.52
1:A:504:LEU:HD11	5:F:91:ALA:CB	2.39	0.52
1:A:535:THR:HG22	1:A:616:VAL:HA	1.91	0.52
2:B:773:MET:C	2:B:775:LYS:N	2.66	0.52
4:E:6:GLU:O	4:E:9:ILE:HG22	2.09	0.52
4:E:127:ILE:O	4:E:127:ILE:HG12	2.08	0.52
1:A:403:LYS:HA	1:A:415:LEU:HB2	1.91	0.52
1:A:639:PRO:HG2	1:A:640:GLN:HG2	1.92	0.52
1:A:885:THR:O	1:A:940:ARG:HG3	2.09	0.52
2:B:737:THR:HG21	7:I:66:PRO:HA	1.91	0.52
2:B:981:ALA:HB3	2:B:1095:LEU:HD11	1.92	0.52
3:C:58:LEU:HD21	8:J:57:ILE:CD1	2.40	0.52
5:F:111:LEU:H	5:F:111:LEU:CD1	2.22	0.52
6:H:58:THR:HG22	6:H:59:ILE:H	1.74	0.52
8:J:45:CYS:HG	8:J:46:CYS:N	2.05	0.52
9:K:49:GLU:C	9:K:51:LEU:N	2.68	0.52
1:A:15:LYS:HE2	2:B:1220:ARG:HG2	1.91	0.52
2:B:864:LYS:HD3	2:B:870:ILE:O	2.10	0.52
2:B:983:ARG:NH1	2:B:1091:TYR:HB3	2.25	0.52
3:C:241:ASP:O	3:C:245:VAL:HG23	2.09	0.52
4:E:2:ASP:O	4:E:3:GLN:CB	2.57	0.52
4:E:30:ILE:HG22	4:E:31:THR:O	2.09	0.52
7:I:99:LEU:O	7:I:111:THR:HG23	2.09	0.52
1:A:161:LEU:O	1:A:162:VAL:O	2.27	0.52
1:A:265:LYS:NZ	1:A:323:LYS:HE2	2.25	0.52
1:A:535:THR:HG23	1:A:575:LYS:HG2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:648:ASN:OD1	1:A:648:ASN:N	2.43	0.52
1:A:1118:VAL:HA	1:A:1327:ILE:HG13	1.90	0.52
2:B:176:SER:O	2:B:182:SER:HB2	2.10	0.52
2:B:864:LYS:HZ1	2:B:867:GLY:CA	2.22	0.52
3:C:16:ASP:O	3:C:233:GLU:HA	2.10	0.52
1:A:417:TYR:O	1:A:418:SER:HB3	2.10	0.52
1:A:1021:LEU:O	1:A:1024:SER:N	2.43	0.52
1:A:1341:ILE:HB	4:E:182:ASP:OD2	2.09	0.52
2:B:363:HIS:O	2:B:364:ILE:CB	2.47	0.52
2:B:516:ASN:HD22	2:B:516:ASN:H	1.56	0.52
3:C:261:ALA:HA	3:C:264:GLN:OE1	2.10	0.52
6:H:84:ALA:C	6:H:86:ASP:H	2.18	0.52
1:A:341:MET:HE2	1:A:1401:SER:HB2	1.92	0.51
2:B:792:MET:HG3	2:B:855:PHE:HE1	1.74	0.51
2:B:912:ILE:O	2:B:938:SER:HB2	2.10	0.51
1:A:134:ARG:HD2	1:A:221:SER:O	2.11	0.51
1:A:575:LYS:HB3	1:A:612:ILE:HG12	1.92	0.51
2:B:204:ILE:HD12	2:B:204:ILE:N	2.25	0.51
2:B:291:ILE:HG22	2:B:297:ILE:HD13	1.91	0.51
2:B:882:THR:CG2	2:B:935:ARG:HA	2.22	0.51
8:J:1:MET:N	8:J:56:LEU:N	2.58	0.51
1:A:565:ILE:HG23	1:A:567:LYS:HE3	1.91	0.51
1:A:863:VAL:O	1:A:864:ILE:HD13	2.10	0.51
2:B:1013:ASN:C	2:B:1015:HIS:H	2.19	0.51
1:A:39:GLU:O	1:A:53:LEU:HB2	2.09	0.51
1:A:251:SER:OG	1:A:252:PHE:N	2.42	0.51
1:A:470:LEU:HD21	1:A:487:MET:HE1	1.92	0.51
1:A:471:ASN:O	1:A:473:SER:N	2.44	0.51
1:A:803:SER:OG	1:A:806:ARG:HD2	2.10	0.51
1:A:1345:ARG:HG3	1:A:1376:THR:HG21	1.91	0.51
2:B:323:VAL:O	2:B:324:ILE:HG13	2.10	0.51
2:B:428:ILE:HD11	2:B:448:ILE:HD13	1.91	0.51
1:A:55:ASP:O	1:A:56:PRO:C	2.52	0.51
1:A:256:GLN:HB3	1:A:257:ARG:HD3	1.90	0.51
1:A:608:ILE:HG12	1:A:613:ILE:HG13	1.93	0.51
1:A:705:LYS:HG3	1:A:713:SER:HB3	1.92	0.51
1:A:858:ASN:HD21	1:A:860:LEU:HB2	1.76	0.51
1:A:1161:THR:HG22	1:A:1163:ILE:H	1.75	0.51
1:A:1161:THR:HG23	1:A:1239:ARG:NH2	2.25	0.51
1:A:1437:GLY:CA	5:F:88:TYR:CD2	2.93	0.51
2:B:64:CYS:HA	2:B:67:SER:HB3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:519:TRP:CD1	2:B:519:TRP:C	2.88	0.51
3:C:226:ASP:O	3:C:227:THR:O	2.29	0.51
6:H:15:VAL:HA	6:H:26:ILE:HD12	1.92	0.51
1:A:401:GLY:CA	1:A:435:HIS:CD2	2.94	0.51
1:A:445:ASN:HB3	1:A:455:MET:HE2	1.91	0.51
1:A:575:LYS:HB3	1:A:612:ILE:CG1	2.40	0.51
1:A:802:ASN:HD21	2:B:729:ILE:N	2.05	0.51
1:A:1155:ASP:OD1	1:A:1162:VAL:HG23	2.10	0.51
1:A:1364:ASN:HD22	1:A:1366:ARG:N	2.08	0.51
1:A:1438:THR:HG23	5:F:92:ARG:HB2	1.92	0.51
2:B:451:LYS:O	2:B:452:THR:C	2.53	0.51
2:B:814:PHE:C	2:B:816:GLU:N	2.67	0.51
2:B:978:ASP:OD1	2:B:1099:VAL:HG23	2.11	0.51
1:A:321:PRO:O	1:A:322:VAL:HG22	2.10	0.51
2:B:498:THR:O	2:B:536:VAL:HA	2.09	0.51
2:B:789:MET:HE1	2:B:965:LYS:O	2.11	0.51
3:C:102:GLN:CG	3:C:154:LYS:HD3	2.26	0.51
3:C:241:ASP:HB3	9:K:109:TRP:CE2	2.46	0.51
6:H:115:TYR:CE2	6:H:124:ARG:HG3	2.45	0.51
1:A:92:HIS:ND1	1:A:236:LEU:HD21	2.25	0.51
1:A:148:CYS:HB3	1:A:168:GLY:HA2	1.93	0.51
1:A:319:GLY:HA2	1:A:320:ARG:HH11	1.57	0.51
1:A:526:ASP:OD2	2:B:829:CYS:HB2	2.10	0.51
1:A:793:SER:O	1:A:794:PRO:C	2.54	0.51
2:B:788:ARG:NH1	2:B:790:ASP:OD1	2.44	0.51
1:A:475:THR:CG2	1:A:476:SER:N	2.74	0.51
1:A:755:PHE:O	1:A:756:ILE:C	2.54	0.51
2:B:696:GLU:O	2:B:699:GLU:HB2	2.11	0.51
3:C:3:GLU:HA	9:K:104:ASN:ND2	2.25	0.51
3:C:42:PRO:HA	3:C:163:ILE:HG23	1.92	0.51
8:J:8:PHE:H	8:J:49:MET:HE3	1.75	0.51
1:A:249:SER:O	1:A:250:ILE:CB	2.59	0.51
1:A:794:PRO:O	1:A:797:LYS:N	2.41	0.51
1:A:857:ARG:HB3	1:A:862:ASN:O	2.11	0.51
1:A:1299:VAL:HG12	1:A:1300:LYS:H	1.75	0.51
1:A:1434:ALA:O	1:A:1436:ILE:N	2.44	0.51
2:B:1023:VAL:O	2:B:1024:ALA:C	2.54	0.51
8:J:7:CYS:CA	8:J:49:MET:HE3	2.40	0.51
1:A:68:GLN:C	1:A:70:CYS:H	2.18	0.50
1:A:93:VAL:HG22	1:A:301:ALA:HA	1.93	0.50
2:B:999:MET:HA	2:B:999:MET:HE3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:999:MET:HE2	2:B:1011:ILE:HD11	1.92	0.50
2:B:1065:GLN:HE21	2:B:1069:PHE:H	1.59	0.50
6:H:109:LYS:HB3	6:H:110:ASP:CG	2.36	0.50
1:A:705:LYS:HE3	1:A:713:SER:CB	2.41	0.50
1:A:1362:TYR:CD1	1:A:1362:TYR:C	2.87	0.50
3:C:66:ARG:NH2	8:J:4:PRO:HA	2.26	0.50
6:H:41:ASP:HB3	6:H:121:LEU:HD22	1.93	0.50
9:K:51:LEU:CD1	9:K:59:ALA:HB3	2.41	0.50
1:A:49:LYS:NZ	1:A:60:SER:HA	2.26	0.50
1:A:412:ARG:NH2	1:A:433:GLU:OE2	2.44	0.50
1:A:965:GLN:HA	1:A:968:GLN:HG2	1.93	0.50
2:B:902:GLY:O	10:L:65:VAL:HG11	2.11	0.50
1:A:609:ASP:C	1:A:611:GLN:H	2.19	0.50
1:A:794:PRO:HA	1:A:797:LYS:HB2	1.93	0.50
2:B:313:MET:HG3	2:B:390:LEU:HD21	1.94	0.50
2:B:485:ARG:CZ	2:B:782:LEU:HD11	2.41	0.50
2:B:843:GLN:NE2	2:B:847:ASP:OD1	2.44	0.50
10:L:34:CYS:O	10:L:35:SER:HB2	2.10	0.50
1:A:351:THR:CG2	1:A:352:VAL:H	2.18	0.50
1:A:658:LEU:HD22	2:B:831:SER:HA	1.92	0.50
2:B:175:ARG:HH11	2:B:175:ARG:HG2	1.77	0.50
2:B:957:ASN:HB3	2:B:961:LEU:HB2	1.92	0.50
2:B:973:ILE:CG2	2:B:974:PRO:HD2	2.41	0.50
4:E:113:GLN:HB3	4:E:137:GLU:OE1	2.11	0.50
9:K:32:VAL:HB	9:K:74:ARG:HG3	1.93	0.50
1:A:99:ILE:HG12	1:A:234:MET:SD	2.51	0.50
1:A:285:PRO:O	1:A:286:HIS:HB2	2.10	0.50
1:A:385:ILE:HD11	1:A:428:TYR:CE2	2.47	0.50
1:A:838:GLN:O	1:A:839:ARG:C	2.55	0.50
1:A:1116:LEU:CD2	1:A:1329:THR:CG2	2.64	0.50
2:B:62:ILE:HD12	2:B:418:LYS:HE2	1.94	0.50
2:B:773:MET:C	2:B:775:LYS:H	2.20	0.50
1:A:361:LEU:HD21	1:A:521:MET:CE	2.39	0.50
2:B:176:SER:O	2:B:182:SER:CB	2.60	0.50
2:B:647:GLY:O	2:B:648:HIS:O	2.30	0.50
2:B:1175:LEU:O	2:B:1176:ASN:HB2	2.11	0.50
4:E:3:GLN:HG2	4:E:5:ASN:H	1.76	0.50
1:A:356:ASP:HB3	1:A:359:LEU:HD12	1.94	0.50
1:A:880:LYS:O	1:A:880:LYS:HG2	2.12	0.50
1:A:1134:ILE:O	1:A:1138:ILE:HG13	2.12	0.50
1:A:1279:ILE:HG22	1:A:1279:ILE:O	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:48:LEU:O	2:B:49:ASP:C	2.55	0.50
2:B:522:VAL:HG11	2:B:537:LYS:HB3	1.93	0.50
4:E:165:LEU:HD13	4:E:170:LEU:O	2.11	0.50
9:K:6:ARG:O	9:K:8:GLU:N	2.45	0.50
1:A:100:LYS:O	1:A:104:GLU:HG3	2.12	0.50
1:A:184:SER:HA	1:A:199:LEU:HD13	1.93	0.50
1:A:590:ARG:HG2	1:A:591:PHE:H	1.77	0.50
1:A:765:VAL:HG21	1:A:800:VAL:CG1	2.41	0.50
2:B:575:PRO:C	2:B:577:ALA:H	2.19	0.50
2:B:648:HIS:O	2:B:649:LYS:O	2.30	0.50
2:B:779:GLY:C	2:B:795:ILE:HG23	2.37	0.50
2:B:864:LYS:CG	2:B:865:LYS:N	2.36	0.50
2:B:1084:GLN:NE2	3:C:192:TRP:H	2.10	0.50
7:I:62:ILE:C	7:I:64:SER:H	2.19	0.50
11:R:3:C:H2'	11:R:4:G:C8	2.46	0.50
1:A:423:ASP:C	1:A:424:ILE:HG13	2.37	0.49
1:A:909:ASP:OD1	1:A:911:SER:HB3	2.11	0.49
2:B:547:VAL:HG12	2:B:612:GLU:OE2	2.12	0.49
2:B:636:PRO:HB2	2:B:637:LEU:CB	2.42	0.49
2:B:737:THR:O	2:B:738:PHE:C	2.56	0.49
2:B:840:ILE:HB	2:B:1011:ILE:HD12	1.93	0.49
2:B:863:GLU:O	2:B:864:LYS:O	2.30	0.49
2:B:1168:LEU:HD21	2:B:1214:PRO:HD2	1.93	0.49
1:A:434:ARG:NH2	1:A:440:ASP:OD2	2.43	0.49
1:A:666:ILE:HG23	2:B:1026:LEU:HD12	1.94	0.49
1:A:672:ASP:N	1:A:736:ASN:HD21	2.11	0.49
2:B:982:SER:O	2:B:1093:GLN:HG3	2.12	0.49
6:H:59:ILE:O	6:H:60:ALA:HB3	2.12	0.49
1:A:527:THR:HG21	1:A:650:GLN:HG2	1.92	0.49
1:A:902:LEU:CG	1:A:926:GLN:HG3	2.42	0.49
2:B:321:GLY:C	2:B:323:VAL:H	2.21	0.49
2:B:647:GLY:O	2:B:648:HIS:C	2.55	0.49
2:B:942:ARG:HB2	2:B:945:GLU:HB2	1.94	0.49
2:B:1006:ILE:HD11	8:J:43:ARG:HB2	1.93	0.49
2:B:1027:ILE:C	2:B:1029:CYS:N	2.69	0.49
2:B:1074:ASN:OD1	2:B:1076:HIS:N	2.45	0.49
5:F:83:PRO:HG2	5:F:84:TYR:HD1	1.77	0.49
1:A:49:LYS:HZ3	1:A:60:SER:HA	1.78	0.49
1:A:100:LYS:HD3	1:A:104:GLU:OE1	2.12	0.49
1:A:596:THR:C	1:A:598:LEU:N	2.67	0.49
1:A:1134:ILE:O	1:A:1138:ILE:CG1	2.61	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:565:PRO:HB2	2:B:567:GLU:OE2	2.13	0.49
1:A:290:GLU:HA	1:A:293:GLU:HG3	1.93	0.49
1:A:314:ALA:HA	1:A:320:ARG:HA	1.95	0.49
1:A:500:GLU:HG2	2:B:1143:ALA:HB1	1.94	0.49
1:A:565:ILE:HG12	1:A:567:LYS:NZ	2.27	0.49
1:A:711:ARG:HH12	7:I:95:THR:HB	1.77	0.49
1:A:777:PHE:HD2	1:A:782:ARG:CA	2.25	0.49
1:A:1116:LEU:HB2	1:A:1308:THR:OG1	2.13	0.49
2:B:515:HIS:H	2:B:518:HIS:HD2	1.58	0.49
2:B:807:ARG:HH11	2:B:807:ARG:CG	2.17	0.49
3:C:181:ASP:CG	3:C:186:LEU:HD13	2.38	0.49
5:F:114:GLU:OE2	5:F:119:ARG:HG2	2.12	0.49
1:A:847:ASP:HB3	1:A:1424:VAL:HG23	1.95	0.49
2:B:319:GLU:C	2:B:321:GLY:H	2.19	0.49
2:B:745:PRO:O	2:B:747:MET:N	2.46	0.49
2:B:797:TYR:HB3	2:B:798:TYR:CD1	2.48	0.49
3:C:20:PHE:HE1	3:C:22:LEU:HD12	1.77	0.49
5:F:116:ASP:HB3	5:F:119:ARG:HB2	1.93	0.49
7:I:35:VAL:CG1	7:I:36:GLU:N	2.76	0.49
1:A:406:ILE:HD13	1:A:431:LYS:CB	2.42	0.49
1:A:540:PHE:HB3	1:A:571:LEU:HD23	1.95	0.49
1:A:808:LEU:HD23	1:A:813:PHE:HA	1.94	0.49
1:A:881:GLN:CD	1:A:959:ASN:HA	2.37	0.49
1:A:991:LYS:O	1:A:994:GLN:HB3	2.11	0.49
1:A:1111:MET:SD	1:A:1114:PRO:HB3	2.50	0.49
2:B:211:VAL:HG12	2:B:212:LEU:N	2.27	0.49
2:B:581:PHE:HB2	2:B:625:LYS:HG2	1.95	0.49
5:F:81:THR:O	5:F:82:THR:C	2.55	0.49
6:H:80:ARG:O	6:H:81:PRO:O	2.30	0.49
12:T:16:DC:C6	12:T:17:DG:C8	3.01	0.49
1:A:18:GLN:HG3	1:A:228:PHE:HE1	1.78	0.49
1:A:130:ASP:C	1:A:132:LYS:N	2.71	0.49
1:A:316:GLN:O	1:A:316:GLN:HG2	2.11	0.49
1:A:445:ASN:HB2	1:A:455:MET:HG2	1.95	0.49
1:A:579:SER:HB3	1:A:611:GLN:HA	1.94	0.49
1:A:672:ASP:N	1:A:736:ASN:ND2	2.60	0.49
1:A:1130:GLN:HG3	1:A:1134:ILE:HD11	1.95	0.49
2:B:200:GLY:HA2	2:B:202:TYR:CE2	2.48	0.49
2:B:310:MET:O	2:B:313:MET:HB2	2.13	0.49
2:B:566:LEU:HD22	2:B:586:TRP:O	2.13	0.49
2:B:1077:THR:HG23	2:B:1079:LYS:H	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1149:GLU:HG3	2:B:1153:GLU:CG	2.30	0.49
1:A:544:ASP:N	1:A:544:ASP:OD1	2.46	0.49
1:A:605:MET:HE1	1:A:612:ILE:HD12	1.95	0.49
1:A:1030:ARG:O	1:A:1031:VAL:C	2.55	0.49
2:B:592:ASN:H	2:B:593:PRO:HD3	1.78	0.49
3:C:29:MET:O	3:C:30:ALA:C	2.55	0.49
8:J:45:CYS:O	8:J:48:ARG:HG3	2.13	0.49
1:A:378:GLU:OE1	1:A:434:ARG:HD3	2.13	0.49
1:A:451:HIS:HB3	1:A:453:MET:N	2.28	0.49
1:A:472:LEU:CD2	2:B:835:GLN:HB3	2.41	0.49
1:A:483:ASP:OD1	11:R:11:U:P	2.71	0.49
1:A:1397:LEU:O	1:A:1400:CYS:HB2	2.12	0.49
2:B:44:VAL:O	2:B:45:SER:C	2.55	0.49
2:B:174:LEU:O	2:B:175:ARG:CB	2.60	0.49
4:E:78:LEU:HD12	4:E:107:THR:HB	1.95	0.49
1:A:249:SER:O	1:A:250:ILE:CG2	2.60	0.48
2:B:23:ALA:HB1	2:B:24:PRO:CD	2.35	0.48
2:B:308:TRP:HA	2:B:311:LEU:HD12	1.95	0.48
7:I:19:ASP:HB3	7:I:24:ARG:H	1.78	0.48
1:A:32:VAL:HB	1:A:57:ARG:HB3	1.95	0.48
1:A:206:GLU:O	1:A:210:ILE:HG12	2.13	0.48
1:A:751:SER:HB2	2:B:1015:HIS:CE1	2.32	0.48
1:A:755:PHE:O	1:A:758:ILE:N	2.46	0.48
1:A:947:PHE:CZ	4:E:203:GLU:HA	2.48	0.48
2:B:288:ALA:HB1	2:B:331:LEU:CD1	2.43	0.48
2:B:292:ILE:HD11	2:B:327:ARG:HG2	1.95	0.48
2:B:483:LEU:O	2:B:484:ASN:HB2	2.13	0.48
2:B:864:LYS:NZ	2:B:867:GLY:CA	2.75	0.48
1:A:341:MET:HE1	1:A:843:LYS:HZ1	1.78	0.48
1:A:407:ARG:HG2	1:A:430:TRP:CH2	2.48	0.48
1:A:410:GLY:O	1:A:411:ASP:O	2.30	0.48
2:B:209:GLU:OE2	2:B:485:ARG:HD2	2.14	0.48
2:B:969:ARG:HD2	3:C:61:GLU:OE2	2.13	0.48
6:H:109:LYS:HB3	6:H:110:ASP:CA	2.43	0.48
1:A:315:LEU:HD23	1:A:316:GLN:CB	2.43	0.48
2:B:843:GLN:HA	2:B:846:ILE:HD12	1.96	0.48
8:J:56:LEU:O	8:J:57:ILE:C	2.54	0.48
10:L:48:CYS:SG	10:L:49:LYS:N	2.85	0.48
1:A:18:GLN:O	2:B:1215:ARG:HG2	2.12	0.48
1:A:18:GLN:HE21	1:A:1418:LEU:HD13	1.78	0.48
1:A:446:ARG:HE	1:A:480:ALA:CB	2.24	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:464:PRO:HG2	9:K:67:PHE:CE1	2.49	0.48
1:A:815:PHE:O	1:A:816:HIS:C	2.56	0.48
2:B:273:LEU:HB2	2:B:276:ILE:HD12	1.96	0.48
2:B:640:VAL:HG23	2:B:740:HIS:HA	1.96	0.48
4:E:205:SER:O	4:E:207:ARG:N	2.47	0.48
1:A:482:PHE:CD1	2:B:836:GLU:HB2	2.48	0.48
1:A:815:PHE:O	1:A:818:MET:N	2.46	0.48
3:C:31:ASN:O	3:C:33:LEU:N	2.47	0.48
8:J:32:GLU:CD	8:J:32:GLU:N	2.68	0.48
1:A:53:LEU:O	1:A:56:PRO:HD2	2.13	0.48
1:A:787:PHE:CE2	1:A:796:SER:HB2	2.48	0.48
1:A:800:VAL:HG13	1:A:812:GLU:HB3	1.96	0.48
2:B:34:ILE:HD13	2:B:542:MET:HE1	1.96	0.48
2:B:235:SER:OG	2:B:236:HIS:CD2	2.66	0.48
2:B:329:THR:HA	2:B:332:ASP:HB2	1.96	0.48
2:B:476:ARG:O	2:B:478:GLY:N	2.47	0.48
2:B:697:GLU:O	2:B:698:GLU:C	2.56	0.48
3:C:249:ASP:O	3:C:253:LYS:HG3	2.12	0.48
4:E:12:LEU:O	4:E:12:LEU:HG	2.13	0.48
4:E:108:GLY:HA3	4:E:132:ILE:HG12	1.96	0.48
6:H:38:LEU:HD12	6:H:124:ARG:O	2.14	0.48
7:I:71:SER:HB3	7:I:85:PHE:HE2	1.78	0.48
7:I:75:CYS:HB3	7:I:110:PHE:CE2	2.48	0.48
1:A:598:LEU:O	1:A:599:SER:C	2.57	0.48
2:B:258:LEU:HB2	2:B:385:LEU:HD21	1.95	0.48
2:B:1002:THR:HG22	2:B:1006:ILE:HB	1.96	0.48
1:A:254:GLU:HA	1:A:255:SER:HA	1.64	0.48
1:A:320:ARG:HB2	1:A:321:PRO:CB	2.43	0.48
1:A:436:ILE:HD11	1:A:491:VAL:HG11	1.96	0.48
1:A:650:GLN:HB3	1:A:654:ASN:ND2	2.29	0.48
1:A:928:LEU:HA	1:A:931:GLU:HB3	1.96	0.48
1:A:942:PHE:HD2	1:A:943:LEU:HD23	1.78	0.48
1:A:943:LEU:C	1:A:945:GLU:N	2.72	0.48
1:A:1215:ARG:O	1:A:1218:GLN:HB2	2.14	0.48
5:F:135:ARG:HG2	5:F:137:TYR:CE1	2.48	0.48
6:H:102:TYR:HE2	6:H:116:TYR:C	2.22	0.48
1:A:608:ILE:CG1	1:A:613:ILE:HG13	2.44	0.47
1:A:731:ARG:HG3	1:A:755:PHE:CE1	2.49	0.47
1:A:1100:ARG:HH21	1:A:1351:GLU:HG3	1.79	0.47
2:B:485:ARG:HG2	2:B:485:ARG:NH1	2.27	0.47
2:B:639:ILE:HG22	2:B:640:VAL:N	2.27	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:123:ASN:ND2	3:C:125:MET:HG2	2.29	0.47
3:C:148:ARG:O	3:C:151:GLN:HG3	2.14	0.47
3:C:167:HIS:HD2	3:C:169:LYS:N	2.09	0.47
4:E:112:TYR:O	4:E:137:GLU:HG3	2.14	0.47
6:H:80:ARG:HB3	6:H:81:PRO:HD2	1.95	0.47
7:I:106:CYS:O	7:I:108:HIS:N	2.47	0.47
8:J:3:VAL:CG2	8:J:18:TRP:CG	2.97	0.47
11:R:3:C:H2'	11:R:4:G:H8	1.78	0.47
1:A:76:GLU:OE2	2:B:1159:ARG:NH1	2.44	0.47
1:A:445:ASN:HD21	1:A:447:GLN:HE21	1.62	0.47
1:A:518:LYS:CB	1:A:519:PRO:HD2	2.44	0.47
1:A:755:PHE:O	1:A:757:ASN:N	2.48	0.47
2:B:361:LEU:CD2	2:B:377:PHE:HD2	2.27	0.47
2:B:416:LEU:CD2	2:B:457:LEU:HD23	2.43	0.47
2:B:633:VAL:O	2:B:694:ASP:HB2	2.14	0.47
2:B:1084:GLN:CD	2:B:1084:GLN:N	2.72	0.47
3:C:18:VAL:O	3:C:231:ASN:HA	2.15	0.47
3:C:196:ASP:O	3:C:200:GLU:HB2	2.14	0.47
6:H:104:PHE:N	6:H:104:PHE:CD1	2.82	0.47
1:A:607:ILE:HG12	1:A:612:ILE:HG22	1.96	0.47
1:A:899:VAL:CB	1:A:929:LEU:HD12	2.45	0.47
2:B:121:ASN:HA	2:B:207:GLY:HA3	1.96	0.47
2:B:424:LEU:O	2:B:428:ILE:HG12	2.13	0.47
6:H:43:ASN:ND2	6:H:46:LEU:HD12	2.30	0.47
8:J:1:MET:H1	8:J:56:LEU:HB2	1.79	0.47
1:A:294:SER:O	1:A:298:PHE:HB2	2.15	0.47
1:A:367:PRO:HB3	1:A:466:SER:HA	1.96	0.47
1:A:385:ILE:HD11	1:A:428:TYR:CZ	2.49	0.47
1:A:556:TRP:CZ2	1:A:560:ILE:HD13	2.49	0.47
1:A:567:LYS:NZ	6:H:97:MET:HG2	2.29	0.47
1:A:962:ARG:C	1:A:964:ILE:N	2.69	0.47
2:B:777:ALA:HA	2:B:1095:LEU:HD23	1.97	0.47
2:B:779:GLY:O	2:B:795:ILE:HA	2.15	0.47
1:A:130:ASP:O	1:A:132:LYS:N	2.48	0.47
1:A:399:HIS:CE1	1:A:462:VAL:HG21	2.49	0.47
1:A:1059:HIS:CE1	5:F:87:LYS:H	2.32	0.47
2:B:365:THR:OG1	2:B:367:LEU:HG	2.14	0.47
2:B:644:GLU:OE1	2:B:644:GLU:HA	2.14	0.47
5:F:109:VAL:CG1	5:F:110:ASP:H	2.17	0.47
8:J:53:HIS:HE1	8:J:55:ASP:OD1	1.96	0.47
1:A:535:THR:CG2	1:A:616:VAL:HA	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:919:ILE:O	1:A:920:LEU:C	2.57	0.47
1:A:1104:ILE:HD13	1:A:1332:PHE:CE2	2.50	0.47
1:A:1111:MET:HG3	1:A:1114:PRO:CD	2.44	0.47
1:A:1407:GLU:O	1:A:1411:GLU:HG2	2.15	0.47
2:B:260:GLY:O	2:B:267:ARG:HD3	2.14	0.47
2:B:577:ALA:HB1	2:B:589:VAL:HG13	1.96	0.47
1:A:276:LEU:CD1	1:A:292:ALA:CB	2.91	0.47
1:A:364:VAL:O	1:A:364:VAL:HG13	2.13	0.47
1:A:700:ASN:ND2	7:I:116:ASN:HD21	2.13	0.47
1:A:1161:THR:HG22	1:A:1162:VAL:N	2.28	0.47
2:B:34:ILE:HD13	2:B:542:MET:CE	2.45	0.47
2:B:758:PHE:CE1	2:B:1027:ILE:HG22	2.50	0.47
2:B:778:MET:HE1	2:B:1094:ARG:NH1	2.23	0.47
2:B:805:THR:HG21	2:B:815:ARG:HD3	1.96	0.47
2:B:957:ASN:ND2	2:B:958:GLN:N	2.63	0.47
7:I:32:CYS:SG	7:I:34:TYR:CB	3.03	0.47
1:A:929:LEU:HD21	1:A:983:ILE:HG23	1.95	0.47
1:A:947:PHE:CD2	1:A:954:TRP:NE1	2.82	0.47
1:A:951:GLU:HA	1:A:951:GLU:OE2	2.14	0.47
1:A:1025:ARG:HG3	1:A:1030:ARG:NH1	2.30	0.47
2:B:332:ASP:C	2:B:334:ILE:H	2.22	0.47
2:B:848:ARG:HH22	2:B:996:ARG:NH1	2.12	0.47
9:K:92:ASN:O	9:K:95:ILE:N	2.47	0.47
1:A:133:LYS:HA	1:A:136:ALA:HB3	1.97	0.47
1:A:244:PRO:HG2	1:A:245:PRO:HD3	1.96	0.47
1:A:848:ILE:O	1:A:1065:GLY:N	2.37	0.47
1:A:982:THR:C	1:A:984:LYS:N	2.71	0.47
1:A:1067:LEU:HD12	1:A:1067:LEU:C	2.40	0.47
2:B:45:SER:OG	2:B:46:GLN:N	2.48	0.47
2:B:552:MET:O	2:B:555:ILE:HB	2.15	0.47
2:B:708:GLU:HG3	2:B:709:ASP:N	2.24	0.47
3:C:185:LYS:CE	3:C:211:ASP:O	2.63	0.47
4:E:168:TYR:CB	4:E:170:LEU:HD11	2.45	0.47
1:A:446:ARG:HH12	1:A:448:PRO:HD2	1.79	0.47
1:A:590:ARG:O	1:A:591:PHE:HD1	1.95	0.47
1:A:833:GLU:O	1:A:834:THR:C	2.58	0.47
2:B:1039:GLY:HA2	8:J:51:LEU:HD22	1.96	0.47
2:B:1084:GLN:NE2	3:C:192:TRP:HB2	2.29	0.47
6:H:76:THR:O	6:H:77:ARG:O	2.33	0.47
9:K:57:LEU:HB2	9:K:76:GLN:HG2	1.97	0.47
1:A:408:ASP:C	1:A:410:GLY:N	2.73	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:583:PRO:O	1:A:610:GLY:HA2	2.15	0.46
1:A:700:ASN:HD22	7:I:116:ASN:HD21	1.64	0.46
1:A:731:ARG:HG3	1:A:755:PHE:CZ	2.51	0.46
1:A:805:LEU:HD21	2:B:1052:VAL:HG21	1.96	0.46
1:A:809:THR:H	1:A:812:GLU:HB2	1.81	0.46
1:A:947:PHE:CE2	1:A:954:TRP:CE2	3.04	0.46
2:B:288:ALA:HA	2:B:331:LEU:CD1	2.45	0.46
9:K:102:LYS:O	9:K:106:GLU:HG2	2.15	0.46
1:A:286:HIS:O	1:A:288:ALA:N	2.42	0.46
1:A:320:ARG:N	1:A:320:ARG:HH11	2.13	0.46
1:A:407:ARG:HA	1:A:430:TRP:CD1	2.50	0.46
2:B:490:SER:OG	2:B:491:THR:N	2.48	0.46
2:B:563:MET:O	2:B:563:MET:HG3	2.13	0.46
2:B:592:ASN:H	2:B:593:PRO:CD	2.27	0.46
2:B:769:TYR:O	2:B:772:ALA:N	2.49	0.46
2:B:1106:ARG:CD	2:B:1126:GLY:O	2.61	0.46
1:A:741:ASN:ND2	1:A:744:LYS:H	1.95	0.46
1:A:1011:GLN:HE22	1:A:1015:VAL:HG21	1.81	0.46
1:A:1100:ARG:HH21	1:A:1351:GLU:CG	2.28	0.46
2:B:286:PHE:HB3	2:B:297:ILE:HD12	1.96	0.46
2:B:573:GLN:O	2:B:575:PRO:HD3	2.16	0.46
2:B:586:TRP:NE1	2:B:588:GLY:O	2.48	0.46
9:K:40:HIS:HE1	9:K:63:VAL:HG22	1.78	0.46
12:T:27:DA:N3	12:T:28:DT:H5'	2.31	0.46
1:A:88:LYS:HA	1:A:89:PRO:HD2	1.53	0.46
1:A:549:MET:O	1:A:552:TRP:HB2	2.16	0.46
1:A:591:PHE:HD2	1:A:595:THR:HB	1.80	0.46
1:A:675:THR:C	1:A:679:ILE:HD12	2.40	0.46
1:A:722:LEU:HD11	1:A:794:PRO:HB3	1.98	0.46
1:A:1325:THR:HA	4:E:147:HIS:HA	1.97	0.46
1:A:1444:MET:HB2	5:F:133:VAL:HG12	1.97	0.46
2:B:1084:GLN:NE2	3:C:192:TRP:N	2.64	0.46
2:B:1166:CYS:O	2:B:1168:LEU:N	2.42	0.46
3:C:102:GLN:HA	3:C:153:LEU:O	2.16	0.46
4:E:175:LEU:HB2	4:E:213:ILE:HG22	1.98	0.46
6:H:22:LYS:HD3	6:H:45:GLU:OE1	2.16	0.46
7:I:40:SER:HB2	7:I:41:PRO:CD	2.45	0.46
1:A:37:PHE:HB2	1:A:52:GLY:CA	2.44	0.46
1:A:93:VAL:HG21	1:A:304:MET:HB3	1.97	0.46
1:A:252:PHE:CD1	1:A:252:PHE:O	2.69	0.46
1:A:360:GLU:O	1:A:363:GLN:HB2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:767:GLN:HE21	1:A:774:ARG:HB3	1.81	0.46
1:A:1261:LYS:C	1:A:1263:ILE:H	2.24	0.46
1:A:1344:GLY:O	1:A:1345:ARG:C	2.56	0.46
2:B:199:MET:SD	2:B:199:MET:N	2.82	0.46
2:B:412:LEU:O	2:B:413:LEU:C	2.57	0.46
9:K:7:PHE:C	9:K:9:LEU:N	2.74	0.46
1:A:403:LYS:HB2	1:A:404:TYR:CD1	2.50	0.46
1:A:997:LEU:O	1:A:1053:PHE:CE2	2.68	0.46
1:A:1072:ILE:O	1:A:1072:ILE:HG22	2.14	0.46
2:B:65:GLU:CD	2:B:66:ASP:H	2.24	0.46
2:B:221:ASN:OD1	2:B:242:SER:HA	2.16	0.46
2:B:554:ILE:O	2:B:555:ILE:C	2.59	0.46
2:B:983:ARG:HH11	2:B:1091:TYR:HB3	1.80	0.46
2:B:1065:GLN:NE2	2:B:1067:ARG:H	2.13	0.46
2:B:1200:ALA:O	2:B:1201:LYS:C	2.57	0.46
3:C:131:HIS:O	3:C:132:PRO:C	2.57	0.46
8:J:6:ARG:HG2	8:J:13:VAL:HA	1.98	0.46
12:T:13:DA:H61	13:N:2:DT:H71	1.79	0.46
1:A:239:LEU:CD1	1:A:240:PRO:HD2	2.35	0.46
1:A:573:SER:N	1:A:576:GLN:HG3	2.07	0.46
1:A:857:ARG:HA	1:A:864:ILE:HG12	1.97	0.46
2:B:555:ILE:CD1	2:B:587:HIS:CE1	2.99	0.46
2:B:600:LEU:HD12	2:B:615:MET:SD	2.56	0.46
2:B:862:GLN:HE21	2:B:961:LEU:HD13	1.81	0.46
3:C:27:LEU:HA	3:C:228:PHE:CZ	2.51	0.46
5:F:83:PRO:O	5:F:151:LEU:HD23	2.16	0.46
1:A:67:CYS:O	1:A:70:CYS:SG	2.74	0.46
1:A:322:VAL:CA	1:A:323:LYS:HD3	2.46	0.46
1:A:442:VAL:CG1	1:A:491:VAL:HG22	2.45	0.46
1:A:839:ARG:O	1:A:843:LYS:HB2	2.16	0.46
1:A:1227:ILE:CG2	1:A:1228:TRP:N	2.79	0.46
2:B:603:LEU:O	2:B:608:ASP:N	2.48	0.46
2:B:681:TRP:O	2:B:684:LEU:HB2	2.16	0.46
3:C:31:ASN:C	3:C:33:LEU:N	2.73	0.46
3:C:33:LEU:HG	3:C:37:MET:CE	2.46	0.46
1:A:251:SER:HB2	11:R:1:A:N3	2.31	0.46
1:A:303:TYR:O	1:A:303:TYR:CD1	2.68	0.46
1:A:596:THR:O	1:A:598:LEU:N	2.48	0.46
1:A:774:ARG:NH2	1:A:794:PRO:HA	2.31	0.46
1:A:1414:ALA:C	1:A:1416:ALA:H	2.24	0.46
3:C:22:LEU:HD22	3:C:25:VAL:HG21	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:125:LEU:C	5:F:127:GLU:N	2.74	0.46
6:H:77:ARG:O	6:H:78:SER:C	2.57	0.46
7:I:33:SER:O	7:I:34:TYR:C	2.59	0.46
1:A:68:GLN:O	1:A:68:GLN:CD	2.59	0.46
1:A:332:LYS:O	1:A:334:GLY:N	2.48	0.46
1:A:629:LEU:CD2	1:A:633:VAL:HG21	2.46	0.46
1:A:968:GLN:HG3	1:A:968:GLN:O	2.16	0.46
1:A:1349:TYR:O	1:A:1350:LYS:C	2.59	0.46
2:B:370:PHE:CD2	2:B:373:ARG:HG3	2.51	0.46
2:B:615:MET:HG2	2:B:626:ILE:HG23	1.98	0.46
3:C:43:THR:HG23	3:C:44:LEU:H	1.80	0.46
3:C:101:LEU:HD21	3:C:113:VAL:HG11	1.98	0.46
9:K:82:ASP:HA	9:K:83:PRO:HD2	1.80	0.46
10:L:26:THR:O	10:L:26:THR:HG22	2.16	0.46
10:L:60:ARG:HG3	10:L:61:THR:N	2.31	0.46
1:A:140:THR:HA	1:A:143:LYS:HE3	1.98	0.45
1:A:381:THR:OG1	1:A:382:PRO:HD2	2.16	0.45
1:A:396:PRO:O	1:A:398:GLU:O	2.34	0.45
1:A:412:ARG:HH22	2:B:1108:ARG:NH2	2.13	0.45
1:A:585:GLY:N	1:A:609:ASP:OD1	2.40	0.45
1:A:694:THR:HA	1:A:714:PHE:CE1	2.50	0.45
1:A:697:ALA:HA	1:A:702:LEU:HB2	1.98	0.45
1:A:996:ASN:C	1:A:998:LEU:N	2.73	0.45
2:B:175:ARG:CG	2:B:175:ARG:NH1	2.77	0.45
2:B:288:ALA:O	2:B:331:LEU:HD11	2.16	0.45
2:B:762:ASN:ND2	2:B:1022:THR:HA	2.31	0.45
2:B:1131:GLY:O	2:B:1132:GLU:C	2.58	0.45
8:J:6:ARG:HA	8:J:12:LYS:O	2.15	0.45
1:A:185:TRP:HZ3	1:A:200:ARG:HB3	1.81	0.45
1:A:315:LEU:CB	1:A:317:LYS:H	2.26	0.45
1:A:375:THR:OG1	1:A:433:GLU:HB3	2.16	0.45
1:A:590:ARG:HG2	1:A:591:PHE:N	2.31	0.45
1:A:922:ASP:OD1	1:A:923:LEU:N	2.46	0.45
1:A:955:PRO:C	1:A:956:LEU:HG	2.41	0.45
2:B:208:SER:OG	2:B:210:LYS:HE2	2.16	0.45
2:B:274:PRO:O	2:B:275:TYR:HB2	2.16	0.45
2:B:955:THR:CG2	2:B:956:THR:N	2.58	0.45
7:I:40:SER:HB2	7:I:41:PRO:HD3	1.97	0.45
1:A:384:ASN:O	1:A:385:ILE:C	2.59	0.45
1:A:482:PHE:HB2	2:B:836:GLU:O	2.17	0.45
1:A:1235:LYS:HG2	1:A:1237:ILE:HD11	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1364:ASN:HD21	1:A:1366:ARG:HG2	1.76	0.45
2:B:95:ILE:HG13	2:B:129:PHE:O	2.16	0.45
2:B:118:ARG:NH2	2:B:194:GLU:OE1	2.49	0.45
2:B:190:TYR:CD2	8:J:62:ARG:HB3	2.52	0.45
2:B:527:THR:OG1	2:B:528:PRO:HD2	2.17	0.45
2:B:763:GLN:O	2:B:766:ARG:HB2	2.16	0.45
2:B:1082:MET:HE2	3:C:188:HIS:C	2.42	0.45
4:E:67:GLU:O	4:E:70:SER:HB3	2.17	0.45
4:E:169:ARG:HG3	5:F:140:ASP:HB3	1.97	0.45
6:H:26:ILE:N	6:H:40:LEU:O	2.50	0.45
6:H:91:ASP:CG	6:H:91:ASP:O	2.59	0.45
10:L:38:LEU:HD21	10:L:49:LYS:HG2	1.98	0.45
1:A:381:THR:HG22	1:A:384:ASN:CG	2.41	0.45
1:A:406:ILE:HB	1:A:431:LYS:HB2	1.98	0.45
1:A:495:GLU:O	1:A:498:ARG:HG3	2.17	0.45
1:A:1392:SER:O	1:A:1394:THR:N	2.48	0.45
2:B:430:ARG:CD	2:B:434:ARG:HH22	2.29	0.45
2:B:515:HIS:CD2	2:B:517:THR:H	2.34	0.45
2:B:589:VAL:CG1	2:B:590:HIS:H	2.30	0.45
2:B:800:GLN:HG2	8:J:52:THR:HG22	1.98	0.45
4:E:178:ILE:HB	4:E:212:ARG:HD3	1.98	0.45
6:H:82:PRO:C	6:H:84:ALA:H	2.25	0.45
7:I:32:CYS:SG	7:I:34:TYR:HB2	2.57	0.45
7:I:111:THR:HG22	7:I:112:SER:N	2.32	0.45
9:K:108:GLU:O	9:K:109:TRP:C	2.59	0.45
1:A:99:ILE:HG13	1:A:99:ILE:H	1.49	0.45
1:A:320:ARG:H	1:A:320:ARG:HH11	1.64	0.45
1:A:575:LYS:CG	1:A:612:ILE:HD11	2.47	0.45
1:A:661:GLY:CA	2:B:1081:LEU:HD22	2.46	0.45
1:A:699:ALA:O	1:A:701:LEU:N	2.49	0.45
1:A:794:PRO:O	1:A:795:GLU:C	2.59	0.45
2:B:796:LEU:HB3	2:B:799:PRO:CD	2.22	0.45
4:E:48:ASP:HB3	4:E:54:GLN:HB2	1.97	0.45
10:L:61:THR:HG21	10:L:63:ARG:HG3	1.98	0.45
1:A:38:PRO:HB3	1:A:270:LEU:HB3	1.98	0.45
1:A:391:LEU:O	1:A:394:ASN:N	2.49	0.45
1:A:550:LEU:HD13	1:A:550:LEU:HA	1.79	0.45
1:A:567:LYS:HG3	1:A:568:PRO:HD2	1.98	0.45
1:A:843:LYS:HD3	1:A:846:GLU:OE2	2.16	0.45
1:A:1098:VAL:N	1:A:1099:PRO:HD2	2.32	0.45
2:B:198:ASP:OD1	2:B:485:ARG:NH2	2.43	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1148:LYS:O	2:B:1152:MET:CB	2.62	0.45
3:C:238:ILE:HG23	3:C:242:GLN:HB2	1.98	0.45
1:A:412:ARG:NH2	2:B:1108:ARG:NH2	2.65	0.45
1:A:672:ASP:HB2	1:A:736:ASN:ND2	2.28	0.45
1:A:699:ALA:C	1:A:701:LEU:H	2.25	0.45
1:A:1048:ASN:O	1:A:1049:ILE:C	2.60	0.45
2:B:361:LEU:N	2:B:362:PRO:HD3	2.32	0.45
2:B:983:ARG:O	2:B:984:HIS:CD2	2.70	0.45
2:B:1149:GLU:CG	2:B:1153:GLU:HG2	2.33	0.45
1:A:1049:ILE:O	1:A:1050:GLU:C	2.60	0.45
1:A:1117:THR:N	1:A:1328:TYR:O	2.50	0.45
2:B:195:CYS:HB3	2:B:782:LEU:HD22	1.99	0.45
3:C:99:LEU:N	3:C:99:LEU:CD2	2.79	0.45
12:T:9:DA:C5	12:T:10:DA:C6	3.05	0.45
12:T:13:DA:H61	13:N:2:DT:H73	1.77	0.45
12:T:26:DG:C2	12:T:27:DA:C8	3.05	0.45
1:A:68:GLN:O	1:A:70:CYS:N	2.50	0.45
1:A:219:PHE:CE1	1:A:230:ARG:HG2	2.52	0.45
1:A:239:LEU:HD12	1:A:240:PRO:N	2.31	0.45
1:A:324:SER:O	1:A:327:ALA:N	2.49	0.45
1:A:557:ASP:HA	9:K:26:LYS:CE	2.45	0.45
1:A:746:MET:HG2	1:A:751:SER:OG	2.17	0.45
1:A:1342:GLU:CG	4:E:212:ARG:HH11	2.25	0.45
2:B:326:ASP:OD1	2:B:329:THR:OG1	2.34	0.45
10:L:25:ALA:N	10:L:27:LEU:HD22	2.32	0.45
1:A:587:HIS:HA	1:A:607:ILE:O	2.17	0.45
1:A:768:GLN:CG	1:A:816:HIS:HA	2.47	0.45
1:A:1370:LEU:O	1:A:1374:VAL:HG23	2.17	0.45
2:B:202:TYR:H	2:B:202:TYR:HD2	1.63	0.45
2:B:845:SER:HB2	8:J:8:PHE:HB3	1.99	0.45
2:B:1006:ILE:HG22	2:B:1087:PHE:HZ	1.82	0.45
3:C:56:THR:CG2	3:C:145:CYS:SG	2.95	0.45
5:F:111:LEU:CD1	5:F:111:LEU:N	2.79	0.45
1:A:382:PRO:N	1:A:428:TYR:HE2	2.14	0.44
1:A:629:LEU:HD23	1:A:633:VAL:HG21	1.99	0.44
2:B:376:PHE:CE2	2:B:569:TYR:HD2	2.34	0.44
2:B:386:LEU:C	2:B:388:CYS:N	2.74	0.44
2:B:870:ILE:O	2:B:870:ILE:HG22	2.16	0.44
4:E:108:GLY:O	4:E:132:ILE:HG23	2.17	0.44
9:K:47:ARG:HD2	9:K:60:ALA:HA	1.98	0.44
12:T:9:DA:C6	12:T:10:DA:N1	2.85	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:T:18:DA:H2'	12:T:19:DT:C6	2.52	0.44
1:A:81:PHE:HE2	1:A:240:PRO:HB2	1.83	0.44
1:A:526:ASP:HB2	2:B:835:GLN:NE2	2.33	0.44
1:A:550:LEU:HD12	1:A:556:TRP:CD1	2.52	0.44
1:A:1351:GLU:O	1:A:1352:VAL:C	2.60	0.44
3:C:37:MET:HE3	3:C:37:MET:HB2	1.85	0.44
9:K:10:PHE:CD1	9:K:11:LEU:HD13	2.52	0.44
11:R:3:C:N4	12:T:26:DG:H1	2.08	0.44
1:A:14:VAL:H	1:A:1432:GLN:NE2	2.15	0.44
1:A:356:ASP:HB2	1:A:469:ARG:HH11	1.83	0.44
1:A:443:LEU:HD21	1:A:455:MET:HB3	1.99	0.44
1:A:445:ASN:CB	1:A:455:MET:HG2	2.46	0.44
1:A:575:LYS:HG2	1:A:612:ILE:HD11	1.99	0.44
1:A:577:ILE:O	1:A:578:LEU:C	2.61	0.44
1:A:599:SER:C	1:A:601:LYS:N	2.75	0.44
1:A:1067:LEU:HD12	1:A:1071:SER:OG	2.18	0.44
1:A:1261:LYS:C	1:A:1263:ILE:N	2.72	0.44
2:B:329:THR:HA	2:B:332:ASP:HB3	1.98	0.44
2:B:405:ARG:HA	2:B:631:GLY:O	2.16	0.44
2:B:859:TYR:N	2:B:859:TYR:CD1	2.86	0.44
2:B:1084:GLN:CD	2:B:1084:GLN:H	2.24	0.44
3:C:8:VAL:HG21	9:K:105:PHE:HB2	1.98	0.44
3:C:251:LEU:HG	9:K:98:LEU:HD11	1.99	0.44
6:H:57:VAL:HG22	6:H:144:ILE:HG12	1.99	0.44
6:H:97:MET:HB2	6:H:118:PHE:CD2	2.52	0.44
1:A:774:ARG:NH1	1:A:797:LYS:HD2	2.32	0.44
1:A:894:GLU:C	1:A:896:ARG:N	2.75	0.44
2:B:487:THR:O	2:B:488:TYR:C	2.59	0.44
2:B:778:MET:CE	2:B:1094:ARG:HH11	2.24	0.44
8:J:7:CYS:CB	8:J:49:MET:HE3	2.48	0.44
1:A:414:ASP:OD1	1:A:416:ARG:CG	2.62	0.44
1:A:947:PHE:HD2	1:A:954:TRP:CE2	2.36	0.44
1:A:1192:LEU:HD11	1:A:1239:ARG:HB3	1.98	0.44
2:B:117:ALA:HA	2:B:122:LEU:HB2	1.99	0.44
2:B:552:MET:N	2:B:553:PRO:HD2	2.33	0.44
1:A:353:ILE:HG22	1:A:468:PHE:HB2	2.00	0.44
1:A:1121:GLU:CG	1:A:1122:PRO:HD2	2.47	0.44
2:B:1159:ARG:HD3	2:B:1193:GLN:CG	2.45	0.44
4:E:184:VAL:O	4:E:187:TYR:N	2.50	0.44
5:F:136:ARG:HD2	5:F:146:TRP:CD1	2.53	0.44
8:J:36:LEU:HD11	8:J:51:LEU:HB2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:J:36:LEU:HD23	8:J:36:LEU:HA	1.85	0.44
11:R:6:G:H2'	11:R:7:A:H8	1.83	0.44
1:A:1340:GLY:O	1:A:1342:GLU:N	2.50	0.44
2:B:273:LEU:HD11	2:B:285:ILE:HD12	2.00	0.44
2:B:377:PHE:CE2	2:B:381:MET:HE2	2.52	0.44
2:B:797:TYR:C	2:B:799:PRO:HD2	2.42	0.44
3:C:77:ILE:HD12	3:C:161:LYS:HG3	1.99	0.44
5:F:116:ASP:HB3	5:F:119:ARG:CB	2.47	0.44
6:H:95:TYR:C	6:H:95:TYR:CD2	2.96	0.44
9:K:83:PRO:O	9:K:86:ALA:HB3	2.18	0.44
1:A:32:VAL:HB	1:A:57:ARG:HB2	2.00	0.44
1:A:315:LEU:N	1:A:315:LEU:HD22	2.33	0.44
1:A:336:ILE:HA	1:A:340:LEU:HD12	2.00	0.44
1:A:466:SER:HB3	9:K:2:ASN:ND2	2.33	0.44
3:C:131:HIS:HA	3:C:132:PRO:HD2	1.92	0.44
4:E:176:PRO:O	4:E:212:ARG:HA	2.18	0.44
1:A:53:LEU:HB3	1:A:54:ASN:H	1.52	0.44
1:A:219:PHE:CZ	1:A:230:ARG:HG2	2.53	0.44
1:A:353:ILE:HD11	1:A:481:ASP:O	2.18	0.44
1:A:474:VAL:HG22	1:A:478:TYR:CE1	2.53	0.44
1:A:626:ASN:C	1:A:628:GLY:H	2.26	0.44
1:A:809:THR:O	1:A:812:GLU:HB2	2.18	0.44
1:A:840:ARG:O	1:A:841:LEU:C	2.61	0.44
1:A:982:THR:C	1:A:984:LYS:H	2.25	0.44
1:A:1080:THR:HG22	1:A:1081:LEU:N	2.33	0.44
2:B:791:THR:O	2:B:792:MET:CB	2.66	0.44
2:B:843:GLN:N	2:B:994:TYR:O	2.43	0.44
2:B:881:ASN:CB	2:B:933:SER:N	2.80	0.44
2:B:999:MET:HG2	2:B:1008:PRO:HD2	2.00	0.44
10:L:53:HIS:C	10:L:55:ILE:H	2.25	0.44
1:A:265:LYS:HD2	1:A:303:TYR:CB	2.48	0.43
1:A:332:LYS:C	1:A:334:GLY:N	2.71	0.43
1:A:352:VAL:CG1	1:A:353:ILE:N	2.81	0.43
1:A:463:ILE:HB	1:A:464:PRO:CD	2.47	0.43
1:A:526:ASP:OD2	2:B:829:CYS:HB3	2.18	0.43
2:B:459:TYR:C	2:B:459:TYR:CD2	2.96	0.43
2:B:806:THR:H	2:B:809:MET:HG3	1.83	0.43
2:B:956:THR:CA	2:B:961:LEU:O	2.63	0.43
2:B:1051:THR:HB	2:B:1054:GLY:H	1.82	0.43
4:E:199:ILE:O	4:E:199:ILE:CG2	2.65	0.43
1:A:337:ARG:HD3	2:B:1132:GLU:OE1	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:777:PHE:HD2	1:A:782:ARG:C	2.27	0.43
2:B:542:MET:SD	2:B:636:PRO:HG3	2.58	0.43
2:B:766:ARG:HA	2:B:769:TYR:CD1	2.52	0.43
2:B:1103:ILE:CD1	2:B:1103:ILE:H	2.29	0.43
4:E:16:PHE:CE2	4:E:20:LYS:HE2	2.53	0.43
8:J:21:TYR:O	8:J:22:LEU:C	2.61	0.43
12:T:25:DC:H2'	12:T:26:DG:H8	1.83	0.43
1:A:66:LYS:C	1:A:68:GLN:H	2.26	0.43
1:A:102:VAL:HB	1:A:211:PHE:HZ	1.83	0.43
1:A:219:PHE:CE2	1:A:231:PRO:HD2	2.53	0.43
1:A:256:GLN:CA	1:A:257:ARG:CB	2.38	0.43
1:A:315:LEU:CD1	1:A:315:LEU:N	2.63	0.43
1:A:737:LEU:HD11	1:A:758:ILE:HG21	2.01	0.43
1:A:1189:SER:O	1:A:1241:ARG:HD3	2.18	0.43
2:B:101:MET:HE3	2:B:169:ARG:NH1	2.27	0.43
2:B:1033:LYS:O	2:B:1036:ALA:HB3	2.18	0.43
2:B:1118:PRO:HD3	2:B:1155:SER:HA	2.00	0.43
7:I:96:SER:HB2	7:I:98:VAL:HG23	2.00	0.43
9:K:36:GLU:O	9:K:37:LYS:C	2.61	0.43
1:A:250:ILE:O	1:A:251:SER:CB	2.64	0.43
1:A:389:THR:OG1	1:A:426:LEU:HD12	2.19	0.43
1:A:402:ALA:O	1:A:415:LEU:HD13	2.19	0.43
1:A:614:PHE:CD1	1:A:614:PHE:C	2.96	0.43
1:A:667:GLY:HA2	1:A:670:ILE:HG12	2.00	0.43
1:A:709:THR:HB	1:A:712:GLU:HG3	2.00	0.43
1:A:809:THR:CB	1:A:810:PRO:HD2	2.47	0.43
1:A:1155:ASP:HB3	1:A:1241:ARG:HH21	1.84	0.43
1:A:1379:GLY:O	4:E:179:GLN:HG2	2.18	0.43
2:B:202:TYR:CD2	2:B:202:TYR:N	2.84	0.43
4:E:205:SER:O	4:E:206:GLY:C	2.62	0.43
5:F:76:LYS:O	5:F:79:ARG:CD	2.67	0.43
5:F:125:LEU:O	5:F:127:GLU:N	2.51	0.43
7:I:75:CYS:HB3	7:I:110:PHE:HE2	1.82	0.43
1:A:152:VAL:O	1:A:162:VAL:CG2	2.65	0.43
1:A:356:ASP:HB2	1:A:469:ARG:NH1	2.33	0.43
1:A:729:ALA:HA	1:A:732:LEU:HB2	2.01	0.43
1:A:1161:THR:CG2	1:A:1163:ILE:H	2.31	0.43
1:A:1242:VAL:HG12	1:A:1243:VAL:H	1.82	0.43
2:B:314:LEU:O	2:B:315:LYS:C	2.60	0.43
6:H:58:THR:CG2	6:H:59:ILE:N	2.79	0.43
8:J:15:GLY:O	8:J:17:LYS:N	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:315:LEU:HB3	1:A:317:LYS:N	2.22	0.43
1:A:924:LYS:HB2	1:A:924:LYS:NZ	2.33	0.43
2:B:333:PHE:O	2:B:333:PHE:CG	2.72	0.43
2:B:637:LEU:HD22	2:B:741:CYS:O	2.17	0.43
2:B:755:ILE:HD13	2:B:755:ILE:HA	1.86	0.43
2:B:763:GLN:HG2	2:B:764:SER:N	2.33	0.43
2:B:1056:SER:CB	2:B:1066:SER:O	2.67	0.43
3:C:41:ILE:HD11	3:C:243:VAL:HG13	2.01	0.43
4:E:3:GLN:HG3	4:E:5:ASN:H	1.82	0.43
4:E:136:ASN:OD1	4:E:137:GLU:N	2.50	0.43
7:I:32:CYS:SG	7:I:33:SER:N	2.91	0.43
12:T:26:DG:N2	12:T:27:DA:H1'	2.34	0.43
1:A:492:PRO:C	1:A:493:GLN:HE21	2.26	0.43
1:A:508:PRO:O	1:A:511:ILE:HG13	2.18	0.43
1:A:686:ALA:O	1:A:690:VAL:HG23	2.18	0.43
1:A:1410:PHE:HD2	2:B:1212:ILE:HD11	1.84	0.43
2:B:108:VAL:CG1	2:B:109:THR:N	2.81	0.43
2:B:792:MET:HE2	2:B:857:ARG:CZ	2.48	0.43
2:B:981:ALA:CB	2:B:1095:LEU:HD11	2.49	0.43
2:B:1056:SER:HB3	2:B:1066:SER:O	2.18	0.43
3:C:5:GLY:O	3:C:6:PRO:C	2.62	0.43
4:E:26:ARG:HD3	4:E:188:LEU:HA	2.01	0.43
7:I:50:THR:HG22	7:I:52:ILE:HG22	2.00	0.43
7:I:99:LEU:HB2	7:I:101:PHE:CE1	2.53	0.43
1:A:172:PRO:HB3	1:A:183:GLY:HA3	2.01	0.43
1:A:366:VAL:O	1:A:367:PRO:C	2.62	0.43
1:A:590:ARG:HB3	1:A:605:MET:N	2.34	0.43
1:A:787:PHE:CD1	1:A:796:SER:HB2	2.53	0.43
1:A:1044:TRP:O	1:A:1045:VAL:C	2.61	0.43
1:A:1364:ASN:ND2	1:A:1366:ARG:N	2.55	0.43
2:B:126:SER:O	2:B:169:ARG:HA	2.19	0.43
2:B:394:ASP:OD2	7:I:91:ARG:HB3	2.18	0.43
2:B:481:GLN:HB2	2:B:494:HIS:HE1	1.83	0.43
2:B:526:GLU:HG2	2:B:538:ASN:ND2	2.33	0.43
6:H:9:ILE:HG12	6:H:56:THR:HG23	2.01	0.43
9:K:43:GLY:HA3	9:K:71:PHE:CE1	2.54	0.43
10:L:68:GLU:H	10:L:68:GLU:HG3	1.57	0.43
11:R:5:A:N3	11:R:6:G:C8	2.87	0.43
1:A:343:LYS:NZ	2:B:1156:ASP:HB2	2.34	0.43
1:A:700:ASN:HD22	7:I:116:ASN:ND2	2.16	0.43
1:A:1072:ILE:HD11	1:A:1368:MET:CA	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:40:GLU:OE2	2:B:681:TRP:HB3	2.19	0.43
2:B:95:ILE:HA	2:B:129:PHE:O	2.19	0.43
2:B:104:GLU:H	2:B:104:GLU:HG2	1.66	0.43
2:B:878:GLN:O	2:B:879:ARG:C	2.62	0.43
2:B:1096:ARG:O	2:B:1097:HIS:HB2	2.19	0.43
7:I:17:ARG:HG2	7:I:18:GLU:N	2.21	0.43
10:L:46:VAL:HG12	10:L:47:ARG:H	1.83	0.43
1:A:922:ASP:O	1:A:923:LEU:HG	2.19	0.43
1:A:1059:HIS:CE1	5:F:86:THR:HA	2.53	0.43
1:A:1398:MET:O	1:A:1401:SER:N	2.44	0.43
2:B:373:ARG:HD3	2:B:566:LEU:HD23	2.01	0.43
2:B:637:LEU:O	2:B:690:VAL:HG13	2.19	0.43
2:B:1168:LEU:HB3	2:B:1169:MET:H	1.63	0.43
3:C:30:ALA:O	3:C:33:LEU:HB3	2.19	0.43
3:C:182:PRO:HG3	3:C:206:ASN:O	2.18	0.43
7:I:69:PRO:HG2	7:I:85:PHE:CE1	2.53	0.43
12:T:19:DT:H2'	12:T:20:DC:O4'	2.19	0.43
1:A:106:VAL:HG11	1:A:214:ILE:HD11	2.00	0.42
1:A:327:ALA:C	1:A:329:LEU:H	2.26	0.42
1:A:902:LEU:HG	1:A:902:LEU:H	1.69	0.42
2:B:555:ILE:HD12	2:B:587:HIS:CE1	2.53	0.42
2:B:1149:GLU:HG2	2:B:1153:GLU:HB2	2.01	0.42
3:C:76:ASP:OD2	3:C:128:ASN:HB3	2.19	0.42
7:I:21:GLU:H	7:I:21:GLU:HG3	1.62	0.42
9:K:78:THR:HG22	9:K:79:GLU:N	2.34	0.42
1:A:282:ASN:HB3	1:A:283:GLY:H	1.60	0.42
1:A:1134:ILE:H	1:A:1134:ILE:HG13	1.51	0.42
1:A:1146:VAL:O	1:A:1197:LEU:HD23	2.19	0.42
2:B:92:PHE:HB3	2:B:130:VAL:HG11	2.01	0.42
2:B:195:CYS:CB	2:B:782:LEU:HD22	2.49	0.42
2:B:458:LYS:O	2:B:462:ALA:HB2	2.18	0.42
2:B:637:LEU:HD23	2:B:742:GLU:OE2	2.18	0.42
2:B:1077:THR:HG22	2:B:1079:LYS:H	1.84	0.42
3:C:115:SER:HB3	3:C:142:VAL:HG12	2.01	0.42
3:C:180:TYR:O	3:C:181:ASP:HB3	2.19	0.42
4:E:12:LEU:HD22	4:E:55:ARG:NH2	2.34	0.42
4:E:16:PHE:O	4:E:19:VAL:N	2.51	0.42
8:J:1:MET:O	8:J:2:ILE:O	2.37	0.42
9:K:102:LYS:O	9:K:106:GLU:CG	2.67	0.42
1:A:416:ARG:HG2	1:A:416:ARG:H	1.52	0.42
1:A:805:LEU:HD12	1:A:806:ARG:N	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:913:LEU:HG	1:A:915:SER:H	1.84	0.42
1:A:1025:ARG:NH1	1:A:1025:ARG:CG	2.77	0.42
2:B:357:GLN:HA	2:B:374:LYS:NZ	2.35	0.42
2:B:530:GLY:O	2:B:531:GLN:C	2.63	0.42
2:B:830:TYR:C	2:B:832:GLY:N	2.77	0.42
2:B:976:ILE:HD11	2:B:992:ILE:HA	2.02	0.42
3:C:77:ILE:C	3:C:79:GLN:H	2.28	0.42
4:E:13:TRP:CE3	4:E:39:LEU:HD13	2.54	0.42
6:H:123:MET:HE1	6:H:142:LEU:HD13	2.01	0.42
1:A:44:THR:O	1:A:45:GLN:HB2	2.20	0.42
1:A:332:LYS:H	1:A:337:ARG:CB	2.33	0.42
1:A:343:LYS:NZ	2:B:1197:PRO:HB3	2.32	0.42
1:A:567:LYS:HD3	6:H:95:TYR:CD1	2.54	0.42
1:A:1336:MET:CE	1:A:1380:GLY:HA2	2.49	0.42
2:B:229:ALA:HB1	2:B:231:PRO:HD2	2.02	0.42
2:B:551:PRO:O	2:B:554:ILE:HB	2.20	0.42
2:B:1156:ASP:HB3	2:B:1198:TYR:H	1.83	0.42
2:B:1207:LEU:HD23	2:B:1207:LEU:HA	1.84	0.42
3:C:171:GLY:HA2	3:C:172:PRO:HD3	1.73	0.42
9:K:61:TYR:HA	9:K:72:LYS:O	2.19	0.42
1:A:98:LYS:C	1:A:100:LYS:N	2.78	0.42
1:A:219:PHE:HB3	1:A:224:PHE:HB2	2.00	0.42
1:A:535:THR:HG21	1:A:617:VAL:H	1.84	0.42
1:A:1390:ASN:ND2	1:A:1402:PHE:HB3	2.35	0.42
1:A:1397:LEU:HB2	1:A:1426:GLU:HG2	2.02	0.42
2:B:980:PHE:CE1	2:B:990:ILE:HD11	2.51	0.42
4:E:114:ASN:O	4:E:115:ASN:HB3	2.19	0.42
6:H:26:ILE:CG2	6:H:40:LEU:HB3	2.49	0.42
9:K:57:LEU:HD12	9:K:76:GLN:HG2	2.01	0.42
1:A:75:ASN:HA	2:B:1116:ARG:HH12	1.84	0.42
1:A:756:ILE:O	1:A:760:GLN:HG3	2.19	0.42
1:A:885:THR:OG1	1:A:1024:SER:HB3	2.20	0.42
1:A:954:TRP:HE3	1:A:955:PRO:HD2	1.84	0.42
1:A:1019:CYS:O	1:A:1022:LEU:HB3	2.19	0.42
1:A:1072:ILE:HD11	1:A:1368:MET:HG2	2.01	0.42
1:A:1336:MET:HE2	1:A:1380:GLY:HA2	2.02	0.42
2:B:635:ARG:C	2:B:636:PRO:O	2.60	0.42
2:B:766:ARG:HA	2:B:766:ARG:HD3	1.78	0.42
2:B:840:ILE:HG23	2:B:992:ILE:HG22	2.02	0.42
2:B:1020:ARG:H	2:B:1020:ARG:HG2	1.64	0.42
2:B:1160:VAL:HG12	2:B:1161:HIS:N	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:82:PRO:C	6:H:84:ALA:N	2.78	0.42
1:A:442:VAL:HG12	1:A:491:VAL:HG22	2.01	0.42
1:A:1191:TRP:CE3	1:A:1191:TRP:HA	2.54	0.42
2:B:276:ILE:CG2	2:B:277:LYS:N	2.83	0.42
2:B:461:LEU:HD12	2:B:461:LEU:HA	1.97	0.42
9:K:63:VAL:HG23	9:K:63:VAL:O	2.19	0.42
1:A:253:ASN:HB2	1:A:256:GLN:CA	2.48	0.42
1:A:346:ASP:N	2:B:1154:ALA:HB1	2.24	0.42
1:A:848:ILE:HD13	1:A:858:ASN:HB3	2.01	0.42
1:A:1313:LEU:O	1:A:1315:GLU:N	2.53	0.42
2:B:43:LEU:HD11	2:B:811:TYR:O	2.20	0.42
2:B:58:THR:O	2:B:62:ILE:HG12	2.20	0.42
2:B:534:GLY:O	2:B:537:LYS:HD3	2.20	0.42
2:B:594:ALA:HB2	7:I:61:ASP:OD1	2.20	0.42
2:B:874:PHE:CD2	2:B:914:LYS:HB3	2.55	0.42
6:H:84:ALA:O	6:H:85:GLY:C	2.61	0.42
9:K:40:HIS:C	9:K:42:LEU:N	2.78	0.42
1:A:602:ASP:HB3	1:A:616:VAL:HG23	2.01	0.42
1:A:884:ASP:OD2	1:A:884:ASP:N	2.50	0.42
1:A:1271:ILE:HG22	1:A:1273:LEU:HD12	2.01	0.42
2:B:801:LYS:O	8:J:52:THR:HG23	2.20	0.42
3:C:33:LEU:HG	3:C:37:MET:HE1	2.02	0.42
4:E:100:ILE:HG12	4:E:105:PHE:HD1	1.83	0.42
9:K:3:ALA:HA	9:K:4:PRO:HD3	1.93	0.42
9:K:4:PRO:HG2	9:K:4:PRO:O	2.20	0.42
10:L:34:CYS:O	10:L:35:SER:CB	2.68	0.42
12:T:11:DG:N2	13:N:5:DT:O2	2.53	0.42
1:A:582:ILE:HA	1:A:583:PRO:HD3	1.75	0.42
1:A:646:PHE:O	1:A:647:GLY:C	2.63	0.42
1:A:841:LEU:O	1:A:845:LEU:HG	2.20	0.42
1:A:996:ASN:C	1:A:998:LEU:H	2.27	0.42
1:A:1191:TRP:HB3	1:A:1260:LEU:HD22	2.01	0.42
2:B:200:GLY:HA2	2:B:202:TYR:HE2	1.85	0.42
2:B:453:ILE:O	2:B:454:THR:C	2.63	0.42
2:B:708:GLU:O	2:B:710:LEU:N	2.53	0.42
2:B:762:ASN:HD21	2:B:1022:THR:HA	1.85	0.42
3:C:10:ILE:HG21	3:C:13:ALA:HB2	2.01	0.42
8:J:15:GLY:C	8:J:17:LYS:N	2.77	0.42
10:L:32:ALA:HB3	10:L:55:ILE:HD12	2.02	0.42
1:A:512:VAL:HG13	1:A:512:VAL:O	2.20	0.41
1:A:566:ILE:O	1:A:567:LYS:O	2.37	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1238:ILE:HG22	1:A:1240:CYS:SG	2.60	0.41
1:A:1313:LEU:C	1:A:1315:GLU:H	2.28	0.41
2:B:430:ARG:HD3	2:B:434:ARG:NH2	2.34	0.41
2:B:450:ALA:O	2:B:451:LYS:C	2.63	0.41
2:B:899:ILE:HD11	2:B:911:ILE:CG1	2.40	0.41
2:B:1096:ARG:HG3	2:B:1097:HIS:N	2.35	0.41
2:B:1099:VAL:HG23	2:B:1099:VAL:H	1.55	0.41
2:B:1138:MET:HG3	2:B:1146:PHE:CE2	2.55	0.41
2:B:1147:LEU:O	2:B:1151:LEU:HB2	2.20	0.41
3:C:78:GLU:OE1	3:C:246:ARG:HD3	2.19	0.41
3:C:97:VAL:HG21	3:C:129:ILE:CG2	2.48	0.41
3:C:204:SER:O	3:C:205:LYS:C	2.63	0.41
4:E:16:PHE:O	4:E:17:ARG:C	2.63	0.41
6:H:23:VAL:HG21	6:H:121:LEU:HD21	2.01	0.41
6:H:39:THR:O	6:H:123:MET:HA	2.20	0.41
1:A:185:TRP:CZ3	1:A:200:ARG:HB3	2.55	0.41
1:A:215:SER:HB3	1:A:218:ASP:OD2	2.20	0.41
1:A:225:ASN:O	1:A:227:VAL:N	2.53	0.41
1:A:548:ASN:HA	9:K:60:ALA:HB1	2.02	0.41
1:A:826:ASP:OD2	1:A:826:ASP:N	2.45	0.41
2:B:37:PHE:HD1	2:B:681:TRP:CE2	2.38	0.41
2:B:189:LEU:O	2:B:190:TYR:C	2.61	0.41
5:F:74:ILE:HD13	5:F:74:ILE:HA	1.90	0.41
1:A:346:ASP:O	1:A:347:PHE:C	2.63	0.41
1:A:518:LYS:CB	1:A:519:PRO:CD	2.99	0.41
1:A:551:TYR:OH	9:K:32:VAL:HG21	2.21	0.41
1:A:567:LYS:HB3	6:H:95:TYR:HA	2.01	0.41
1:A:1059:HIS:ND1	5:F:87:LYS:HG2	2.35	0.41
1:A:1166:ASP:OD1	1:A:1194:ARG:NH2	2.44	0.41
1:A:1323:ASP:OD1	1:A:1325:THR:HG22	2.20	0.41
2:B:99:LYS:HA	2:B:100:PRO:HD2	1.76	0.41
2:B:263:GLY:O	2:B:264:SER:C	2.64	0.41
2:B:293:PRO:C	2:B:294:ASP:O	2.63	0.41
2:B:377:PHE:O	2:B:380:TYR:N	2.51	0.41
2:B:956:THR:HB	10:L:46:VAL:HG21	2.03	0.41
2:B:997:GLU:CD	3:C:39:ALA:HB2	2.46	0.41
3:C:41:ILE:HG13	3:C:172:PRO:CG	2.48	0.41
4:E:191:LYS:HE3	4:E:191:LYS:HB2	1.84	0.41
8:J:8:PHE:N	8:J:49:MET:HE3	2.35	0.41
12:T:9:DA:C6	12:T:10:DA:C6	3.08	0.41
1:A:423:ASP:HB3	1:A:424:ILE:H	1.26	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:650:GLN:O	1:A:651:LYS:C	2.62	0.41
1:A:794:PRO:O	1:A:796:SER:N	2.54	0.41
1:A:1021:LEU:O	1:A:1023:ARG:N	2.54	0.41
2:B:516:ASN:H	2:B:516:ASN:ND2	2.17	0.41
2:B:639:ILE:CG2	2:B:640:VAL:N	2.83	0.41
2:B:658:ILE:O	2:B:661:LEU:HB2	2.20	0.41
2:B:710:LEU:O	2:B:711:GLU:HB3	2.21	0.41
2:B:911:ILE:O	2:B:912:ILE:HG13	2.20	0.41
2:B:1033:LYS:N	2:B:1089:PRO:HG2	2.35	0.41
4:E:124:VAL:H	4:E:125:PRO:CD	2.34	0.41
8:J:7:CYS:HA	8:J:49:MET:HE3	2.02	0.41
9:K:88:LYS:O	9:K:89:ASN:C	2.62	0.41
1:A:232:GLU:HG2	1:A:233:TRP:CD1	2.56	0.41
1:A:278:THR:O	1:A:278:THR:HG22	2.19	0.41
1:A:609:ASP:O	1:A:611:GLN:N	2.53	0.41
1:A:1041:ALA:O	1:A:1045:VAL:HG23	2.21	0.41
2:B:384:ARG:HH22	2:B:621:GLU:CG	2.32	0.41
2:B:1107:ALA:O	2:B:1108:ARG:CB	2.68	0.41
4:E:165:LEU:HD22	4:E:165:LEU:HA	1.90	0.41
6:H:93:TYR:CD2	6:H:145:ARG:HD3	2.56	0.41
6:H:118:PHE:O	6:H:119:GLY:C	2.63	0.41
1:A:37:PHE:HA	1:A:38:PRO:HD3	1.91	0.41
1:A:353:ILE:HG13	1:A:485:ASP:O	2.20	0.41
1:A:794:PRO:C	1:A:796:SER:N	2.79	0.41
1:A:809:THR:HB	1:A:810:PRO:CD	2.51	0.41
1:A:1080:THR:HG22	1:A:1081:LEU:H	1.84	0.41
2:B:129:PHE:HE2	2:B:166:PHE:HB2	1.79	0.41
2:B:309:GLN:OE1	7:I:52:ILE:HG23	2.21	0.41
4:E:59:SER:O	4:E:79:TRP:CH2	2.73	0.41
4:E:63:ASN:HB3	4:E:64:PRO:HD3	1.99	0.41
5:F:93:ILE:HD11	5:F:134:ILE:HD11	2.03	0.41
8:J:36:LEU:O	8:J:41:LEU:HB2	2.21	0.41
8:J:44:TYR:CD1	8:J:44:TYR:C	2.98	0.41
1:A:274:ILE:O	1:A:274:ILE:HG22	2.21	0.41
1:A:345:VAL:HA	2:B:1118:PRO:HG2	2.02	0.41
1:A:406:ILE:HG22	1:A:407:ARG:N	2.36	0.41
1:A:444:PHE:HE2	1:A:470:LEU:HD23	1.79	0.41
1:A:446:ARG:HD3	1:A:478:TYR:O	2.20	0.41
1:A:911:SER:O	1:A:978:PRO:HB3	2.21	0.41
1:A:1349:TYR:HA	1:A:1372:VAL:HG21	2.02	0.41
2:B:60:GLN:O	2:B:63:ILE:HG22	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:276:ILE:HG22	2:B:277:LYS:N	2.36	0.41
2:B:879:ARG:HB2	2:B:880:THR:H	1.33	0.41
8:J:2:ILE:O	8:J:2:ILE:CG2	2.69	0.41
1:A:805:LEU:CD1	1:A:806:ARG:N	2.82	0.41
1:A:844:ALA:HB2	1:A:1389:PHE:CZ	2.56	0.41
1:A:1336:MET:HE2	1:A:1341:ILE:HD13	2.03	0.41
2:B:248:SER:HB3	2:B:249:ARG:H	1.65	0.41
2:B:638:PHE:CD1	2:B:743:ILE:HD13	2.56	0.41
4:E:62:ALA:C	4:E:63:ASN:HD22	2.29	0.41
4:E:179:GLN:O	4:E:182:ASP:HB2	2.21	0.41
5:F:90:ARG:O	5:F:91:ALA:C	2.64	0.41
1:A:214:ILE:HD13	1:A:214:ILE:HA	1.84	0.41
1:A:335:ARG:HE	1:A:335:ARG:HA	1.86	0.41
1:A:443:LEU:HD12	2:B:1146:PHE:CZ	2.56	0.41
1:A:819:GLY:C	1:A:821:ARG:H	2.28	0.41
1:A:863:VAL:HG11	1:A:866:PHE:CD2	2.56	0.41
1:A:869:GLY:C	1:A:871:ASP:H	2.28	0.41
1:A:1121:GLU:HG3	1:A:1122:PRO:HD2	2.02	0.41
1:A:1408:ILE:O	1:A:1412:ALA:HB2	2.20	0.41
2:B:519:TRP:O	2:B:519:TRP:HD1	2.02	0.41
2:B:520:GLY:HA3	2:B:635:ARG:CD	2.51	0.41
2:B:562:GLY:O	2:B:563:MET:C	2.63	0.41
2:B:792:MET:HE1	12:T:24:DT:OP1	2.20	0.41
2:B:999:MET:HB3	2:B:1007:VAL:HG22	2.02	0.41
2:B:1053:GLU:HB3	2:B:1057:LYS:HE3	2.02	0.41
2:B:1055:ILE:HD13	2:B:1055:ILE:HA	1.94	0.41
2:B:1074:ASN:OD1	2:B:1074:ASN:C	2.64	0.41
2:B:1158:PHE:CD2	2:B:1198:TYR:HD1	2.38	0.41
2:B:1200:ALA:C	2:B:1202:LEU:N	2.76	0.41
8:J:48:ARG:C	8:J:48:ARG:HD2	2.46	0.41
1:A:965:GLN:H	1:A:965:GLN:HG3	1.65	0.41
2:B:62:ILE:HG23	2:B:418:LYS:HG2	2.03	0.41
2:B:655:LYS:O	2:B:658:ILE:HG22	2.21	0.41
2:B:762:ASN:HD22	2:B:763:GLN:H	1.69	0.41
2:B:975:GLN:CG	2:B:976:ILE:N	2.78	0.41
2:B:1155:SER:OG	2:B:1156:ASP:N	2.53	0.41
5:F:73:ALA:O	5:F:74:ILE:HG12	2.21	0.41
5:F:75:PRO:O	5:F:77:ASP:O	2.39	0.41
9:K:40:HIS:CE1	9:K:63:VAL:CG2	3.03	0.41
1:A:4:GLN:HE22	2:B:1159:ARG:H	1.67	0.40
1:A:362:ASP:OD1	1:A:459:ARG:HD3	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:491:VAL:O	1:A:493:GLN:NE2	2.54	0.40
1:A:532:ARG:O	1:A:535:THR:N	2.50	0.40
1:A:590:ARG:CG	1:A:591:PHE:H	2.33	0.40
1:A:598:LEU:HD13	6:H:25:ARG:HH12	1.86	0.40
1:A:845:LEU:O	1:A:846:GLU:C	2.64	0.40
1:A:872:GLY:C	1:A:1058:VAL:HG23	2.45	0.40
1:A:929:LEU:CD2	1:A:983:ILE:CG2	2.99	0.40
1:A:1364:ASN:O	1:A:1365:TYR:C	2.64	0.40
2:B:26:THR:O	2:B:27:ALA:C	2.63	0.40
2:B:405:ARG:HB3	2:B:631:GLY:HA3	2.03	0.40
7:I:111:THR:CG2	7:I:112:SER:N	2.84	0.40
7:I:119:THR:O	7:I:120:GLN:HG2	2.21	0.40
10:L:53:HIS:O	10:L:55:ILE:N	2.50	0.40
11:R:6:G:N3	11:R:7:A:C8	2.90	0.40
1:A:32:VAL:HB	1:A:57:ARG:HD2	2.02	0.40
1:A:214:ILE:HG22	1:A:215:SER:O	2.22	0.40
1:A:302:THR:C	1:A:304:MET:H	2.30	0.40
1:A:645:LEU:O	1:A:646:PHE:C	2.65	0.40
1:A:664:THR:OG1	2:B:1014:PRO:HB2	2.21	0.40
1:A:712:GLU:C	1:A:714:PHE:H	2.29	0.40
1:A:930:ASP:O	1:A:931:GLU:C	2.64	0.40
1:A:1053:PHE:O	1:A:1055:ARG:N	2.53	0.40
2:B:205:ILE:O	2:B:208:SER:N	2.48	0.40
2:B:235:SER:OG	2:B:236:HIS:HD2	2.03	0.40
2:B:859:TYR:CZ	2:B:941:LEU:HD22	2.55	0.40
3:C:31:ASN:O	3:C:34:ARG:N	2.54	0.40
3:C:46:ILE:CD1	3:C:72:LEU:HD11	2.51	0.40
12:T:17:DG:H2'	12:T:17:DG:N3	2.36	0.40
1:A:343:LYS:HZ1	2:B:1156:ASP:HB2	1.85	0.40
1:A:444:PHE:O	1:A:478:TYR:CE2	2.75	0.40
1:A:666:ILE:HG23	2:B:1026:LEU:CD1	2.52	0.40
2:B:99:LYS:HB3	2:B:180:TYR:CE2	2.56	0.40
2:B:174:LEU:HD12	2:B:174:LEU:HA	1.90	0.40
2:B:827:ILE:HD12	2:B:1086:PHE:CD2	2.56	0.40
2:B:1032:SER:O	2:B:1033:LYS:C	2.65	0.40
2:B:1177:HIS:C	2:B:1179:GLN:H	2.29	0.40
3:C:76:ASP:O	3:C:79:GLN:HG2	2.22	0.40
7:I:15:TYR:N	7:I:15:TYR:CD1	2.89	0.40
13:N:2:DT:O2	13:N:2:DT:H2'	2.22	0.40
1:A:442:VAL:O	1:A:457:ALA:HA	2.21	0.40
1:A:1044:TRP:C	1:A:1046:LEU:N	2.79	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:115:GLN:O	2:B:119:LEU:HD12	2.21	0.40
2:B:291:ILE:CG2	2:B:297:ILE:HD13	2.50	0.40
2:B:839:MET:O	2:B:990:ILE:HA	2.21	0.40
2:B:992:ILE:HG21	2:B:994:TYR:CE2	2.56	0.40
4:E:161:LYS:C	4:E:163:GLU:N	2.78	0.40
1:A:244:PRO:C	1:A:246:VAL:N	2.80	0.40
1:A:249:SER:C	1:A:250:ILE:CG2	2.79	0.40
1:A:1404:GLU:HB3	1:A:1407:GLU:HG2	2.02	0.40
2:B:287:ARG:HA	2:B:291:ILE:O	2.20	0.40
2:B:426:LYS:HG3	2:B:430:ARG:HH12	1.87	0.40
2:B:745:PRO:O	2:B:748:ILE:HG12	2.22	0.40
2:B:821:GLN:HE22	2:B:851:PHE:H	1.69	0.40
2:B:1156:ASP:HB3	2:B:1157:ALA:H	1.55	0.40
3:C:46:ILE:H	3:C:46:ILE:HG12	1.58	0.40
3:C:46:ILE:HD12	3:C:157:CYS:HB3	2.02	0.40
4:E:117:THR:HA	4:E:118:PRO:HD2	1.88	0.40
8:J:35:ALA:O	8:J:39:LEU:CD1	2.62	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	
1	A	1383/1733 (80%)	1038 (75%)	233 (17%)	112 (8%)	1	11
2	B	1088/1224 (89%)	822 (76%)	188 (17%)	78 (7%)	1	13
3	C	264/318 (83%)	209 (79%)	48 (18%)	7 (3%)	4	28
4	E	212/215 (99%)	162 (76%)	39 (18%)	11 (5%)	1	18
5	F	82/155 (53%)	65 (79%)	13 (16%)	4 (5%)	1	19
6	H	129/146 (88%)	97 (75%)	21 (16%)	11 (8%)	0	11
7	I	117/122 (96%)	83 (71%)	25 (21%)	9 (8%)	1	12

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	J	63/70 (90%)	45 (71%)	14 (22%)	4 (6%)	1	15
9	K	112/120 (93%)	89 (80%)	16 (14%)	7 (6%)	1	15
10	L	44/70 (63%)	24 (54%)	9 (20%)	11 (25%)	0	1
All	All	3494/4173 (84%)	2634 (75%)	606 (17%)	254 (7%)	1	13

All (254) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	42	ASP
1	A	54	ASN
1	A	55	ASP
1	A	56	PRO
1	A	93	VAL
1	A	130	ASP
1	A	162	VAL
1	A	214	ILE
1	A	248	PRO
1	A	250	ILE
1	A	251	SER
1	A	253	ASN
1	A	257	ARG
1	A	315	LEU
1	A	322	VAL
1	A	324	SER
1	A	325	ILE
1	A	331	GLY
1	A	399	HIS
1	A	402	ALA
1	A	411	ASP
1	A	428	TYR
1	A	567	LYS
1	A	568	PRO
1	A	591	PHE
1	A	700	ASN
1	A	846	GLU
1	A	998	LEU
1	A	1036	ARG
1	A	1255	GLU
1	A	1393	ASN
2	B	100	PRO
2	B	176	SER

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Mol	Chain	Res	Type
2	B	229	ALA
2	B	249	ARG
2	B	436	VAL
2	B	466	TRP
2	B	477	ALA
2	B	484	ASN
2	B	531	GLN
2	B	592	ASN
2	B	636	PRO
2	B	648	HIS
2	B	649	LYS
2	B	650	GLU
2	B	711	GLU
2	B	731	VAL
2	B	734	HIS
2	B	751	VAL
2	B	831	SER
2	B	864	LYS
2	B	865	LYS
2	B	981	ALA
2	B	1046	PRO
2	B	1157	ALA
2	B	1181	GLU
3	C	142	VAL
3	C	149	LYS
3	C	227	THR
4	E	3	GLN
4	E	59	SER
4	E	172	GLU
4	E	173	SER
5	F	74	ILE
6	H	77	ARG
6	H	81	PRO
6	H	140	ALA
7	I	20	LYS
7	I	47	GLU
7	I	107	SER
8	J	2	ILE
8	J	6	ARG
9	K	71	PHE
10	L	26	THR
10	L	35	SER

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Mol	Chain	Res	Type
1	A	50	ILE
1	A	68	GLN
1	A	226	GLU
1	A	266	LEU
1	A	312	PRO
1	A	313	GLN
1	A	409	SER
1	A	472	LEU
1	A	515	GLN
1	A	517	ASN
1	A	592	ASP
1	A	597	LEU
1	A	610	GLY
1	A	756	ILE
1	A	972	HIS
1	A	986	ILE
1	A	1048	ASN
1	A	1054	LEU
1	A	1341	ILE
1	A	1388	GLY
1	A	1399	ARG
2	B	53	GLN
2	B	58	THR
2	B	475	SER
2	B	516	ASN
2	B	540	SER
2	B	708	GLU
2	B	709	ASP
2	B	1028	GLU
2	B	1166	CYS
2	B	1176	ASN
3	C	110	THR
4	E	192	ARG
4	E	206	GLY
5	F	81	THR
6	H	32	THR
6	H	82	PRO
6	H	85	GLY
6	H	134	ASN
7	I	21	GLU
7	I	34	TYR
7	I	86	PHE

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Mol	Chain	Res	Type
8	J	16	ASP
9	K	81	TYR
10	L	54	ARG
10	L	55	ILE
10	L	64	LEU
1	A	69	THR
1	A	76	GLU
1	A	89	PRO
1	A	128	ILE
1	A	131	SER
1	A	167	CYS
1	A	178	GLY
1	A	282	ASN
1	A	424	ILE
1	A	593	GLU
1	A	708	MET
1	A	755	PHE
1	A	810	PRO
1	A	895	LYS
1	A	903	ASN
1	A	922	ASP
1	A	957	PRO
1	A	963	ILE
1	A	1022	LEU
1	A	1062	GLU
1	A	1188	GLN
1	A	1223	ASP
1	A	1261	LYS
1	A	1270	ASN
1	A	1274	ARG
1	A	1314	SER
1	A	1327	ILE
1	A	1398	MET
1	A	1435	PRO
2	B	21	GLU
2	B	67	SER
2	B	248	SER
2	B	333	PHE
2	B	555	ILE
2	B	563	MET
2	B	738	PHE
2	B	879	ARG

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Mol	Chain	Res	Type
2	B	881	ASN
2	B	958	GLN
2	B	1047	PHE
2	B	1156	ASP
2	B	1167	GLY
2	B	1201	LYS
3	C	215	GLU
4	E	36	GLU
5	F	73	ALA
5	F	126	ALA
6	H	62	SER
7	I	54	GLU
9	K	5	ASP
9	K	46	ILE
10	L	45	ALA
1	A	287	HIS
1	A	318	SER
1	A	404	TYR
1	A	484	GLY
1	A	923	LEU
1	A	994	GLN
1	A	1021	LEU
1	A	1221	LYS
1	A	1438	THR
2	B	45	SER
2	B	266	ALA
2	B	367	LEU
2	B	418	LYS
2	B	712	PRO
2	B	746	SER
2	B	876	LYS
2	B	878	GLN
2	B	891	ASP
2	B	997	GLU
2	B	1186	ASP
2	B	1222	ARG
2	B	1223	ASP
4	E	124	VAL
6	H	43	ASN
6	H	90	ALA
9	K	7	PHE
10	L	37	LYS

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Mol	Chain	Res	Type
10	L	59	ALA
1	A	87	ALA
1	A	274	ILE
1	A	332	LYS
1	A	335	ARG
1	A	418	SER
1	A	514	PRO
1	A	576	GLN
1	A	958	VAL
2	B	365	THR
2	B	483	LEU
2	B	488	TYR
2	B	791	THR
2	B	792	MET
2	B	799	PRO
2	B	1021	MET
2	B	1061	GLU
3	C	6	PRO
3	C	144	ILE
10	L	39	SER
10	L	56	LEU
1	A	367	PRO
1	A	546	VAL
1	A	583	PRO
1	A	795	GLU
1	A	1122	PRO
1	A	1424	VAL
2	B	575	PRO
2	B	613	VAL
2	B	647	GLY
2	B	1027	ILE
2	B	1178	ASN
4	E	76	GLY
7	I	63	GLY
9	K	4	PRO
9	K	50	LEU
10	L	53	HIS
1	A	400	PRO
2	B	1017	ILE
4	E	51	GLY
8	J	33	GLY
1	A	829	VAL

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Mol	Chain	Res	Type
1	A	1437	GLY
4	E	118	PRO
6	H	59	ILE
1	A	916	GLY
2	B	1103	ILE
2	B	1165	ILE
7	I	76	PRO
1	A	599	SER
1	A	1049	ILE
1	A	1107	VAL
1	A	321	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1218/1520 (80%)	953 (78%)	265 (22%)	1	6
2	B	960/1061 (90%)	751 (78%)	209 (22%)	1	6
3	C	234/274 (85%)	187 (80%)	47 (20%)	1	9
4	E	196/197 (100%)	162 (83%)	34 (17%)	2	13
5	F	74/137 (54%)	60 (81%)	14 (19%)	1	11
6	H	117/128 (91%)	94 (80%)	23 (20%)	1	9
7	I	113/116 (97%)	94 (83%)	19 (17%)	2	13
8	J	60/65 (92%)	48 (80%)	12 (20%)	1	9
9	K	99/102 (97%)	80 (81%)	19 (19%)	1	10
10	L	40/57 (70%)	30 (75%)	10 (25%)	0	4
All	All	3111/3657 (85%)	2459 (79%)	652 (21%)	1	7

All (652) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	SER
1	A	12	ARG

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Mol	Chain	Res	Type
1	A	18	GLN
1	A	26	GLU
1	A	32	VAL
1	A	40	THR
1	A	44	THR
1	A	47	ARG
1	A	53	LEU
1	A	58	LEU
1	A	60	SER
1	A	71	GLN
1	A	80	HIS
1	A	81	PHE
1	A	84	ILE
1	A	93	VAL
1	A	98	LYS
1	A	99	ILE
1	A	100	LYS
1	A	102	VAL
1	A	105	CYS
1	A	110	CYS
1	A	116	ASP
1	A	128	ILE
1	A	129	LYS
1	A	130	ASP
1	A	140	THR
1	A	162	VAL
1	A	169	ASN
1	A	170	THR
1	A	180	LYS
1	A	184	SER
1	A	185	TRP
1	A	199	LEU
1	A	206	GLU
1	A	208	LEU
1	A	214	ILE
1	A	215	SER
1	A	221	SER
1	A	222	LEU
1	A	225	ASN
1	A	235	ILE
1	A	250	ILE
1	A	254	GLU

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Mol	Chain	Res	Type
1	A	255	SER
1	A	257	ARG
1	A	266	LEU
1	A	270	LEU
1	A	271	LYS
1	A	277	GLU
1	A	282	ASN
1	A	286	HIS
1	A	287	HIS
1	A	295	LEU
1	A	297	GLN
1	A	303	TYR
1	A	306	ASN
1	A	307	ASP
1	A	308	ILE
1	A	313	GLN
1	A	315	LEU
1	A	316	GLN
1	A	318	SER
1	A	320	ARG
1	A	323	LYS
1	A	335	ARG
1	A	337	ARG
1	A	344	ARG
1	A	379	VAL
1	A	381	THR
1	A	403	LYS
1	A	405	VAL
1	A	406	ILE
1	A	413	ILE
1	A	416	ARG
1	A	419	LYS
1	A	423	ASP
1	A	424	ILE
1	A	434	ARG
1	A	436	ILE
1	A	442	VAL
1	A	443	LEU
1	A	445	ASN
1	A	450	LEU
1	A	452	LYS
1	A	453	MET

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Mol	Chain	Res	Type
1	A	455	MET
1	A	460	VAL
1	A	463	ILE
1	A	469	ARG
1	A	470	LEU
1	A	475	THR
1	A	481	ASP
1	A	485	ASP
1	A	486	GLU
1	A	496	GLU
1	A	498	ARG
1	A	504	LEU
1	A	513	SER
1	A	518	LYS
1	A	523	ILE
1	A	524	VAL
1	A	527	THR
1	A	534	LEU
1	A	550	LEU
1	A	566	ILE
1	A	576	GLN
1	A	577	ILE
1	A	588	LEU
1	A	590	ARG
1	A	595	THR
1	A	596	THR
1	A	597	LEU
1	A	599	SER
1	A	602	ASP
1	A	612	ILE
1	A	618	GLU
1	A	619	LYS
1	A	621	THR
1	A	625	SER
1	A	630	ILE
1	A	648	ASN
1	A	663	SER
1	A	666	ILE
1	A	680	THR
1	A	682	THR
1	A	687	LYS
1	A	688	LYS

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Mol	Chain	Res	Type
1	A	702	LEU
1	A	705	LYS
1	A	713	SER
1	A	720	ARG
1	A	732	LEU
1	A	740	LEU
1	A	743	VAL
1	A	752	LYS
1	A	756	ILE
1	A	758	ILE
1	A	764	CYS
1	A	768	GLN
1	A	771	GLU
1	A	775	ILE
1	A	782	ARG
1	A	783	THR
1	A	788	SER
1	A	795	GLU
1	A	796	SER
1	A	797	LYS
1	A	800	VAL
1	A	801	GLU
1	A	803	SER
1	A	805	LEU
1	A	826	ASP
1	A	829	VAL
1	A	830	LYS
1	A	831	THR
1	A	838	GLN
1	A	855	THR
1	A	858	ASN
1	A	867	ILE
1	A	879	GLU
1	A	880	LYS
1	A	885	THR
1	A	886	ILE
1	A	895	LYS
1	A	896	ARG
1	A	897	TYR
1	A	902	LEU
1	A	905	ASP
1	A	907	THR

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Mol	Chain	Res	Type
1	A	911	SER
1	A	914	GLU
1	A	918	GLU
1	A	924	LYS
1	A	929	LEU
1	A	949	ASP
1	A	960	ILE
1	A	966	ASN
1	A	969	GLN
1	A	982	THR
1	A	988	LEU
1	A	990	VAL
1	A	996	ASN
1	A	997	LEU
1	A	1000	LEU
1	A	1006	ILE
1	A	1007	ILE
1	A	1017	LEU
1	A	1025	ARG
1	A	1029	ARG
1	A	1033	GLN
1	A	1037	LEU
1	A	1048	ASN
1	A	1052	GLN
1	A	1057	VAL
1	A	1058	VAL
1	A	1067	LEU
1	A	1081	LEU
1	A	1094	VAL
1	A	1095	THR
1	A	1110	ASN
1	A	1111	MET
1	A	1118	VAL
1	A	1120	LEU
1	A	1129	GLU
1	A	1134	ILE
1	A	1135	ARG
1	A	1142	THR
1	A	1146	VAL
1	A	1152	ILE
1	A	1159	ARG
1	A	1160	SER

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Mol	Chain	Res	Type
1	A	1161	THR
1	A	1165	GLU
1	A	1170	ILE
1	A	1172	LEU
1	A	1173	HIS
1	A	1187	GLN
1	A	1193	LEU
1	A	1199	ARG
1	A	1219	THR
1	A	1222	ASN
1	A	1232	ASN
1	A	1235	LYS
1	A	1240	CYS
1	A	1255	GLU
1	A	1262	LYS
1	A	1264	GLU
1	A	1267	MET
1	A	1272	THR
1	A	1273	LEU
1	A	1276	VAL
1	A	1280	GLU
1	A	1282	VAL
1	A	1285	MET
1	A	1291	VAL
1	A	1299	VAL
1	A	1300	LYS
1	A	1301	GLU
1	A	1315	GLU
1	A	1322	ILE
1	A	1325	THR
1	A	1333	ILE
1	A	1336	MET
1	A	1350	LYS
1	A	1351	GLU
1	A	1354	ASN
1	A	1355	VAL
1	A	1359	ASP
1	A	1364	ASN
1	A	1372	VAL
1	A	1376	THR
1	A	1385	THR
1	A	1391	ARG

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Mol	Chain	Res	Type
1	A	1394	THR
1	A	1398	MET
1	A	1400	CYS
1	A	1403	GLU
1	A	1405	THR
1	A	1406	VAL
1	A	1407	GLU
1	A	1420	ASP
1	A	1425	SER
1	A	1428	VAL
1	A	1445	ILE
2	B	34	ILE
2	B	40	GLU
2	B	63	ILE
2	B	66	ASP
2	B	67	SER
2	B	90	ILE
2	B	94	LYS
2	B	95	ILE
2	B	97	VAL
2	B	98	THR
2	B	104	GLU
2	B	106	ASP
2	B	109	THR
2	B	119	LEU
2	B	120	ARG
2	B	126	SER
2	B	128	LEU
2	B	172	ILE
2	B	175	ARG
2	B	177	LYS
2	B	187	SER
2	B	188	ASP
2	B	199	MET
2	B	202	TYR
2	B	222	ILE
2	B	225	VAL
2	B	234	ILE
2	B	244	LEU
2	B	246	LYS
2	B	248	SER
2	B	249	ARG

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Mol	Chain	Res	Type
2	B	261	ARG
2	B	262	GLU
2	B	264	SER
2	B	268	THR
2	B	272	THR
2	B	276	ILE
2	B	282	ILE
2	B	283	VAL
2	B	298	LEU
2	B	305	VAL
2	B	313	MET
2	B	315	LYS
2	B	319	GLU
2	B	324	ILE
2	B	347	LYS
2	B	354	ASP
2	B	387	LEU
2	B	391	ASP
2	B	393	LYS
2	B	398	ARG
2	B	404	LYS
2	B	408	LEU
2	B	416	LEU
2	B	420	LEU
2	B	424	LEU
2	B	425	THR
2	B	426	LYS
2	B	427	ASP
2	B	429	PHE
2	B	432	MET
2	B	435	THR
2	B	437	GLU
2	B	461	LEU
2	B	463	THR
2	B	468	GLU
2	B	473	MET
2	B	479	VAL
2	B	482	VAL
2	B	483	LEU
2	B	485	ARG
2	B	487	THR
2	B	489	SER

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Mol	Chain	Res	Type
2	B	490	SER
2	B	500	THR
2	B	502	ILE
2	B	513	GLN
2	B	516	ASN
2	B	527	THR
2	B	537	LYS
2	B	539	LEU
2	B	542	MET
2	B	545	ILE
2	B	549	THR
2	B	552	MET
2	B	563	MET
2	B	567	GLU
2	B	570	VAL
2	B	582	VAL
2	B	591	ARG
2	B	595	ARG
2	B	600	LEU
2	B	604	ARG
2	B	612	GLU
2	B	613	VAL
2	B	614	SER
2	B	633	VAL
2	B	637	LEU
2	B	641	GLU
2	B	644	GLU
2	B	649	LYS
2	B	651	LEU
2	B	653	VAL
2	B	658	ILE
2	B	668	ASP
2	B	682	SER
2	B	694	ASP
2	B	701	ILE
2	B	705	MET
2	B	714	GLU
2	B	731	VAL
2	B	737	THR
2	B	751	VAL
2	B	755	ILE
2	B	762	ASN

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Mol	Chain	Res	Type
2	B	764	SER
2	B	778	MET
2	B	787	VAL
2	B	790	ASP
2	B	791	THR
2	B	794	ASN
2	B	807	ARG
2	B	812	LEU
2	B	815	ARG
2	B	822	ASN
2	B	825	VAL
2	B	829	CYS
2	B	830	TYR
2	B	835	GLN
2	B	847	ASP
2	B	861	ASP
2	B	862	GLN
2	B	864	LYS
2	B	865	LYS
2	B	866	TYR
2	B	868	MET
2	B	869	SER
2	B	872	GLU
2	B	878	GLN
2	B	879	ARG
2	B	880	THR
2	B	882	THR
2	B	883	LEU
2	B	886	LYS
2	B	892	LYS
2	B	895	ASP
2	B	899	ILE
2	B	905	VAL
2	B	906	SER
2	B	911	ILE
2	B	944	THR
2	B	945	GLU
2	B	951	GLN
2	B	953	LEU
2	B	957	ASN
2	B	958	GLN
2	B	959	ASP

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Mol	Chain	Res	Type
2	B	968	VAL
2	B	970	THR
2	B	971	THR
2	B	973	ILE
2	B	976	ILE
2	B	983	ARG
2	B	986	GLN
2	B	989	THR
2	B	997	GLU
2	B	998	ASP
2	B	999	MET
2	B	1002	THR
2	B	1007	VAL
2	B	1010	LEU
2	B	1012	ILE
2	B	1017	ILE
2	B	1020	ARG
2	B	1022	THR
2	B	1028	GLU
2	B	1050	ILE
2	B	1051	THR
2	B	1062	HIS
2	B	1072	MET
2	B	1077	THR
2	B	1082	MET
2	B	1090	THR
2	B	1093	GLN
2	B	1096	ARG
2	B	1098	MET
2	B	1099	VAL
2	B	1103	ILE
2	B	1113	VAL
2	B	1115	THR
2	B	1124	ARG
2	B	1132	GLU
2	B	1141	HIS
2	B	1147	LEU
2	B	1151	LEU
2	B	1152	MET
2	B	1153	GLU
2	B	1159	ARG
2	B	1165	ILE

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Mol	Chain	Res	Type
2	B	1166	CYS
2	B	1178	ASN
2	B	1189	ILE
2	B	1191	ILE
2	B	1194	ILE
2	B	1196	ILE
2	B	1202	LEU
2	B	1212	ILE
2	B	1218	THR
2	B	1223	ASP
3	C	3	GLU
3	C	4	GLU
3	C	10	ILE
3	C	15	LYS
3	C	16	ASP
3	C	18	VAL
3	C	25	VAL
3	C	26	ASP
3	C	27	LEU
3	C	34	ARG
3	C	36	VAL
3	C	38	ILE
3	C	41	ILE
3	C	43	THR
3	C	49	VAL
3	C	55	THR
3	C	56	THR
3	C	63	ILE
3	C	77	ILE
3	C	83	SER
3	C	89	GLU
3	C	93	ASP
3	C	99	LEU
3	C	102	GLN
3	C	119	VAL
3	C	129	ILE
3	C	133	ILE
3	C	134	ILE
3	C	138	GLU
3	C	142	VAL
3	C	143	LEU
3	C	145	CYS

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Mol	Chain	Res	Type
3	C	163	ILE
3	C	165	LYS
3	C	166	GLU
3	C	183	TRP
3	C	195	GLN
3	C	196	ASP
3	C	203	GLN
3	C	215	GLU
3	C	227	THR
3	C	233	GLU
3	C	235	VAL
3	C	240	VAL
3	C	244	VAL
3	C	254	LYS
3	C	267	GLN
4	E	3	GLN
4	E	4	GLU
4	E	9	ILE
4	E	32	GLN
4	E	37	LEU
4	E	43	LYS
4	E	61	GLN
4	E	65	THR
4	E	66	GLU
4	E	77	SER
4	E	78	LEU
4	E	83	CYS
4	E	92	THR
4	E	97	VAL
4	E	101	GLN
4	E	104	ASN
4	E	107	THR
4	E	119	SER
4	E	127	ILE
4	E	131	THR
4	E	134	THR
4	E	146	HIS
4	E	150	VAL
4	E	156	LEU
4	E	162	ARG
4	E	165	LEU
4	E	169	ARG

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Mol	Chain	Res	Type
4	E	170	LEU
4	E	171	LYS
4	E	184	VAL
4	E	196	VAL
4	E	203	GLU
4	E	204	THR
4	E	212	ARG
5	F	74	ILE
5	F	77	ASP
5	F	79	ARG
5	F	90	ARG
5	F	97	ARG
5	F	99	LEU
5	F	111	LEU
5	F	112	GLU
5	F	114	GLU
5	F	118	LEU
5	F	120	ILE
5	F	123	LYS
5	F	133	VAL
5	F	155	LEU
6	H	2	SER
6	H	11	GLN
6	H	27	GLU
6	H	33	GLN
6	H	37	LYS
6	H	49	VAL
6	H	54	SER
6	H	55	LEU
6	H	56	THR
6	H	80	ARG
6	H	86	ASP
6	H	89	LEU
6	H	94	ASP
6	H	95	TYR
6	H	102	TYR
6	H	107	VAL
6	H	110	ASP
6	H	112	ILE
6	H	121	LEU
6	H	132	LEU
6	H	135	LEU

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Mol	Chain	Res	Type
6	H	136	LYS
6	H	139	ASN
7	I	3	THR
7	I	5	ARG
7	I	8	ARG
7	I	9	ASP
7	I	10	CYS
7	I	11	ASN
7	I	12	ASN
7	I	13	MET
7	I	28	GLU
7	I	30	ARG
7	I	37	GLU
7	I	50	THR
7	I	52	ILE
7	I	62	ILE
7	I	78	CYS
7	I	83	ASN
7	I	114	GLN
7	I	117	LYS
7	I	119	THR
8	J	7	CYS
8	J	9	SER
8	J	14	VAL
8	J	24	LEU
8	J	27	GLU
8	J	32	GLU
8	J	34	THR
8	J	42	LYS
8	J	43	ARG
8	J	48	ARG
8	J	55	ASP
8	J	59	LYS
9	K	9	LEU
9	K	18	LYS
9	K	20	LYS
9	K	31	VAL
9	K	33	ILE
9	K	47	ARG
9	K	50	LEU
9	K	51	LEU
9	K	56	VAL

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Mol	Chain	Res	Type
9	K	64	GLU
9	K	71	PHE
9	K	73	LEU
9	K	75	ILE
9	K	77	THR
9	K	79	GLU
9	K	102	LYS
9	K	107	THR
9	K	113	THR
9	K	114	LEU
10	L	31	CYS
10	L	38	LEU
10	L	46	VAL
10	L	51	CYS
10	L	55	ILE
10	L	61	THR
10	L	63	ARG
10	L	65	VAL
10	L	66	GLN
10	L	68	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (92) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4	GLN
1	A	18	GLN
1	A	54	ASN
1	A	80	HIS
1	A	169	ASN
1	A	171	GLN
1	A	282	ASN
1	A	299	HIS
1	A	313	GLN
1	A	394	ASN
1	A	435	HIS
1	A	445	ASN
1	A	451	HIS
1	A	493	GLN
1	A	517	ASN
1	A	626	ASN
1	A	654	ASN
1	A	736	ASN

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Mol	Chain	Res	Type
1	A	741	ASN
1	A	742	ASN
1	A	745	GLN
1	A	757	ASN
1	A	858	ASN
1	A	906	HIS
1	A	926	GLN
1	A	965	GLN
1	A	966	ASN
1	A	968	GLN
1	A	975	HIS
1	A	1040	GLN
1	A	1171	GLN
1	A	1173	HIS
1	A	1278	ASN
1	A	1312	ASN
1	A	1364	ASN
1	A	1390	ASN
1	A	1432	GLN
2	B	47	GLN
2	B	121	ASN
2	B	236	HIS
2	B	433	GLN
2	B	449	ASN
2	B	484	ASN
2	B	515	HIS
2	B	516	ASN
2	B	518	HIS
2	B	531	GLN
2	B	587	HIS
2	B	657	HIS
2	B	686	ASN
2	B	706	GLN
2	B	734	HIS
2	B	744	HIS
2	B	762	ASN
2	B	794	ASN
2	B	822	ASN
2	B	834	ASN
2	B	842	ASN
2	B	862	GLN
2	B	946	ASN

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Mol	Chain	Res	Type
2	B	957	ASN
2	B	1015	HIS
2	B	1040	ASN
2	B	1065	GLN
2	B	1084	GLN
2	B	1211	ASN
3	C	73	GLN
3	C	79	GLN
3	C	123	ASN
3	C	167	HIS
3	C	188	HIS
3	C	203	GLN
3	C	206	ASN
4	E	32	GLN
4	E	61	GLN
4	E	63	ASN
4	E	99	HIS
4	E	114	ASN
4	E	146	HIS
4	E	147	HIS
6	H	11	GLN
6	H	33	GLN
6	H	52	GLN
6	H	134	ASN
6	H	137	GLN
6	H	139	ASN
7	I	83	ASN
7	I	116	ASN
9	K	40	HIS
9	K	65	HIS
9	K	92	ASN
10	L	53	HIS

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
11	R	11/15 (73%)	3 (27%)	0

All (3) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
11	R	4	G
11	R	10	A
11	R	12	G

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 9 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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	A	1395/1733 (80%)	-0.03	13 (0%) 81 64	76, 116, 186, 214	0
2	B	1106/1224 (90%)	-0.01	7 (0%) 85 71	72, 109, 156, 180	0
3	C	266/318 (83%)	-0.27	0 100 100	83, 106, 145, 154	0
4	E	214/215 (99%)	-0.03	3 (1%) 73 55	104, 151, 192, 196	0
5	F	84/155 (54%)	-0.27	0 100 100	99, 123, 142, 147	0
6	H	133/146 (91%)	-0.06	2 (1%) 72 54	123, 143, 165, 167	0
7	I	119/122 (97%)	0.03	1 (0%) 82 65	113, 132, 150, 160	0
8	J	65/70 (92%)	-0.33	0 100 100	77, 94, 126, 131	0
9	K	114/120 (95%)	-0.24	0 100 100	87, 108, 124, 131	0
10	L	46/70 (65%)	0.27	1 (2%) 62 46	100, 161, 179, 181	0
11	R	12/15 (80%)	-0.02	0 100 100	100, 128, 185, 192	0
12	T	28/28 (100%)	0.26	0 100 100	102, 210, 322, 325	0
13	N	14/14 (100%)	0.62	1 (7%) 22 21	287, 311, 317, 318	0
All	All	3596/4230 (85%)	-0.05	28 (0%) 82 65	72, 116, 181, 325	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	56	PRO	4.0
1	A	311	GLN	4.0
1	A	820	GLY	3.7
2	B	335	GLY	3.5
1	A	397	ASN	3.3
7	I	13	MET	3.2
1	A	1434	ALA	3.2
6	H	134	ASN	3.1
2	B	816	GLU	2.8

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Mol	Chain	Res	Type	RSRZ
2	B	813	LYS	2.5
2	B	446	LEU	2.5
1	A	149	GLU	2.5
1	A	314	ALA	2.3
4	E	110	PHE	2.3
13	N	1	DC	2.2
6	H	86	ASP	2.2
2	B	899	ILE	2.2
2	B	882	THR	2.2
1	A	318	SER	2.2
1	A	386	ASP	2.1
10	L	45	ALA	2.1
4	E	126	SER	2.1
1	A	1332	PHE	2.1
1	A	307	ASP	2.1
2	B	954	VAL	2.0
1	A	317	LYS	2.0
1	A	396	PRO	2.0
4	E	124	VAL	2.0

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

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

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($\text{\AA}^2$)	Q<0.9
15	MG	A	1736	1/1	0.87	0.11	92,92,92,92	0
14	ZN	A	1734	1/1	0.94	0.05	212,212,212,212	0
14	ZN	A	1735	1/1	0.95	0.05	155,155,155,155	0
14	ZN	L	105	1/1	0.98	0.03	169,169,169,169	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
14	ZN	B	1307	1/1	0.98	0.04	158,158,158,158	0
14	ZN	I	203	1/1	0.99	0.03	123,123,123,123	0
14	ZN	I	204	1/1	0.99	0.04	131,131,131,131	0
14	ZN	C	319	1/1	1.00	0.03	97,97,97,97	0
14	ZN	J	101	1/1	1.00	0.04	93,93,93,93	0

6.5 Other polymers [i](#)

There are no such residues in this entry.