



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:40 PM UTC

PDB ID : 1R9S / pdb_00001r9s
Title : RNA POLYMERASE II STRAND SEPARATED ELONGATION COM-
PLEX, MATCHED NUCLEOTIDE
Authors : Westover, K.D.; Bushnell, D.A.; Kornberg, R.D.
Deposited on : 2003-10-30
Resolution : 4.25 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

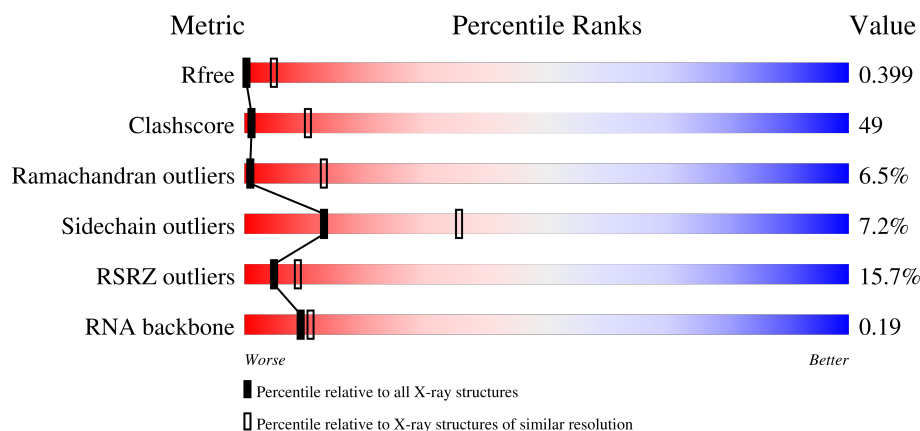
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.25 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	1029 (4.62-3.90)
Clashscore	190562	1074 (4.62-3.90)
Ramachandran outliers	187476	1001 (4.62-3.88)
Sidechain outliers	187428	1021 (4.66-3.86)
RSRZ outliers	180081	1026 (4.62-3.90)
RNA backbone	3983	1028 (5.40-3.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	R	10	50% 50%
2	T	14	36% 21% 64% 14%
3	A	1733	13% 28% 42% 9% 20%
4	B	1224	14% 28% 50% 10% 10%

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

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	UTP	R	3000	X	-	-	-

2 Entry composition [i](#)

There are 15 unique types of molecules in this entry. The entry contains 28491 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called RNA strand.

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

- Molecule 2 is a DNA chain called DNA strand.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	T	14	Total	C	N	O	P	0	0	0
			279	135	48	83	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	1381	Total	C	N	O	S	0	0	0
			10857	6851	1899	2046	61			

- Molecule 4 is a protein called DNA-directed RNA polymerase II 140 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	B	1097	Total	C	N	O	S	0	0	0
			8720	5526	1523	1617	54			

- Molecule 5 is a protein called DNA-directed RNA polymerase II 45 kDa polypeptide.

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

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III 27 kDa polypeptide.

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

- Molecule 7 is a protein called DNA-directed RNA polymerases I, II, and III 23 kDa polypeptide.

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

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III 14.5 kDa polypeptide.

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

- Molecule 9 is a protein called DNA-directed RNA polymerase II 14.2 kDa polypeptide.

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

- Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III 8.3 kDa polypeptide.

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

- Molecule 11 is a protein called DNA-directed RNA polymerase II 13.6 kDa polypeptide.

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

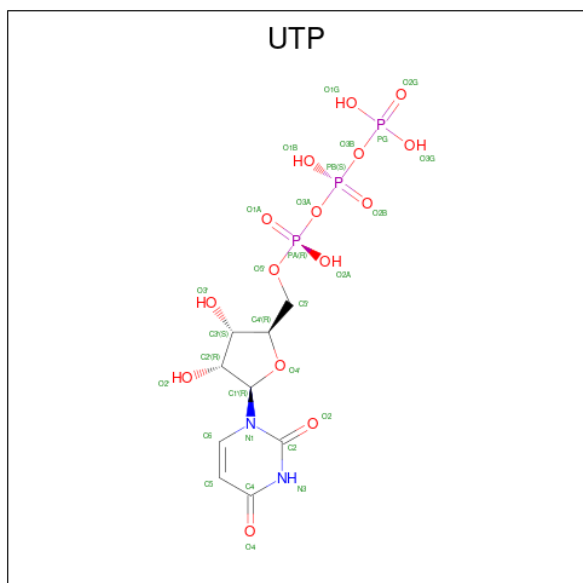
- Molecule 12 is a protein called DNA-directed RNA polymerases I, II, and III 7.7 kDa polypeptide.

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

- Molecule 13 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 14 is URIDINE 5'-TRIPHOSPHATE (CCD ID: UTP) (formula: C₉H₁₅N₂O₁₅P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
14	R	1	Total	C	N	O	P	0	0
			29	9	2	15	3		

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

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

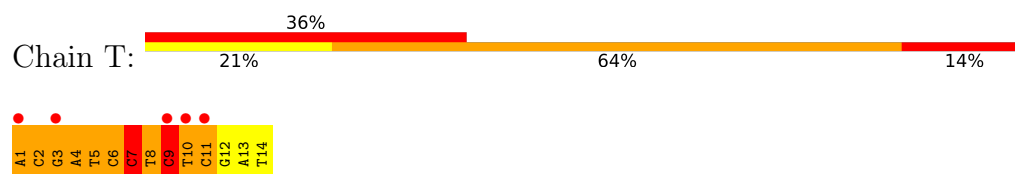
3 Residue-property plots

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

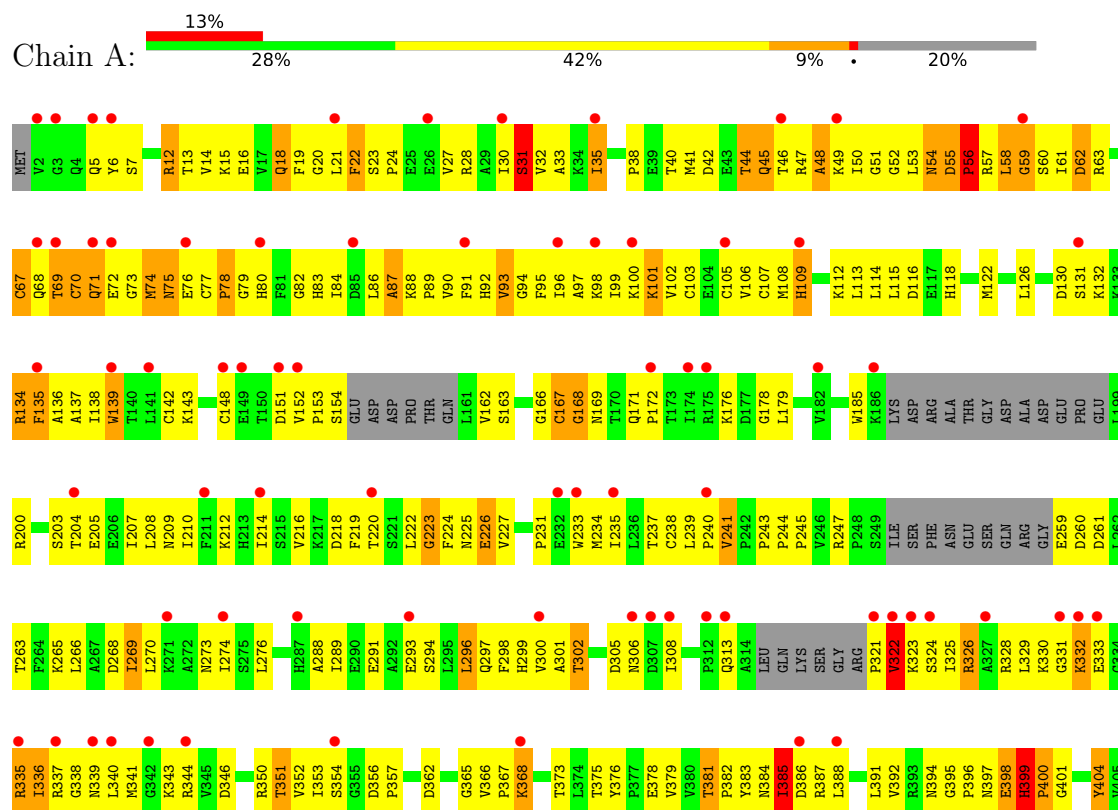
• Molecule 1: RNA strand



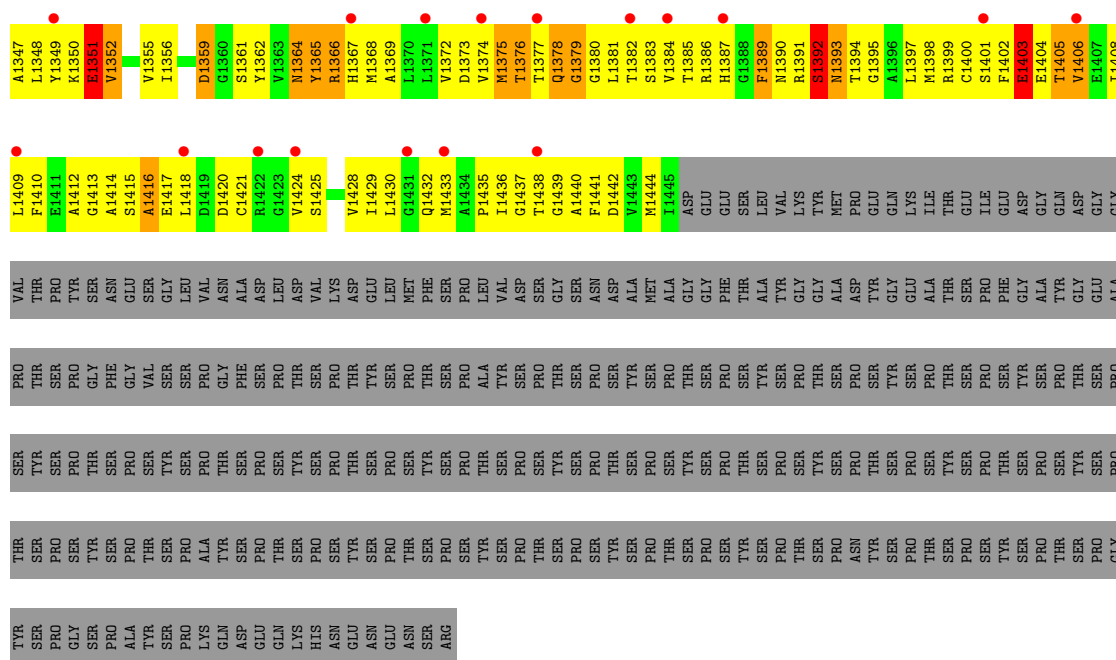
• Molecule 2: DNA strand

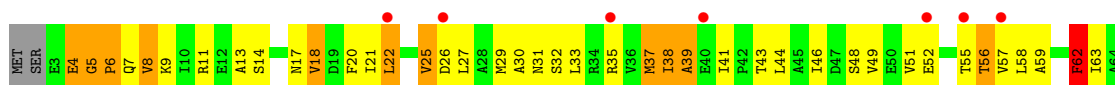


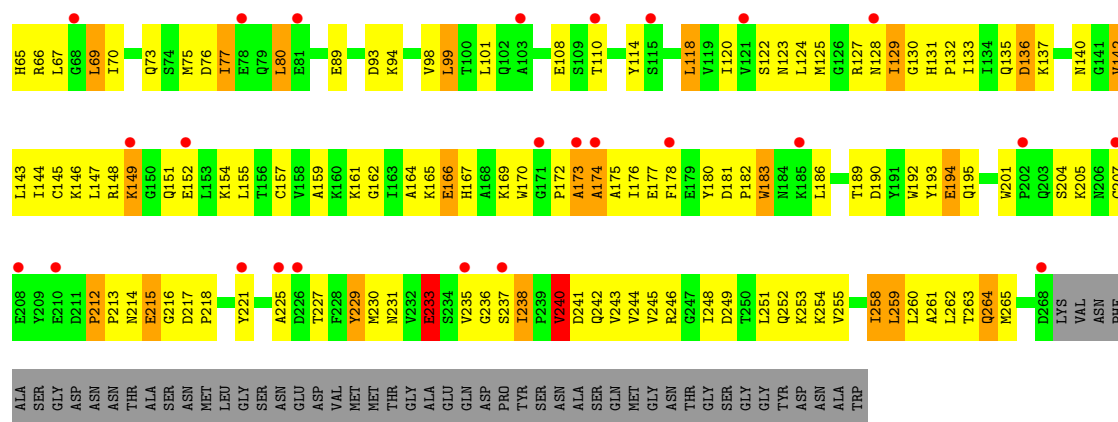
• Molecule 3: DNA-directed RNA polymerase II largest subunit



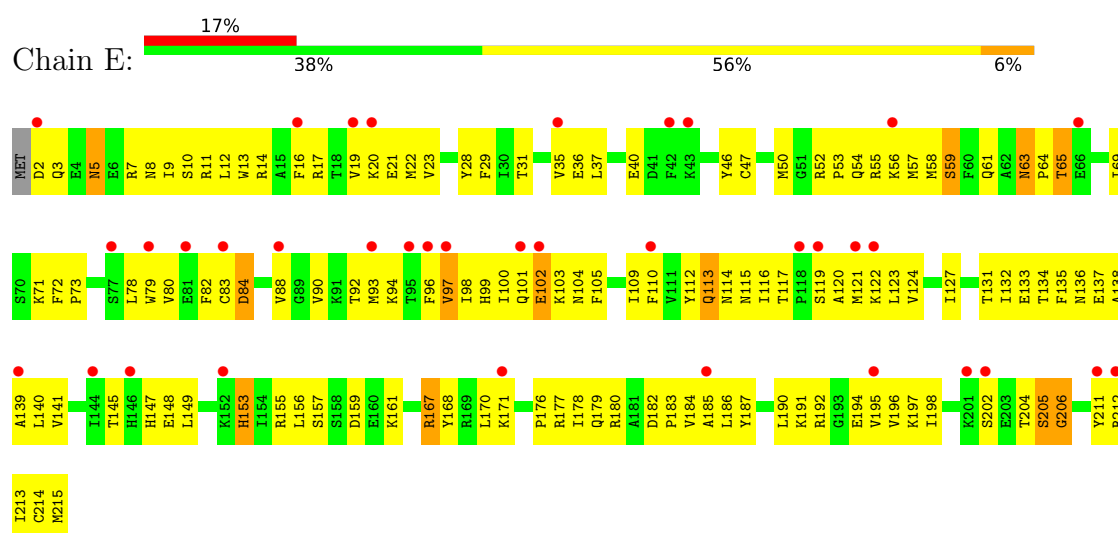




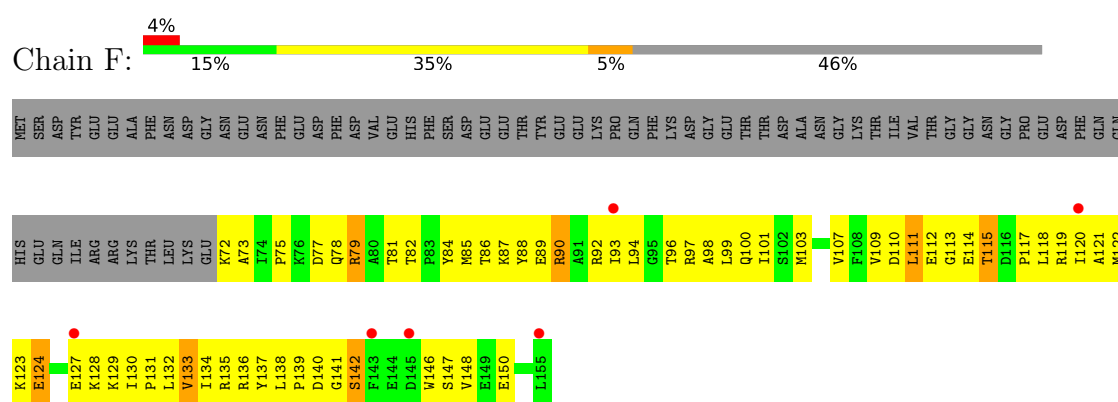




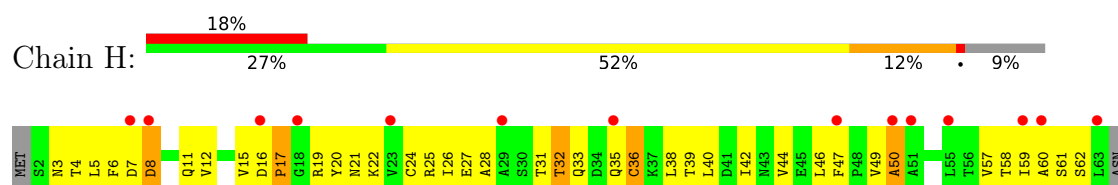
• Molecule 6: DNA-directed RNA polymerases I, II, and III 27 kDa polypeptide



• Molecule 7: DNA-directed RNA polymerases I, II, and III 23 kDa polypeptide

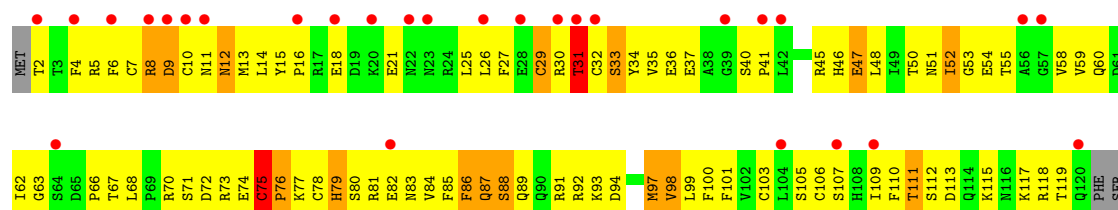


• Molecule 8: DNA-directed RNA polymerases I, II, and III 14.5 kDa polypeptide





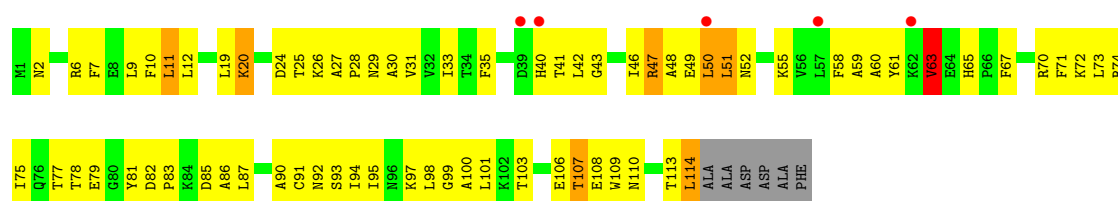
• Molecule 9: DNA-directed RNA polymerase II 14.2 kDa polypeptide



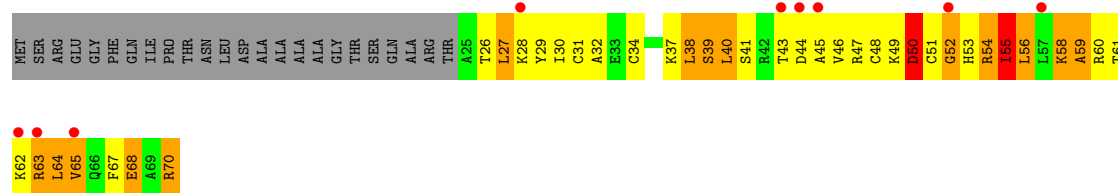
• Molecule 10: DNA-directed RNA polymerases I, II, and III 8.3 kDa polypeptide



• Molecule 11: DNA-directed RNA polymerase II 13.6 kDa polypeptide



• Molecule 12: DNA-directed RNA polymerases I, II, and III 7.7 kDa polypeptide



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	169.65Å 222.34Å 194.32Å 90.00° 101.67° 90.00°	Depositor
Resolution (Å)	40.00 – 4.25 40.00 – 4.25	Depositor EDS
% Data completeness (in resolution range)	95.8 (40.00-4.25) 84.4 (40.00-4.25)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.00 (at 4.13Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.349 , 0.398 0.345 , 0.399	Depositor DCC
R_{free} test set	5207 reflections (10.13%)	wwPDB-VP
Wilson B-factor (Å ²)	96.8	Xtriage
Anisotropy	0.402	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 152.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.80	EDS
Total number of atoms	28491	wwPDB-VP
Average B, all atoms (Å ²)	130.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.04% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	R	3.17	19/244 (7.8%)	3.31	32/380 (8.4%)
2	T	3.01	13/311 (4.2%)	3.52	40/477 (8.4%)
3	A	0.53	0/11048	1.06	72/14936 (0.5%)
4	B	0.56	0/8890	1.07	58/11990 (0.5%)
5	C	0.60	0/2133	1.19	27/2891 (0.9%)
6	E	0.42	0/1788	1.03	12/2406 (0.5%)
7	F	0.48	0/691	0.99	2/933 (0.2%)
8	H	0.46	0/1086	1.11	11/1470 (0.7%)
9	I	0.53	0/989	1.10	7/1331 (0.5%)
10	J	0.67	0/541	1.09	4/727 (0.6%)
11	K	0.54	0/937	0.95	3/1265 (0.2%)
12	L	0.53	0/365	1.10	5/485 (1.0%)
All	All	0.68	32/29023 (0.1%)	1.18	273/39291 (0.7%)

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
1	R	0	1
2	T	1	2
All	All	1	3

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	T	3	DG	O3'-P	-28.47	1.18	1.61
2	T	4	DA	O3'-P	-24.21	1.24	1.61
1	R	10	A	P-OP1	-20.25	1.08	1.49
1	R	5	A	O3'-P	-18.20	1.33	1.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	T	7	DC	O3'-P	-14.37	1.39	1.61
1	R	10	A	P-O5'	12.28	1.78	1.59
2	T	7	DC	O5'-C5'	11.78	1.78	1.42
1	R	8	G	C3'-O3'	10.41	1.57	1.42
1	R	4	G	P-OP1	10.36	1.69	1.49
1	R	7	A	C5'-C4'	-9.98	1.36	1.51
2	T	3	DG	P-OP1	9.96	1.68	1.48
2	T	8	DT	P-OP2	9.72	1.67	1.48
1	R	1	A	O3'-P	-9.55	1.46	1.61
1	R	10	A	C5'-C4'	-8.78	1.38	1.51
1	R	4	G	C3'-O3'	8.78	1.55	1.42
1	R	5	A	P-O5'	8.76	1.72	1.59
1	R	4	G	O3'-P	8.62	1.74	1.61
2	T	3	DG	C3'-O3'	-8.43	1.17	1.42
1	R	9	G	O3'-P	8.08	1.73	1.61
1	R	6	G	P-OP2	7.72	1.64	1.49
1	R	2	U	P-OP2	7.38	1.63	1.49
1	R	2	U	C3'-O3'	-7.01	1.31	1.42
1	R	10	A	P-OP2	-6.54	1.35	1.49
2	T	9	DC	O3'-P	-6.35	1.51	1.61
1	R	3	C	C3'-O3'	6.20	1.51	1.42
2	T	9	DC	C4'-O4'	-6.16	1.33	1.45
2	T	2	DC	C3'-O3'	6.08	1.60	1.42
1	R	1	A	C3'-O3'	5.85	1.50	1.42
2	T	10	DT	P-OP1	-5.50	1.37	1.48
2	T	5	DT	P-OP2	5.46	1.59	1.48
1	R	9	G	P-OP1	-5.35	1.38	1.49
2	T	7	DC	C3'-C2'	-5.08	1.42	1.52

All (273) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	T	3	DG	O3'-P-O5'	-35.52	50.72	104.00
1	R	9	G	P-O3'-C3'	22.07	153.31	120.20
2	T	3	DG	P-O3'-C3'	-20.68	89.17	120.20
1	R	3	C	O3'-P-O5'	-20.25	73.63	104.00
1	R	4	G	OP2-P-O3'	-19.73	48.80	108.00
2	T	9	DC	C4'-C3'-O3'	19.25	138.88	110.00
1	R	4	G	O3'-P-O5'	17.52	130.28	104.00
2	T	7	DC	C4'-C3'-O3'	17.23	135.85	110.00
2	T	6	DC	OP1-P-O3'	-17.11	56.68	108.00
2	T	13	DA	OP1-P-O3'	-16.71	57.88	108.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	T	7	DC	C5'-C4'-C3'	15.40	138.00	114.90
1	R	8	G	OP1-P-O3'	-12.82	69.53	108.00
4	B	296	GLU	N-CA-C	-12.31	97.62	112.89
1	R	9	G	O3'-P-O5'	-11.68	86.48	104.00
1	R	1	A	C2'-C3'-O3'	11.68	131.21	113.70
2	T	6	DC	C4'-C3'-O3'	11.31	126.96	110.00
5	C	173	ALA	N-CA-C	11.17	123.45	111.28
3	A	452	LYS	N-CA-C	-10.88	97.32	112.45
3	A	474	VAL	N-CA-C	-10.82	102.51	112.90
2	T	7	DC	O5'-P-OP1	10.68	141.02	109.00
1	R	5	A	C2'-C3'-O3'	10.41	129.31	113.70
1	R	7	A	P-O5'-C5'	-10.01	105.88	120.90
1	R	10	A	O5'-C5'-C4'	-10.00	96.51	111.50
9	I	75	CYS	N-CA-C	-9.99	97.06	109.65
1	R	5	A	C5'-C4'-C3'	9.97	130.95	116.00
1	R	8	G	OP2-P-O3'	9.94	137.82	108.00
5	C	39	ALA	N-CA-C	9.51	127.34	114.12
1	R	3	C	OP1-P-O3'	9.20	135.59	108.00
2	T	3	DG	C4'-C3'-O3'	9.14	123.71	110.00
5	C	183	TRP	N-CA-C	-9.11	95.84	110.32
2	T	9	DC	C5'-C4'-O4'	8.85	122.67	109.40
3	A	1311	VAL	N-CA-C	8.84	121.21	108.48
4	B	976	ILE	N-CA-C	8.82	118.89	110.42
1	R	10	A	C5'-C4'-C3'	8.63	128.95	116.00
2	T	7	DC	C4'-C3'-C2'	8.58	115.28	102.40
2	T	6	DC	OP2-P-O3'	8.54	133.62	108.00
4	B	736	THR	N-CA-C	-8.43	100.03	110.65
8	H	85	GLY	N-CA-C	-8.42	105.06	114.40
1	R	7	A	C4'-C3'-O3'	8.39	125.58	113.00
2	T	13	DA	OP2-P-O3'	8.32	132.96	108.00
1	R	4	G	P-O3'-C3'	8.22	132.53	120.20
8	H	80	ARG	CA-C-N	-8.17	111.96	120.38
8	H	80	ARG	C-N-CA	-8.17	111.96	120.38
3	A	1392	SER	N-CA-C	8.09	128.02	110.80
3	A	693	VAL	N-CA-C	-7.83	103.62	110.74
3	A	950	GLY	N-CA-C	-7.62	104.53	115.27
4	B	606	LYS	N-CA-C	-7.61	103.25	112.54
6	E	171	LYS	N-CA-C	-7.61	100.72	110.53
2	T	3	DG	C4'-C3'-C2'	7.57	113.76	102.40
3	A	241	VAL	N-CA-C	7.57	115.05	107.55
3	A	398	GLU	N-CA-C	-7.50	95.41	108.69
2	T	10	DT	C6-N1-C1'	7.49	130.58	119.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	514	LEU	N-CA-C	-7.48	98.74	109.96
4	B	392	ARG	N-CA-C	-7.46	104.32	113.50
8	H	81	PRO	N-CA-C	7.46	119.80	110.70
4	B	591	ARG	N-CA-C	-7.43	101.27	110.41
2	T	8	DT	O3'-P-O5'	-7.41	92.89	104.00
3	A	1215	ARG	N-CA-C	-7.38	102.62	111.69
3	A	564	ALA	N-CA-C	-7.34	103.31	111.82
3	A	481	ASP	N-CA-C	-7.31	97.61	108.79
4	B	851	PHE	N-CA-C	7.19	121.31	111.39
3	A	417	TYR	N-CA-C	-7.14	98.21	109.50
2	T	10	DT	C2-N1-C1'	-7.13	108.66	119.35
6	E	5	ASN	N-CA-C	-7.12	102.94	111.69
2	T	4	DA	C2'-C3'-O3'	7.06	122.09	111.50
12	L	58	LYS	N-CA-C	7.01	121.57	110.70
2	T	13	DA	O3'-P-O5'	7.00	114.50	104.00
3	A	1440	ALA	N-CA-C	-6.97	104.64	113.43
4	B	1077	THR	N-CA-C	6.97	121.01	112.23
5	C	137	LYS	N-CA-C	-6.97	103.41	112.68
2	T	5	DT	C2'-C3'-O3'	-6.91	101.13	111.50
3	A	1338	VAL	N-CA-C	6.91	117.88	111.45
9	I	119	THR	N-CA-C	-6.91	104.88	113.38
1	R	6	G	P-O5'-C5'	-6.91	110.54	120.90
2	T	1	DA	O5'-C5'-C4'	6.89	121.14	110.80
5	C	233	GLU	N-CA-C	-6.88	100.34	110.52
3	A	296	LEU	N-CA-C	-6.86	103.73	111.07
4	B	351	TYR	N-CA-C	-6.85	102.89	111.11
7	F	112	GLU	N-CA-C	-6.84	105.01	113.15
6	E	202	SER	N-CA-C	6.82	119.80	109.23
4	B	363	HIS	N-CA-C	-6.82	101.54	110.33
3	A	71	GLN	CB-CA-C	-6.72	108.81	116.54
6	E	65	THR	N-CA-C	-6.70	102.17	110.41
3	A	1403	GLU	N-CA-C	6.69	125.05	110.80
8	H	122	LEU	N-CA-C	6.66	120.74	110.42
3	A	797	LYS	N-CA-C	6.65	120.09	112.57
4	B	1130	PHE	N-CA-C	-6.61	102.49	111.55
5	C	89	GLU	N-CA-C	-6.60	98.47	108.96
4	B	703	ILE	N-CA-C	6.56	117.33	107.75
3	A	1269	GLU	N-CA-C	6.55	122.35	113.97
12	L	65	VAL	N-CA-C	6.50	117.94	108.58
4	B	712	PRO	N-CA-C	-6.49	99.11	112.47
1	R	5	A	C4'-C3'-O3'	6.47	122.70	113.00
5	C	194	GLU	N-CA-C	-6.46	105.98	114.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	R	10	A	N9-C1'-C2'	6.45	121.68	112.00
3	A	466	SER	N-CA-C	6.41	124.45	110.80
10	J	2	ILE	N-CA-C	6.40	122.65	109.34
3	A	643	ALA	N-CA-C	-6.39	104.23	111.07
3	A	1262	LYS	N-CA-C	-6.38	104.76	112.54
4	B	99	LYS	N-CA-C	-6.38	101.81	110.36
2	T	4	DA	OP1-P-O3'	-6.38	88.88	108.00
4	B	761	HIS	N-CA-C	-6.36	102.93	112.54
3	A	1010	ALA	N-CA-C	-6.35	103.98	111.03
3	A	491	VAL	N-CA-C	6.34	114.81	107.89
3	A	729	ALA	N-CA-C	-6.34	104.37	111.28
12	L	67	PHE	N-CA-C	6.33	119.81	109.24
3	A	776	ALA	N-CA-C	6.30	119.05	110.35
5	C	41	ILE	CA-C-N	6.29	126.26	120.03
5	C	41	ILE	C-N-CA	6.29	126.26	120.03
9	I	111	THR	N-CA-C	6.28	119.88	110.14
6	E	97	VAL	N-CA-C	-6.27	104.23	110.62
4	B	1085	ILE	N-CA-C	6.25	118.47	108.85
4	B	56	ASP	N-CA-C	6.24	118.63	111.02
1	R	9	G	OP1-P-O3'	6.23	126.69	108.00
6	E	153	HIS	N-CA-C	-6.22	100.44	110.32
3	A	399	HIS	N-CA-C	6.20	123.51	109.81
1	R	8	G	O3'-P-O5'	-6.17	94.74	104.00
2	T	14	DT	N1-C1'-C2'	6.17	122.75	113.50
4	B	801	LYS	N-CA-C	-6.17	101.99	109.83
1	R	6	G	OP1-P-OP2	-6.15	101.14	119.60
2	T	9	DC	O3'-P-O5'	6.15	113.23	104.00
4	B	681	TRP	N-CA-C	-6.15	104.85	112.90
3	A	602	ASP	N-CA-C	-6.12	102.95	111.39
4	B	1009	ASP	N-CA-C	-6.12	105.65	113.23
3	A	1021	LEU	N-CA-C	-6.11	103.57	111.02
8	H	50	ALA	N-CA-C	6.11	115.91	107.73
1	R	10	A	P-O5'-C5'	6.10	130.05	120.90
4	B	1103	ILE	N-CA-C	6.10	122.02	109.34
2	T	9	DC	C2-N1-C1'	-6.07	110.60	119.70
5	C	166	GLU	N-CA-C	-6.07	104.78	111.82
3	A	938	LYS	N-CA-C	-6.02	104.80	111.36
2	T	14	DT	C2'-C3'-O3'	6.02	120.53	111.50
1	R	7	A	C2'-C3'-O3'	-5.95	104.77	113.70
1	R	7	A	O3'-P-O5'	5.93	112.90	104.00
3	A	496	GLU	N-CA-C	-5.93	104.45	111.03
2	T	11	DC	N1-C1'-C2'	-5.91	104.63	113.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1170	ILE	N-CA-C	5.86	116.04	110.53
2	T	5	DT	OP2-P-O3'	-5.84	90.47	108.00
9	I	31	THR	N-CA-C	-5.84	106.28	113.41
4	B	706	GLN	N-CA-C	-5.84	102.25	110.31
4	B	599	THR	N-CA-C	-5.83	104.56	111.03
3	A	325	ILE	N-CA-C	-5.83	107.18	111.90
5	C	108	GLU	N-CA-C	-5.83	105.98	112.57
4	B	541	LEU	N-CA-C	5.81	117.41	111.14
8	H	36	CYS	N-CA-C	5.80	118.98	109.76
3	A	749	ALA	N-CA-C	-5.78	105.06	111.36
3	A	266	LEU	N-CA-C	-5.76	106.09	113.23
1	R	4	G	OP1-P-O3'	5.75	125.26	108.00
3	A	710	LEU	N-CA-C	-5.73	104.42	111.75
9	I	11	ASN	N-CA-C	5.72	119.45	111.90
5	C	237	SER	N-CA-C	-5.71	105.41	112.38
3	A	399	HIS	CA-C-N	-5.71	112.70	119.84
3	A	399	HIS	C-N-CA	-5.71	112.70	119.84
5	C	259	LEU	N-CA-C	-5.69	105.00	111.14
3	A	553	VAL	CA-C-N	5.67	125.35	119.05
3	A	553	VAL	C-N-CA	5.67	125.35	119.05
4	B	900	ALA	CA-C-N	5.67	126.93	119.84
4	B	900	ALA	C-N-CA	5.67	126.93	119.84
3	A	395	GLY	CA-C-N	5.67	126.93	119.84
3	A	395	GLY	C-N-CA	5.67	126.93	119.84
4	B	165	VAL	N-CA-C	5.67	116.46	108.36
3	A	468	PHE	N-CA-C	-5.66	101.90	110.28
4	B	172	ILE	N-CA-C	5.65	116.72	108.58
3	A	524	VAL	N-CA-C	5.64	121.08	109.34
4	B	640	VAL	N-CA-C	5.64	119.06	113.53
2	T	9	DC	C5'-C4'-C3'	-5.64	106.45	114.90
4	B	294	ASP	N-CA-C	-5.60	98.88	110.80
4	B	109	THR	N-CA-C	-5.59	100.13	109.24
10	J	45	CYS	N-CA-C	-5.58	105.20	111.28
3	A	1162	VAL	N-CA-C	-5.58	105.49	113.07
2	T	7	DC	O4'-C4'-C3'	-5.57	97.05	105.40
3	A	44	THR	N-CA-C	-5.57	105.11	112.24
4	B	413	LEU	N-CA-C	-5.56	105.22	111.28
5	C	62	PHE	N-CA-C	-5.56	105.13	111.14
2	T	9	DC	C2'-C3'-O3'	-5.55	103.17	111.50
11	K	63	VAL	N-CA-C	-5.55	98.45	106.88
7	F	124	GLU	N-CA-C	-5.54	106.02	112.89
1	R	5	A	OP2-P-O3'	5.54	124.61	108.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	936	ASP	N-CA-C	5.53	118.47	110.28
5	C	8	VAL	N-CA-C	5.53	117.09	109.46
3	A	750	GLY	N-CA-C	-5.53	100.08	113.18
5	C	41	ILE	N-CA-C	-5.52	103.88	108.63
2	T	5	DT	C5'-C4'-O4'	5.51	117.67	109.40
3	A	827	THR	N-CA-C	-5.51	105.19	111.14
6	E	180	ARG	N-CA-C	-5.51	105.27	111.28
8	H	3	ASN	N-CA-C	5.51	115.56	108.34
3	A	330	LYS	N-CA-C	5.51	118.00	110.24
5	C	94	LYS	N-CA-C	-5.50	106.93	113.97
2	T	5	DT	P-O5'-C5'	-5.50	111.75	120.00
3	A	1391	ARG	N-CA-C	-5.49	104.93	111.69
4	B	894	ASP	N-CA-C	-5.49	101.88	110.17
6	E	161	LYS	N-CA-C	-5.49	105.30	111.28
5	C	37	MET	N-CA-C	-5.48	105.20	111.07
2	T	10	DT	N1-C1'-C2'	-5.48	105.28	113.50
4	B	647	GLY	N-CA-C	5.47	126.15	113.18
5	C	118	LEU	N-CA-C	-5.47	102.92	110.35
3	A	666	ILE	CB-CA-C	-5.46	104.98	111.97
1	R	8	G	C4'-C3'-O3'	5.45	121.18	113.00
3	A	1307	GLU	N-CA-C	-5.45	101.40	110.17
11	K	52	ASN	N-CA-C	-5.44	106.81	113.50
6	E	63	ASN	CA-C-N	5.44	125.36	119.76
6	E	63	ASN	C-N-CA	5.44	125.36	119.76
12	L	68	GLU	N-CA-C	-5.44	101.81	109.96
5	C	225	ALA	N-CA-C	5.43	117.08	108.67
2	T	6	DC	C2'-C3'-O3'	-5.42	103.38	111.50
4	B	1023	VAL	N-CA-C	5.41	116.13	110.62
3	A	143	LYS	N-CA-C	-5.40	107.06	113.97
8	H	103	LYS	N-CA-C	5.39	117.69	108.90
1	R	9	G	O5'-P-OP1	5.39	124.18	108.00
6	E	113	GLN	N-CA-C	5.39	119.86	113.12
3	A	288	ALA	N-CA-C	-5.38	105.39	113.89
3	A	562	THR	CA-C-N	5.33	125.33	119.89
3	A	562	THR	C-N-CA	5.33	125.33	119.89
3	A	1389	PHE	N-CA-C	5.33	119.64	113.18
4	B	648	HIS	N-CA-C	5.33	122.16	110.80
5	C	56	THR	N-CA-C	5.33	116.80	110.19
4	B	112	LEU	N-CA-C	5.33	118.30	109.46
3	A	847	ASP	N-CA-C	5.31	119.47	113.15
4	B	693	ILE	N-CA-C	5.31	115.61	108.17
8	H	16	ASP	N-CA-C	5.30	118.00	109.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	I	18	GLU	N-CA-C	5.30	117.87	109.24
4	B	1114	LEU	N-CA-C	5.29	117.13	111.36
4	B	253	THR	N-CA-C	5.28	118.16	109.76
2	T	14	DT	C6-N1-C1'	5.27	127.25	119.35
4	B	1123	SER	N-CA-C	-5.25	105.97	112.38
5	C	80	LEU	N-CA-C	-5.24	100.48	109.24
3	A	1216	ILE	CB-CA-C	-5.24	104.99	112.22
5	C	240	VAL	N-CA-C	5.24	115.86	110.36
4	B	278	GLN	N-CA-C	5.24	116.16	107.73
8	H	107	VAL	N-CA-C	-5.23	106.11	112.76
4	B	1203	LEU	N-CA-C	-5.22	105.28	110.97
5	C	258	ILE	N-CA-C	-5.22	105.31	111.00
3	A	861	GLY	N-CA-C	-5.20	107.36	114.64
4	B	739	THR	N-CA-C	-5.20	107.60	114.31
3	A	693	VAL	CB-CA-C	-5.20	105.08	111.94
3	A	628	GLY	N-CA-C	5.19	125.48	113.18
4	B	317	CYS	N-CA-C	-5.18	105.31	111.69
6	E	205	SER	N-CA-C	-5.18	99.66	108.26
9	I	10	CYS	N-CA-C	5.18	119.22	113.01
3	A	580	VAL	N-CA-C	-5.17	105.50	110.72
10	J	5	VAL	N-CA-C	-5.17	102.01	108.84
2	T	9	DC	C4'-C3'-C2'	5.16	110.14	102.40
4	B	756	ILE	CB-CA-C	-5.16	106.14	110.94
3	A	1188	GLN	N-CA-C	5.16	117.82	110.24
4	B	69	LEU	N-CA-C	5.15	117.99	109.85
4	B	743	ILE	N-CA-C	-5.15	105.48	110.42
5	C	193	TYR	N-CA-C	5.15	117.24	109.41
4	B	66	ASP	N-CA-C	-5.14	106.77	112.57
3	A	1113	THR	CA-C-N	5.13	126.26	119.84
3	A	1113	THR	C-N-CA	5.13	126.26	119.84
4	B	110	HIS	N-CA-C	5.13	118.10	109.95
4	B	886	LYS	N-CA-C	5.13	117.47	109.52
2	T	9	DC	C6-N1-C1'	5.12	127.37	119.70
1	R	6	G	C2'-C3'-O3'	-5.11	106.03	113.70
1	R	1	A	OP2-P-O3'	5.10	123.30	108.00
2	T	2	DC	OP1-P-O3'	5.09	123.27	108.00
4	B	107	GLY	N-CA-C	5.09	118.41	110.88
4	B	604	ARG	N-CA-C	-5.09	106.92	113.23
3	A	12	ARG	N-CA-C	5.09	116.54	108.96
4	B	659	ALA	N-CA-C	-5.08	105.87	111.71
5	C	129	ILE	N-CA-C	5.07	114.55	108.06
11	K	20	LYS	N-CA-C	-5.06	99.73	108.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	L	40	LEU	N-CA-C	5.06	116.50	108.96
10	J	10	CYS	N-CA-C	5.06	119.72	113.50
1	R	2	U	O3'-P-O5'	-5.05	96.42	104.00
3	A	696	GLU	N-CA-C	-5.05	105.47	110.97
3	A	415	LEU	N-CA-C	5.04	121.53	110.80
4	B	293	PRO	N-CA-C	5.04	118.79	111.03
3	A	886	ILE	N-CA-C	5.03	116.12	111.45
3	A	1078	GLN	N-CA-C	-5.03	106.07	113.61
5	C	38	ILE	N-CA-C	5.02	115.74	110.62
3	A	445	ASN	N-CA-C	5.01	117.00	109.23
4	B	854	LEU	N-CA-C	-5.01	102.66	110.42

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	T	7	DC	C3'

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	R	10	A	Sidechain
2	T	7	DC	Sidechain
2	T	9	DC	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	R	217	0	110	48	0
2	T	279	0	160	69	0
3	A	10857	0	10959	1097	18
4	B	8720	0	8746	950	13
5	C	2095	0	2052	175	0
6	E	1752	0	1776	145	0
7	F	679	0	701	73	0
8	H	1068	0	1040	135	0
9	I	971	0	933	108	59

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	J	532	0	544	78	0
11	K	919	0	929	92	0
12	L	363	0	388	59	0
13	A	1	0	0	0	0
13	R	1	0	0	0	0
14	R	29	0	8	8	0
15	A	2	0	0	0	0
15	B	1	0	0	0	0
15	C	1	0	0	0	0
15	I	2	0	0	1	0
15	J	1	0	0	1	0
15	L	1	0	0	0	0
All	All	28491	0	28346	2764	59

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 49.

All (2764) 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:R:10:A:P	1:R:10:A:OP1	1.08	1.47
2:T:6:DC:H2''	2:T:7:DC:C5'	1.54	1.36
2:T:7:DC:C5'	2:T:7:DC:O5'	1.78	1.30
3:A:353:ILE:HD13	3:A:487:MET:HE3	1.23	1.20
3:A:567:LYS:HB2	3:A:568:PRO:HD2	1.18	1.17
2:T:6:DC:C2'	2:T:7:DC:H5'	1.75	1.15
9:I:111:THR:HG22	9:I:113:ASP:H	1.05	1.15
4:B:345:LYS:HA	4:B:348:ARG:HE	1.11	1.15
3:A:666:ILE:HD11	4:B:1030:LEU:HD13	1.27	1.12
12:L:60:ARG:HG3	12:L:61:THR:H	1.05	1.12
3:A:1329:THR:HG22	3:A:1331:SER:H	1.16	1.11
3:A:855:THR:HG21	3:A:857:ARG:HE	1.12	1.11
6:E:124:VAL:HG13	6:E:132:ILE:HB	1.33	1.10
4:B:1051:THR:HG22	4:B:1053:GLU:H	1.00	1.09
3:A:1364:ASN:ND2	3:A:1366:ARG:HG2	1.65	1.09
4:B:570:VAL:HB	4:B:573:GLN:HB3	1.36	1.08
1:R:8:G:O2'	1:R:9:G:H5'	1.55	1.06
4:B:512:ARG:HH21	4:B:535:LEU:HD11	1.17	1.06
3:A:1161:THR:HG22	3:A:1163:ILE:H	1.18	1.06
3:A:704:ALA:HB2	3:A:710:LEU:HG	1.34	1.06
2:T:1:DA:H2''	2:T:2:DC:O5'	1.46	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:1:DA:C2	2:T:2:DC:H5	1.74	1.05
4:B:708:GLU:HG3	4:B:709:ASP:H	1.17	1.04
4:B:287:ARG:HG2	4:B:292:ILE:HA	1.38	1.04
3:A:93:VAL:HG13	3:A:301:ALA:HB1	1.33	1.03
5:C:80:LEU:HD22	5:C:129:ILE:HD11	1.41	1.03
4:B:1159:ARG:HE	4:B:1193:GLN:NE2	1.56	1.03
7:F:81:THR:HG21	7:F:136:ARG:HD3	1.38	1.03
4:B:977:GLY:HA3	4:B:1099:VAL:HG21	1.41	1.03
12:L:32:ALA:HB3	12:L:55:ILE:HD12	1.39	1.02
3:A:1111:MET:HE2	3:A:1114:PRO:HA	1.39	1.01
3:A:567:LYS:CB	3:A:568:PRO:HD2	1.91	1.01
4:B:1159:ARG:NE	4:B:1193:GLN:HE21	1.57	1.00
3:A:902:LEU:HG	3:A:926:GLN:HG3	1.40	1.00
5:C:57:VAL:HG11	10:J:60:PHE:HB3	1.44	1.00
4:B:1002:THR:HG22	4:B:1006:ILE:H	1.22	0.99
11:K:113:THR:O	11:K:114:LEU:HB2	1.60	0.99
3:A:913:LEU:HD12	3:A:914:GLU:H	1.25	0.99
4:B:120:ARG:HG2	4:B:955:THR:HG21	1.40	0.99
5:C:56:THR:HG22	5:C:57:VAL:H	1.28	0.98
6:E:135:PHE:HB3	6:E:140:LEU:HD11	1.45	0.98
4:B:842:ASN:ND2	4:B:845:SER:H	1.62	0.97
3:A:567:LYS:HB3	8:H:96:VAL:H	1.26	0.97
4:B:174:LEU:O	4:B:175:ARG:HB2	1.64	0.97
2:T:1:DA:C2	2:T:2:DC:C5	2.53	0.97
4:B:1100:ASP:HA	4:B:1103:ILE:HD11	1.46	0.97
1:R:5:A:C2	1:R:6:G:C5	2.52	0.96
5:C:167:HIS:CD2	5:C:169:LYS:H	1.83	0.96
3:A:115:LEU:HB2	3:A:122:MET:HE2	1.45	0.96
4:B:1051:THR:HG22	4:B:1053:GLU:N	1.81	0.96
4:B:200:GLY:HA2	4:B:202:TYR:CE2	2.02	0.95
4:B:392:ARG:HH21	9:I:52:ILE:HD11	1.30	0.95
4:B:639:ILE:HD11	4:B:691:GLU:HG3	1.47	0.94
4:B:737:THR:HG21	9:I:66:PRO:O	1.68	0.94
3:A:244:PRO:HG2	3:A:245:PRO:HD3	1.46	0.94
3:A:338:GLY:HA2	4:B:1129:ARG:HH22	1.33	0.94
3:A:1116:LEU:HD12	3:A:1329:THR:OG1	1.67	0.94
3:A:783:THR:HG22	3:A:784:LEU:HG	1.48	0.93
4:B:824:ILE:HG12	10:J:48:ARG:HH12	1.32	0.93
4:B:1159:ARG:HD3	4:B:1193:GLN:HG3	1.47	0.93
9:I:7:CYS:HB2	9:I:14:LEU:HD21	1.47	0.92
4:B:955:THR:HG22	4:B:956:THR:H	1.31	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1435:PRO:HA	3:A:1439:GLY:O	1.69	0.92
3:A:1281:ARG:HD2	3:A:1309:ASP:OD2	1.68	0.92
12:L:60:ARG:HG3	12:L:61:THR:N	1.85	0.92
1:R:9:G:C6	1:R:10:A:N6	2.37	0.91
10:J:46:CYS:HG	15:J:101:ZN:ZN	0.78	0.91
5:C:73:GLN:HE21	5:C:75:MET:H	1.14	0.91
9:I:75:CYS:HG	15:I:204:ZN:ZN	0.68	0.91
10:J:1:MET:H1	10:J:56:LEU:HB2	1.34	0.91
3:A:15:LYS:HB3	4:B:1220:ARG:HG2	1.51	0.91
3:A:381:THR:HG22	3:A:383:TYR:H	1.35	0.91
3:A:1399:ARG:HB3	3:A:1408:ILE:HD13	1.50	0.91
3:A:1194:ARG:NH2	3:A:1237:ILE:HD13	1.87	0.90
4:B:1002:THR:HG22	4:B:1006:ILE:N	1.84	0.90
4:B:842:ASN:HD22	4:B:845:SER:H	1.17	0.90
4:B:956:THR:HA	4:B:961:LEU:O	1.71	0.90
5:C:22:LEU:HD22	5:C:25:VAL:HG21	1.53	0.90
3:A:590:ARG:HG3	3:A:590:ARG:NH1	1.86	0.90
3:A:1105:LEU:HD22	3:A:1384:VAL:HG21	1.53	0.90
4:B:955:THR:HG22	4:B:956:THR:N	1.85	0.90
7:F:93:ILE:HD11	7:F:134:ILE:HD11	1.54	0.90
3:A:351:THR:HG23	4:B:1103:ILE:HA	1.53	0.90
4:B:1159:ARG:HE	4:B:1193:GLN:HE21	0.93	0.89
9:I:111:THR:HG22	9:I:113:ASP:N	1.86	0.89
3:A:868:TYR:HD2	3:A:1058:VAL:HG21	1.38	0.89
3:A:1410:PHE:CD2	4:B:1212:ILE:HD11	2.08	0.89
2:T:2:DC:H2'	2:T:3:DG:C8	2.07	0.89
4:B:800:GLN:HB3	10:J:52:THR:HG21	1.54	0.89
6:E:5:ASN:HD21	6:E:52:ARG:HG2	1.35	0.89
3:A:549:MET:SD	3:A:577:ILE:HD12	2.12	0.88
3:A:567:LYS:HB2	3:A:568:PRO:CD	2.02	0.88
4:B:1077:THR:HG22	4:B:1079:LYS:H	1.35	0.88
4:B:955:THR:CG2	4:B:956:THR:H	1.87	0.88
4:B:519:TRP:HZ2	4:B:705:MET:HE1	1.37	0.88
1:R:9:G:O6	1:R:10:A:N6	2.07	0.88
3:A:666:ILE:CD1	4:B:1030:LEU:HD13	2.04	0.87
3:A:886:ILE:HD11	3:A:943:LEU:HB3	1.56	0.87
4:B:512:ARG:HH21	4:B:535:LEU:CD1	1.88	0.87
3:A:567:LYS:NZ	8:H:46:LEU:HB2	1.87	0.87
3:A:590:ARG:HG3	3:A:590:ARG:HH11	1.37	0.87
4:B:1065:GLN:HE21	4:B:1067:ARG:N	1.73	0.87
5:C:57:VAL:HG11	10:J:60:PHE:CB	2.03	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:8:DT:H2''	2:T:9:DC:O5'	1.74	0.87
3:A:61:ILE:HG22	3:A:62:ASP:H	1.37	0.87
4:B:345:LYS:CA	4:B:348:ARG:HE	1.87	0.87
4:B:744:HIS:HD2	4:B:746:SER:H	1.22	0.87
3:A:1192:LEU:HD11	3:A:1239:ARG:HB3	1.56	0.87
3:A:667:GLY:HA2	3:A:670:ILE:HD12	1.56	0.87
3:A:337:ARG:NH1	3:A:839:ARG:HH12	1.72	0.87
5:C:44:LEU:HB2	5:C:77:ILE:HD11	1.55	0.87
3:A:962:ARG:HA	3:A:965:GLN:HE21	1.38	0.86
2:T:3:DG:H5'	3:A:836:TYR:CD1	2.09	0.86
4:B:130:VAL:HG21	4:B:167:ILE:HD12	1.56	0.86
4:B:977:GLY:HA3	4:B:1099:VAL:CG2	2.04	0.86
2:T:11:DC:H2''	2:T:12:DG:H5'	1.56	0.86
3:A:443:LEU:HD22	3:A:455:MET:HE2	1.58	0.86
3:A:1242:VAL:HG12	3:A:1243:VAL:H	1.40	0.86
4:B:1106:ARG:HH21	4:B:1109:GLY:H	1.24	0.86
4:B:801:LYS:O	10:J:52:THR:HG23	1.75	0.86
4:B:912:ILE:O	4:B:938:SER:HB2	1.76	0.86
5:C:167:HIS:HD2	5:C:169:LYS:H	0.90	0.85
3:A:269:ILE:HD11	3:A:300:VAL:HA	1.57	0.85
11:K:10:PHE:CD1	11:K:11:LEU:HD13	2.11	0.85
4:B:345:LYS:HA	4:B:348:ARG:NE	1.91	0.85
3:A:417:TYR:O	3:A:418:SER:HB2	1.75	0.85
3:A:804:TYR:HE1	4:B:1021:MET:HE3	1.40	0.85
2:T:6:DC:H4'	3:A:447:GLN:NE2	1.91	0.85
3:A:1348:LEU:HD23	3:A:1372:VAL:HG13	1.59	0.85
3:A:1039:LYS:O	3:A:1043:ASP:HB2	1.76	0.85
1:R:5:A:N1	1:R:6:G:C6	2.44	0.84
3:A:709:THR:HG21	9:I:93:LYS:O	1.78	0.84
4:B:1106:ARG:NH1	4:B:1118:PRO:HB3	1.91	0.84
4:B:519:TRP:CZ2	4:B:705:MET:HE1	2.11	0.84
8:H:125:LEU:HG	8:H:130:ARG:NH1	1.92	0.84
6:E:177:ARG:HD3	6:E:215:MET:SD	2.18	0.84
2:T:9:DC:OP1	4:B:1123:SER:HB3	1.77	0.84
3:A:1118:VAL:CG2	3:A:1306:LEU:HB2	2.08	0.84
3:A:1390:ASN:ND2	3:A:1399:ARG:HA	1.93	0.84
11:K:12:LEU:H	11:K:12:LEU:HD12	1.42	0.84
3:A:353:ILE:CD1	3:A:487:MET:HE3	2.07	0.84
4:B:228:LYS:HD3	4:B:234:ILE:HD13	1.57	0.84
2:T:6:DC:H4'	3:A:447:GLN:HE22	1.42	0.83
7:F:147:SER:OG	7:F:150:GLU:HG3	1.78	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:605:MET:HE3	3:A:614:PHE:O	1.78	0.83
4:B:200:GLY:HA2	4:B:202:TYR:HE2	1.43	0.83
4:B:637:LEU:HD12	4:B:693:ILE:HD12	1.60	0.83
4:B:1002:THR:CG2	4:B:1006:ILE:H	1.91	0.83
5:C:11:ARG:NH2	5:C:229:TYR:HD2	1.77	0.82
3:A:535:THR:HG21	3:A:617:VAL:H	1.43	0.82
3:A:1111:MET:HE1	3:A:1330:ASN:OD1	1.79	0.82
3:A:565:ILE:HG23	3:A:567:LYS:HG2	1.62	0.82
3:A:885:THR:HG23	3:A:893:PHE:HE1	1.43	0.82
4:B:108:VAL:HG12	4:B:109:THR:H	1.42	0.82
4:B:269:ILE:HD11	4:B:386:LEU:HD21	1.62	0.82
3:A:683:ILE:HD11	3:A:764:CYS:HB2	1.61	0.82
6:E:2:ASP:O	6:E:3:GLN:HG2	1.78	0.82
4:B:763:GLN:HG2	4:B:765:PRO:HD2	1.61	0.82
4:B:999:MET:HG3	4:B:1000:PRO:HD2	1.61	0.82
3:A:563:PRO:HG3	3:A:572:TRP:CZ2	2.14	0.81
8:H:81:PRO:HB2	8:H:82:PRO:HD3	1.62	0.81
8:H:93:TYR:HB3	8:H:144:ILE:O	1.80	0.81
10:J:3:VAL:HG21	10:J:18:TRP:HB2	1.61	0.81
10:J:48:ARG:HH21	10:J:49:MET:HE1	1.42	0.81
3:A:1017:LEU:HB2	6:E:206:GLY:H	1.45	0.81
4:B:1106:ARG:HE	4:B:1109:GLY:N	1.79	0.81
4:B:800:GLN:HB3	10:J:52:THR:CG2	2.11	0.81
3:A:208:LEU:HD22	3:A:212:LYS:HE3	1.62	0.81
3:A:511:ILE:HG12	3:A:521:MET:HE3	1.62	0.81
3:A:742:ASN:HA	3:A:745:GLN:HB2	1.63	0.81
4:B:1106:ARG:HE	4:B:1109:GLY:H	1.29	0.81
5:C:37:MET:HG2	5:C:243:VAL:HG12	1.62	0.81
4:B:121:ASN:N	4:B:121:ASN:HD22	1.79	0.81
9:I:50:THR:CG2	9:I:52:ILE:HG23	2.11	0.81
3:A:472:LEU:O	3:A:475:THR:HB	1.81	0.81
8:H:81:PRO:HB2	8:H:82:PRO:CD	2.11	0.81
4:B:899:ILE:HD11	4:B:911:ILE:HA	1.62	0.80
3:A:337:ARG:NH1	3:A:839:ARG:NH1	2.29	0.80
4:B:244:LEU:O	4:B:249:ARG:HG2	1.81	0.80
5:C:148:ARG:NH1	10:J:64:ASN:HA	1.96	0.80
3:A:406:ILE:HB	3:A:431:LYS:HB2	1.61	0.80
3:A:868:TYR:CE1	3:A:1064:VAL:HG11	2.17	0.80
4:B:796:LEU:HB3	4:B:799:PRO:HG3	1.63	0.80
4:B:1106:ARG:HH21	4:B:1109:GLY:N	1.78	0.80
9:I:75:CYS:SG	9:I:78:CYS:SG	2.80	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:6:DC:C2'	2:T:7:DC:C5'	2.45	0.80
4:B:1100:ASP:HA	4:B:1103:ILE:CD1	2.12	0.80
10:J:3:VAL:HG21	10:J:18:TRP:CB	2.12	0.80
3:A:523:ILE:HD12	3:A:622:VAL:CG2	2.12	0.80
3:A:1118:VAL:HG22	3:A:1306:LEU:HB2	1.64	0.79
1:R:5:A:H2'	1:R:6:G:C8	2.18	0.79
3:A:93:VAL:CG1	3:A:301:ALA:HB1	2.11	0.79
4:B:118:ARG:HH22	4:B:194:GLU:CD	1.90	0.79
2:T:3:DG:H5'	3:A:836:TYR:CE1	2.18	0.79
3:A:40:THR:HG22	3:A:41:MET:HG3	1.64	0.79
4:B:293:PRO:HG2	4:B:296:GLU:CB	2.12	0.79
4:B:487:THR:HG22	4:B:489:SER:H	1.48	0.79
3:A:32:VAL:HG21	3:A:68:GLN:NE2	1.97	0.79
3:A:298:PHE:O	3:A:302:THR:HB	1.83	0.79
4:B:1065:GLN:HE21	4:B:1067:ARG:H	1.29	0.79
4:B:1106:ARG:NH2	4:B:1109:GLY:H	1.79	0.79
5:C:56:THR:HG22	5:C:57:VAL:N	1.97	0.79
3:A:768:GLN:CG	3:A:816:HIS:HA	2.13	0.79
3:A:913:LEU:HD12	3:A:914:GLU:N	1.98	0.79
3:A:1299:VAL:HG12	3:A:1300:LYS:H	1.47	0.78
4:B:834:ASN:HB3	4:B:840:ILE:HG13	1.63	0.78
10:J:64:ASN:HB3	10:J:65:PRO:HD3	1.63	0.78
3:A:666:ILE:HD13	4:B:1030:LEU:HD22	1.65	0.78
3:A:1281:ARG:O	3:A:1282:VAL:HG23	1.83	0.78
8:H:5:LEU:HD11	8:H:135:LEU:HG	1.63	0.78
3:A:58:LEU:HD22	3:A:80:HIS:O	1.83	0.78
8:H:40:LEU:HD23	8:H:42:ILE:HD11	1.66	0.78
3:A:313:GLN:HB2	3:A:322:VAL:CG2	2.14	0.78
4:B:102:VAL:HG23	4:B:112:LEU:HB2	1.65	0.78
3:A:783:THR:HG21	3:A:815:PHE:CZ	2.19	0.78
4:B:855:PHE:HZ	4:B:857:ARG:NH1	1.81	0.78
3:A:70:CYS:O	3:A:72:GLU:HG2	1.84	0.78
3:A:679:ILE:HG23	3:A:729:ALA:HB1	1.63	0.78
3:A:1076:ALA:HA	3:A:1079:MET:HE2	1.65	0.78
4:B:392:ARG:NH2	9:I:52:ILE:HD11	1.98	0.78
4:B:583:ASN:HD21	4:B:628:THR:HB	1.49	0.78
4:B:496:ARG:NH1	4:B:539:LEU:HB2	1.99	0.77
5:C:165:LYS:O	11:K:6:ARG:NH1	2.17	0.77
3:A:313:GLN:HB2	3:A:322:VAL:HG23	1.64	0.77
4:B:542:MET:HE3	4:B:747:MET:HG3	1.63	0.77
3:A:901:LEU:H	3:A:926:GLN:NE2	1.82	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:102:VAL:CG2	4:B:112:LEU:HB2	2.13	0.77
4:B:1100:ASP:OD1	4:B:1103:ILE:HD11	1.84	0.77
8:H:89:LEU:C	8:H:91:ASP:H	1.90	0.77
4:B:842:ASN:ND2	4:B:845:SER:N	2.31	0.77
4:B:1166:CYS:O	4:B:1168:LEU:N	2.18	0.77
10:J:12:LYS:O	10:J:14:VAL:HG23	1.85	0.77
11:K:47:ARG:HB3	11:K:47:ARG:HH11	1.49	0.77
3:A:855:THR:HG21	3:A:857:ARG:NE	1.95	0.77
4:B:232:SER:OG	4:B:234:ILE:HD12	1.84	0.77
3:A:31:SER:CB	3:A:83:HIS:HB2	2.15	0.77
3:A:1438:THR:HB	4:B:1144:ALA:HB3	1.66	0.77
10:J:10:CYS:SG	10:J:46:CYS:SG	2.83	0.77
3:A:23:SER:HB3	3:A:233:TRP:CZ2	2.19	0.77
3:A:1345:ARG:HD2	3:A:1373:ASP:OD1	1.84	0.77
3:A:24:PRO:HB3	3:A:237:THR:HB	1.67	0.76
3:A:326:ARG:HG2	3:A:1406:VAL:HG21	1.67	0.76
3:A:567:LYS:HZ1	8:H:46:LEU:HB2	1.49	0.76
3:A:896:ARG:HD3	3:A:897:TYR:CE1	2.21	0.76
4:B:707:PRO:HG2	4:B:708:GLU:H	1.49	0.76
4:B:1096:ARG:O	4:B:1097:HIS:HB2	1.85	0.76
4:B:899:ILE:CD1	4:B:911:ILE:HA	2.16	0.76
6:E:69:ILE:HG23	6:E:73:PRO:HA	1.68	0.76
3:A:849:MET:HE3	3:A:1061:GLY:HA2	1.67	0.76
2:T:6:DC:H2''	2:T:7:DC:H5'	0.79	0.76
3:A:399:HIS:O	3:A:401:GLY:N	2.17	0.76
3:A:223:GLY:O	3:A:1415:SER:HA	1.86	0.76
4:B:842:ASN:HD22	4:B:845:SER:N	1.83	0.76
5:C:57:VAL:CG1	10:J:60:PHE:HB3	2.15	0.76
5:C:166:GLU:HG3	11:K:10:PHE:HZ	1.51	0.76
3:A:1094:VAL:HG13	3:A:1113:THR:HG21	1.66	0.76
4:B:996:ARG:NH2	5:C:174:ALA:O	2.19	0.76
3:A:336:ILE:HD12	3:A:1405:THR:HG21	1.68	0.75
3:A:541:ILE:HG12	3:A:549:MET:HE1	1.66	0.75
4:B:542:MET:HG3	4:B:747:MET:HE3	1.66	0.75
5:C:124:LEU:O	5:C:127:ARG:HG2	1.85	0.75
8:H:93:TYR:HA	8:H:145:ARG:HB3	1.68	0.75
3:A:469:ARG:HH21	4:B:976:ILE:HD13	1.50	0.75
4:B:118:ARG:HG3	4:B:204:ILE:HD13	1.68	0.75
4:B:211:VAL:HG21	4:B:483:LEU:HD13	1.67	0.75
4:B:711:GLU:N	4:B:712:PRO:HD3	2.01	0.75
4:B:882:THR:HG22	4:B:884:ARG:H	1.50	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1323:ASP:OD1	3:A:1325:THR:HB	1.85	0.75
3:A:41:MET:HA	3:A:49:LYS:HA	1.68	0.75
3:A:341:MET:HE1	3:A:1401:SER:HB2	1.68	0.75
3:A:804:TYR:CE1	4:B:1021:MET:HE3	2.21	0.75
11:K:55:LYS:HB3	11:K:81:TYR:HD1	1.50	0.75
7:F:111:LEU:HD12	7:F:111:LEU:N	2.02	0.75
4:B:708:GLU:HG3	4:B:709:ASP:N	1.98	0.75
3:A:265:LYS:NZ	3:A:323:LYS:H	1.84	0.74
3:A:1436:ILE:HG22	3:A:1437:GLY:H	1.52	0.74
4:B:62:ILE:HG23	4:B:418:LYS:HG2	1.69	0.74
12:L:38:LEU:O	12:L:39:SER:HB3	1.85	0.74
2:T:2:DC:OP1	3:A:1403:GLU:O	2.04	0.74
3:A:458:HIS:CE1	3:A:507:VAL:HG21	2.22	0.74
3:A:1146:VAL:HG11	3:A:1202:MET:SD	2.27	0.74
3:A:535:THR:CG2	3:A:616:VAL:HA	2.17	0.74
3:A:575:LYS:HB3	3:A:612:ILE:CG2	2.17	0.74
3:A:1436:ILE:HG22	3:A:1437:GLY:N	2.03	0.74
4:B:708:GLU:CG	4:B:709:ASP:H	1.97	0.74
3:A:693:VAL:HG21	3:A:721:PHE:HE1	1.51	0.74
6:E:61:GLN:HE21	6:E:105:PHE:HE2	1.34	0.74
3:A:95:PHE:O	3:A:99:ILE:HG13	1.85	0.74
3:A:853:ASP:OD1	3:A:855:THR:HB	1.88	0.74
4:B:521:LEU:HD22	4:B:633:VAL:HG12	1.69	0.74
4:B:423:LYS:HA	4:B:426:LYS:HE2	1.68	0.74
3:A:443:LEU:HD21	3:A:455:MET:HB3	1.70	0.74
4:B:770:GLN:HG2	4:B:983:ARG:O	1.86	0.74
3:A:154:SER:HB3	3:A:162:VAL:CG2	2.17	0.74
3:A:710:LEU:H	3:A:710:LEU:HD12	1.52	0.74
3:A:1436:ILE:CG2	4:B:1142:GLY:HA2	2.17	0.74
4:B:542:MET:HE1	4:B:743:ILE:HG21	1.69	0.74
8:H:123:MET:HE1	8:H:142:LEU:CD1	2.17	0.74
3:A:1299:VAL:HG12	3:A:1300:LYS:N	2.02	0.74
4:B:313:MET:HE3	4:B:386:LEU:HD22	1.68	0.74
5:C:167:HIS:HD2	5:C:169:LYS:N	1.76	0.74
8:H:5:LEU:HB3	8:H:133:ASN:O	1.88	0.74
11:K:65:HIS:CD2	11:K:67:PHE:H	2.06	0.74
4:B:172:ILE:HD13	4:B:178:ASN:HB3	1.70	0.73
3:A:500:GLU:OE2	4:B:1145:SER:HB2	1.88	0.73
11:K:65:HIS:HD2	11:K:67:PHE:H	1.35	0.73
2:T:1:DA:N3	2:T:1:DA:H2'	2.03	0.73
3:A:828:ALA:HB2	4:B:530:GLY:HA2	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:651:LEU:HD11	4:B:707:PRO:HB3	1.69	0.73
3:A:321:PRO:O	3:A:322:VAL:HB	1.87	0.73
3:A:417:TYR:O	3:A:418:SER:CB	2.36	0.73
3:A:857:ARG:HD3	3:A:861:GLY:O	1.88	0.73
3:A:1441:PHE:CZ	7:F:89:GLU:HA	2.23	0.73
6:E:124:VAL:HA	6:E:132:ILE:HD12	1.70	0.73
3:A:268:ASP:HB3	3:A:299:HIS:CE1	2.23	0.73
6:E:61:GLN:NE2	6:E:105:PHE:HE2	1.86	0.73
3:A:32:VAL:HB	3:A:57:ARG:HD2	1.71	0.73
4:B:1106:ARG:NE	4:B:1109:GLY:H	1.85	0.73
1:R:10:A:OP1	1:R:10:A:OP2	1.99	0.73
3:A:534:LEU:O	3:A:574:GLY:HA3	1.88	0.73
8:H:35:GLN:HB3	8:H:111:LEU:HD21	1.70	0.73
3:A:567:LYS:HB3	8:H:96:VAL:N	2.02	0.73
3:A:691:LEU:HD11	3:A:695:LYS:HE3	1.71	0.73
1:R:9:G:N1	1:R:10:A:N6	2.36	0.73
3:A:75:ASN:O	3:A:76:GLU:HB3	1.88	0.73
4:B:234:ILE:HD12	4:B:234:ILE:H	1.54	0.73
4:B:313:MET:CE	4:B:386:LEU:HD22	2.19	0.73
4:B:363:HIS:O	4:B:364:ILE:HB	1.88	0.73
3:A:1152:ILE:HG23	3:A:1260:LEU:HD23	1.71	0.73
4:B:708:GLU:O	4:B:710:LEU:N	2.22	0.73
4:B:980:PHE:CE2	4:B:1094:ARG:HG3	2.23	0.73
4:B:570:VAL:HG21	4:B:573:GLN:NE2	2.04	0.72
3:A:445:ASN:HB2	3:A:455:MET:HG2	1.70	0.72
3:A:858:ASN:C	3:A:858:ASN:HD22	1.95	0.72
3:A:868:TYR:CD2	3:A:1058:VAL:HG21	2.23	0.72
3:A:899:VAL:HB	3:A:929:LEU:HD12	1.71	0.72
4:B:46:GLN:HG3	4:B:47:GLN:N	2.03	0.72
4:B:193:LYS:HD3	4:B:787:VAL:HG11	1.70	0.72
3:A:337:ARG:NE	3:A:839:ARG:HH22	1.88	0.72
3:A:598:LEU:HD22	8:H:25:ARG:NH1	2.05	0.72
3:A:925:LEU:O	3:A:929:LEU:HD23	1.88	0.72
3:A:1399:ARG:HB2	3:A:1408:ILE:HG21	1.70	0.72
4:B:570:VAL:HB	4:B:573:GLN:CB	2.18	0.72
8:H:89:LEU:HB3	8:H:91:ASP:OD1	1.88	0.72
8:H:123:MET:HE1	8:H:142:LEU:HD13	1.69	0.72
1:R:4:G:H1	2:T:11:DC:H42	1.37	0.72
3:A:1258:HIS:ND1	3:A:1262:LYS:HE3	2.04	0.72
11:K:55:LYS:HD3	11:K:78:THR:CB	2.20	0.72
3:A:48:ALA:O	3:A:49:LYS:HG3	1.89	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:353:ILE:HD13	3:A:487:MET:CE	2.14	0.72
3:A:901:LEU:HG	3:A:926:GLN:HE21	1.55	0.72
4:B:879:ARG:HB3	4:B:883:LEU:HD23	1.70	0.72
4:B:999:MET:HE2	4:B:1011:ILE:HD11	1.71	0.72
2:T:2:DC:H2'	2:T:3:DG:H8	1.55	0.72
3:A:1209:MET:SD	3:A:1236:LEU:HB3	2.30	0.72
4:B:58:THR:O	4:B:62:ILE:HG13	1.89	0.72
3:A:399:HIS:HB3	3:A:400:PRO:HD3	1.70	0.72
3:A:445:ASN:CB	3:A:455:MET:HG2	2.19	0.72
4:B:745:PRO:O	4:B:748:ILE:HG12	1.88	0.72
3:A:567:LYS:HD3	8:H:95:TYR:CD1	2.25	0.72
3:A:1397:LEU:O	3:A:1400:CYS:HB2	1.89	0.72
3:A:340:LEU:HD21	4:B:1200:ALA:HB2	1.72	0.71
4:B:309:GLN:HG3	9:I:52:ILE:HD13	1.72	0.71
4:B:1007:VAL:HG22	4:B:1008:PRO:HD2	1.71	0.71
5:C:18:VAL:HG23	5:C:240:VAL:HG11	1.72	0.71
6:E:168:TYR:HB3	6:E:170:LEU:HD21	1.72	0.71
4:B:637:LEU:CD1	4:B:693:ILE:HD12	2.20	0.71
4:B:737:THR:HG23	9:I:66:PRO:CB	2.20	0.71
4:B:1072:MET:HE3	4:B:1085:ILE:HD12	1.70	0.71
9:I:74:GLU:HB3	9:I:79:HIS:HA	1.70	0.71
11:K:7:PHE:HB2	11:K:11:LEU:HD22	1.71	0.71
14:R:3000:UTP:O2	2:T:4:DA:C2	2.44	0.71
3:A:567:LYS:HE3	8:H:46:LEU:HD12	1.72	0.71
3:A:575:LYS:HB3	3:A:612:ILE:HG23	1.71	0.71
4:B:1066:SER:O	4:B:1067:ARG:HD3	1.90	0.71
4:B:108:VAL:HG12	4:B:109:THR:N	2.06	0.71
5:C:98:VAL:C	5:C:99:LEU:HD23	2.16	0.71
3:A:672:ASP:HB2	3:A:736:ASN:OD1	1.90	0.71
3:A:675:THR:HG21	3:A:736:ASN:ND2	2.06	0.71
4:B:281:PRO:HG2	4:B:284:ILE:HD12	1.73	0.71
4:B:792:MET:HA	4:B:856:PHE:O	1.91	0.71
3:A:855:THR:HG23	3:A:857:ARG:HG3	1.72	0.70
3:A:900:ASP:OD2	3:A:903:ASN:HB2	1.90	0.70
3:A:1015:VAL:HG12	3:A:1019:CYS:SG	2.31	0.70
4:B:555:ILE:HD13	4:B:587:HIS:CE1	2.26	0.70
1:R:5:A:C2	1:R:6:G:C6	2.79	0.70
3:A:225:ASN:O	3:A:227:VAL:N	2.21	0.70
3:A:741:ASN:HD22	3:A:741:ASN:C	1.99	0.70
4:B:1056:SER:HB3	4:B:1066:SER:HB2	1.73	0.70
3:A:451:HIS:NE2	3:A:1074:GLU:HG3	2.07	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:343:LYS:HE3	4:B:1151:LEU:O	1.92	0.70
3:A:367:PRO:HB3	3:A:466:SER:HA	1.73	0.70
3:A:675:THR:CB	3:A:736:ASN:HD21	2.04	0.70
3:A:994:GLN:HE22	3:A:1023:ARG:HE	1.38	0.70
4:B:636:PRO:O	4:B:637:LEU:HG	1.90	0.70
4:B:957:ASN:HD22	4:B:961:LEU:HD12	1.57	0.70
6:E:56:LYS:HG3	6:E:84:ASP:HB2	1.73	0.70
8:H:49:VAL:HG12	8:H:50:ALA:N	2.07	0.70
3:A:44:THR:O	3:A:45:GLN:HB2	1.91	0.70
4:B:955:THR:HG23	12:L:54:ARG:O	1.91	0.70
4:B:65:GLU:HG3	4:B:66:ASP:H	1.56	0.70
3:A:351:THR:HG21	4:B:1103:ILE:HG23	1.72	0.70
3:A:463:ILE:HB	3:A:464:PRO:HD2	1.74	0.70
3:A:503:GLN:HE21	7:F:90:ARG:NH2	1.88	0.70
3:A:1394:THR:HG23	3:A:1398:MET:HE3	1.73	0.70
4:B:638:PHE:CE1	4:B:743:ILE:HA	2.26	0.70
3:A:1095:THR:HG22	3:A:1100:ARG:HB2	1.74	0.69
11:K:55:LYS:HD3	11:K:78:THR:HB	1.72	0.69
12:L:60:ARG:CG	12:L:61:THR:H	1.94	0.69
2:T:8:DT:C2'	2:T:9:DC:O5'	2.39	0.69
3:A:1208:THR:HB	3:A:1211:GLN:HG3	1.74	0.69
3:A:472:LEU:HD11	4:B:835:GLN:NE2	2.07	0.69
4:B:378:LEU:O	4:B:382:ILE:HG13	1.92	0.69
12:L:47:ARG:HG2	12:L:52:GLY:HA2	1.72	0.69
3:A:335:ARG:HA	3:A:339:ASN:HD22	1.56	0.69
3:A:383:TYR:HB3	7:F:115:THR:HG22	1.73	0.69
4:B:130:VAL:HG12	4:B:131:ASP:N	2.07	0.69
4:B:293:PRO:HG2	4:B:296:GLU:HB3	1.74	0.69
4:B:54:PHE:HA	4:B:58:THR:HB	1.74	0.69
5:C:80:LEU:HD22	5:C:129:ILE:CD1	2.21	0.69
3:A:567:LYS:HE3	8:H:46:LEU:CD1	2.22	0.69
4:B:463:THR:CG2	4:B:465:ASN:HD22	2.05	0.69
4:B:839:MET:HE3	4:B:1010:LEU:HD11	1.74	0.69
8:H:36:CYS:SG	8:H:130:ARG:NH2	2.65	0.69
2:T:1:DA:N1	2:T:2:DC:C5	2.61	0.69
3:A:392:VAL:HG13	3:A:415:LEU:HD11	1.74	0.69
3:A:414:ASP:OD1	3:A:416:ARG:HG2	1.93	0.69
3:A:763:ALA:O	3:A:803:SER:HB3	1.92	0.69
3:A:1332:PHE:H	3:A:1332:PHE:HD2	1.38	0.69
7:F:81:THR:HG21	7:F:136:ARG:CD	2.20	0.69
3:A:340:LEU:HD13	3:A:1429:ILE:HG23	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:768:GLN:HG2	3:A:816:HIS:HA	1.75	0.69
3:A:786:HIS:HE1	4:B:742:GLU:OE1	1.76	0.69
4:B:314:LEU:O	4:B:317:CYS:HB2	1.92	0.69
4:B:884:ARG:O	4:B:936:ASP:HB3	1.93	0.69
5:C:39:ALA:HA	5:C:164:ALA:HB3	1.75	0.68
6:E:83:CYS:SG	6:E:88:VAL:HG22	2.32	0.68
3:A:391:LEU:HD22	3:A:400:PRO:O	1.93	0.68
4:B:288:ALA:HB1	4:B:331:LEU:HD12	1.75	0.68
3:A:584:ASN:O	3:A:637:LYS:HE3	1.92	0.68
3:A:1390:ASN:HD22	3:A:1399:ARG:HA	1.57	0.68
12:L:40:LEU:HD13	12:L:44:ASP:CG	2.19	0.68
4:B:22:SER:O	4:B:654:ARG:HD2	1.94	0.68
4:B:46:GLN:HG3	4:B:47:GLN:H	1.59	0.68
4:B:542:MET:CE	4:B:747:MET:HG3	2.22	0.68
3:A:72:GLU:OE2	4:B:1175:LEU:HD12	1.92	0.68
3:A:693:VAL:CG2	3:A:721:PHE:HE1	2.07	0.68
4:B:954:VAL:O	12:L:55:ILE:O	2.11	0.68
3:A:599:SER:HB2	3:A:603:ASN:H	1.58	0.68
4:B:280:ILE:CD1	4:B:334:ILE:HG12	2.23	0.68
5:C:51:VAL:HG22	5:C:155:LEU:HD22	1.76	0.68
3:A:563:PRO:HB2	3:A:565:ILE:O	1.94	0.68
4:B:562:GLY:HA3	4:B:590:HIS:CE1	2.29	0.68
8:H:7:ASP:O	8:H:8:ASP:HB2	1.92	0.68
11:K:47:ARG:HB3	11:K:47:ARG:NH1	2.09	0.68
3:A:535:THR:HG21	3:A:617:VAL:N	2.08	0.68
4:B:709:ASP:O	4:B:710:LEU:HD23	1.94	0.68
4:B:986:GLN:OE1	4:B:986:GLN:HA	1.92	0.68
3:A:590:ARG:HH11	3:A:590:ARG:CG	2.06	0.68
3:A:974:ASP:HB2	8:H:136:LYS:HZ1	1.59	0.68
5:C:254:LYS:HB3	11:K:42:LEU:HD11	1.75	0.68
2:T:1:DA:C6	2:T:2:DC:C5	2.81	0.67
3:A:994:GLN:HE21	3:A:1019:CYS:HB3	1.59	0.67
4:B:280:ILE:HG22	4:B:285:ILE:HG13	1.76	0.67
4:B:842:ASN:ND2	4:B:844:SER:HB2	2.09	0.67
4:B:514:LEU:HD12	4:B:515:HIS:N	2.09	0.67
5:C:166:GLU:HG3	11:K:10:PHE:CZ	2.29	0.67
4:B:121:ASN:HA	4:B:207:GLY:HA3	1.77	0.67
5:C:5:GLY:O	5:C:7:GLN:HG3	1.95	0.67
12:L:46:VAL:HG13	12:L:56:LEU:HD12	1.76	0.67
9:I:53:GLY:O	9:I:89:GLN:HB2	1.94	0.67
9:I:75:CYS:SG	9:I:103:CYS:SG	2.92	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:351:THR:CG2	4:B:1103:ILE:HG23	2.24	0.67
3:A:535:THR:HG21	3:A:616:VAL:HA	1.75	0.67
5:C:8:VAL:HG12	5:C:9:LYS:N	2.09	0.67
3:A:814:PHE:O	3:A:817:ALA:HB3	1.95	0.67
4:B:976:ILE:O	4:B:990:ILE:HB	1.94	0.67
4:B:1147:LEU:HD22	4:B:1151:LEU:HD22	1.77	0.67
2:T:1:DA:C1'	3:A:1386:ARG:HH12	2.08	0.67
4:B:711:GLU:N	4:B:712:PRO:CD	2.57	0.67
4:B:864:LYS:HB3	4:B:872:GLU:H	1.59	0.67
2:T:1:DA:C4	2:T:2:DC:C5	2.83	0.67
3:A:16:GLU:HB3	3:A:1418:LEU:HD11	1.77	0.67
3:A:450:LEU:HD13	3:A:1074:GLU:HG2	1.77	0.67
3:A:694:THR:O	3:A:698:GLN:HG3	1.94	0.67
5:C:93:ASP:O	5:C:127:ARG:NH2	2.27	0.67
5:C:260:LEU:O	5:C:264:GLN:HG3	1.95	0.67
4:B:566:LEU:HD13	4:B:588:GLY:HA2	1.77	0.67
6:E:78:LEU:HD23	6:E:78:LEU:C	2.20	0.67
3:A:828:ALA:CB	4:B:530:GLY:HA2	2.25	0.66
3:A:1267:MET:HA	3:A:1271:ILE:HD12	1.77	0.66
3:A:1342:GLU:OE2	6:E:212:ARG:NH1	2.28	0.66
4:B:711:GLU:H	4:B:712:PRO:HD3	1.60	0.66
4:B:882:THR:HG21	4:B:935:ARG:HA	1.75	0.66
4:B:1039:GLY:HA2	10:J:51:LEU:HD21	1.77	0.66
8:H:26:ILE:HD12	8:H:42:ILE:HD12	1.77	0.66
8:H:106:GLU:C	8:H:108:SER:H	2.02	0.66
8:H:115:TYR:CE2	8:H:124:ARG:HG3	2.30	0.66
3:A:305:ASP:HB3	3:A:308:ILE:HD11	1.77	0.66
3:A:525:GLN:CB	4:B:835:GLN:HG2	2.25	0.66
3:A:897:TYR:CD2	3:A:936:LEU:HD13	2.30	0.66
3:A:1193:LEU:HD21	3:A:1267:MET:HE2	1.77	0.66
4:B:957:ASN:O	4:B:959:ASP:N	2.29	0.66
3:A:446:ARG:HG2	3:A:446:ARG:HH11	1.59	0.66
3:A:453:MET:HB3	3:A:477:PRO:HB3	1.76	0.66
3:A:1348:LEU:HD21	3:A:1375:MET:SD	2.35	0.66
4:B:986:GLN:HE22	4:B:1020:ARG:CZ	2.08	0.66
6:E:127:ILE:O	6:E:127:ILE:HG13	1.93	0.66
8:H:95:TYR:CE2	8:H:97:MET:HG3	2.31	0.66
9:I:55:THR:HG23	9:I:58:VAL:HG21	1.76	0.66
3:A:590:ARG:HB3	3:A:605:MET:N	2.10	0.66
3:A:1333:ILE:O	3:A:1336:MET:HB3	1.96	0.66
3:A:1364:ASN:ND2	3:A:1365:TYR:N	2.43	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:1002:THR:HG23	4:B:1004:GLU:N	2.10	0.66
8:H:38:LEU:HD13	8:H:125:LEU:HD13	1.77	0.66
3:A:76:GLU:OE2	4:B:1159:ARG:NH1	2.28	0.66
3:A:88:LYS:HD2	3:A:293:GLU:CD	2.20	0.66
3:A:1042:PHE:CE2	3:A:1046:LEU:HD11	2.31	0.66
4:B:287:ARG:NH2	4:B:294:ASP:OD2	2.28	0.66
4:B:1051:THR:CG2	4:B:1053:GLU:H	1.93	0.66
3:A:90:VAL:CG1	3:A:297:GLN:HA	2.26	0.66
5:C:56:THR:HG21	5:C:145:CYS:SG	2.35	0.66
8:H:97:MET:HE2	8:H:142:LEU:HD23	1.76	0.66
12:L:45:ALA:O	12:L:46:VAL:HG23	1.95	0.66
3:A:381:THR:HG22	3:A:383:TYR:N	2.09	0.66
4:B:363:HIS:O	4:B:364:ILE:CB	2.44	0.66
2:T:6:DC:C4	2:T:7:DC:C5	2.84	0.66
4:B:311:LEU:HB3	9:I:4:PHE:CZ	2.31	0.66
4:B:349:ILE:O	4:B:352:ALA:HB3	1.96	0.66
4:B:1106:ARG:CZ	4:B:1109:GLY:H	2.07	0.66
9:I:32:CYS:SG	9:I:33:SER:N	2.69	0.66
10:J:58:GLU:HA	10:J:61:LEU:HD12	1.76	0.66
3:A:1364:ASN:HD22	3:A:1364:ASN:C	2.04	0.66
4:B:751:VAL:O	4:B:754:SER:HB2	1.95	0.66
3:A:306:ASN:HD21	3:A:324:SER:H	1.43	0.66
3:A:1193:LEU:HB2	3:A:1260:LEU:HD11	1.78	0.66
4:B:1001:PHE:CZ	4:B:1073:TYR:HB2	2.30	0.66
5:C:11:ARG:HH21	5:C:229:TYR:HD2	1.44	0.66
6:E:176:PRO:O	6:E:212:ARG:HA	1.95	0.66
3:A:736:ASN:O	3:A:737:LEU:C	2.38	0.65
3:A:751:SER:O	3:A:752:LYS:HG2	1.95	0.65
3:A:95:PHE:HE2	3:A:1414:ALA:HB2	1.62	0.65
3:A:102:VAL:HG21	3:A:234:MET:HE1	1.77	0.65
3:A:914:GLU:HB2	3:A:979:SER:O	1.95	0.65
3:A:715:GLU:O	3:A:719:VAL:HG23	1.96	0.65
4:B:128:LEU:HB3	4:B:167:ILE:O	1.95	0.65
4:B:211:VAL:HG23	4:B:483:LEU:HB2	1.78	0.65
4:B:603:LEU:HB3	4:B:609:ILE:HG13	1.76	0.65
7:F:111:LEU:HD12	7:F:111:LEU:H	1.62	0.65
5:C:8:VAL:HG12	5:C:9:LYS:H	1.60	0.65
12:L:51:CYS:O	12:L:53:HIS:N	2.28	0.65
1:R:8:G:N2	2:T:8:DT:N3	2.45	0.65
3:A:329:LEU:HD23	3:A:335:ARG:HG3	1.78	0.65
3:A:816:HIS:CE1	4:B:764:SER:HB2	2.30	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:994:GLN:HE22	3:A:1023:ARG:NE	1.95	0.65
4:B:293:PRO:HG2	4:B:296:GLU:HB2	1.79	0.65
9:I:111:THR:HG21	9:I:113:ASP:HB2	1.78	0.65
3:A:1242:VAL:HG12	3:A:1243:VAL:N	2.12	0.65
4:B:911:ILE:CG2	4:B:966:VAL:HG11	2.26	0.65
5:C:22:LEU:HD22	5:C:25:VAL:CG2	2.25	0.65
7:F:109:VAL:HG12	7:F:110:ASP:N	2.10	0.65
8:H:24:CYS:HB2	8:H:44:VAL:CG2	2.27	0.65
3:A:1319:VAL:HG13	3:A:1320:PRO:HD2	1.79	0.65
4:B:805:THR:HG21	4:B:815:ARG:HE	1.62	0.65
4:B:1197:PRO:HG2	4:B:1200:ALA:HB2	1.79	0.65
12:L:48:CYS:SG	12:L:49:LYS:N	2.70	0.65
14:R:3000:UTP:O2	2:T:4:DA:H2	1.80	0.65
4:B:101:MET:HE3	4:B:169:ARG:HH22	1.62	0.65
4:B:512:ARG:NH2	4:B:535:LEU:HD11	2.02	0.65
3:A:381:THR:HG21	3:A:383:TYR:CD1	2.31	0.65
4:B:120:ARG:CG	4:B:955:THR:HG21	2.23	0.65
4:B:1162:ILE:HD11	4:B:1194:ILE:HD13	1.77	0.65
8:H:40:LEU:HD13	8:H:123:MET:HE3	1.79	0.65
2:T:8:DT:OP2	2:T:8:DT:H71	1.97	0.64
4:B:824:ILE:CG1	10:J:48:ARG:HH12	2.08	0.64
10:J:9:SER:OG	10:J:48:ARG:NH2	2.30	0.64
3:A:541:ILE:HG21	3:A:549:MET:HE3	1.78	0.64
4:B:686:ASN:C	4:B:688:GLY:H	2.04	0.64
7:F:96:THR:O	7:F:100:GLN:HG3	1.97	0.64
7:F:109:VAL:HG21	7:F:124:GLU:HA	1.79	0.64
2:T:1:DA:N1	2:T:2:DC:H5	1.94	0.64
4:B:1170:THR:O	4:B:1170:THR:HG22	1.97	0.64
5:C:241:ASP:HB3	11:K:109:TRP:CE2	2.32	0.64
6:E:96:PHE:CZ	6:E:100:ILE:HD11	2.32	0.64
8:H:12:VAL:HA	8:H:28:ALA:CB	2.28	0.64
3:A:87:ALA:HB3	3:A:276:LEU:HD23	1.79	0.64
3:A:475:THR:HG22	3:A:476:SER:N	2.12	0.64
3:A:512:VAL:HA	3:A:519:PRO:HA	1.79	0.64
4:B:788:ARG:NH1	4:B:790:ASP:OD1	2.31	0.64
4:B:879:ARG:HB3	4:B:883:LEU:CD2	2.27	0.64
3:A:1035:TYR:O	3:A:1037:LEU:N	2.30	0.64
3:A:1224:LEU:HD12	3:A:1241:ARG:O	1.97	0.64
4:B:46:GLN:HE22	4:B:496:ARG:HA	1.62	0.64
4:B:649:LYS:HE2	4:B:738:PHE:O	1.96	0.64
8:H:107:VAL:HG21	8:H:126:GLU:HG3	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:901:LEU:HA	3:A:907:THR:HG23	1.80	0.64
3:A:1115:SER:HA	3:A:1308:THR:HG22	1.77	0.64
3:A:1394:THR:CG2	3:A:1395:GLY:N	2.61	0.64
4:B:25:ILE:HG22	4:B:29:ASP:HB2	1.79	0.64
4:B:1001:PHE:CE1	4:B:1073:TYR:HB2	2.33	0.64
5:C:114:TYR:CD2	5:C:140:ASN:HB3	2.32	0.64
2:T:4:DA:H2''	2:T:5:DT:H5'	1.80	0.64
3:A:443:LEU:CD2	3:A:455:MET:HE2	2.27	0.64
4:B:446:LEU:O	4:B:447:ALA:HB3	1.97	0.64
4:B:1072:MET:CE	4:B:1085:ILE:HB	2.28	0.64
6:E:124:VAL:HG22	6:E:132:ILE:HG21	1.78	0.64
3:A:84:ILE:HG23	3:A:239:LEU:HB3	1.80	0.64
3:A:244:PRO:CG	3:A:245:PRO:HD3	2.27	0.64
3:A:381:THR:CG2	3:A:383:TYR:H	2.09	0.64
4:B:842:ASN:HD21	4:B:844:SER:HB2	1.63	0.64
1:R:5:A:H2'	1:R:6:G:O4'	1.98	0.63
3:A:225:ASN:O	3:A:226:GLU:HG2	1.99	0.63
4:B:1034:VAL:HG23	4:B:1059:LEU:HB2	1.80	0.63
3:A:778:GLY:HA3	4:B:516:ASN:HB2	1.80	0.63
4:B:515:HIS:HD2	4:B:517:THR:OG1	1.81	0.63
4:B:519:TRP:C	4:B:519:TRP:CD1	2.76	0.63
3:A:1402:PHE:CD2	3:A:1403:GLU:HG3	2.33	0.63
3:A:1436:ILE:HB	4:B:1144:ALA:HB2	1.80	0.63
4:B:114:PRO:HG3	4:B:181:LEU:HD11	1.79	0.63
4:B:577:ALA:HB1	4:B:589:VAL:CG1	2.27	0.63
4:B:1201:LYS:O	4:B:1205:GLN:HG3	1.97	0.63
8:H:101:ALA:HB2	8:H:116:TYR:CE2	2.33	0.63
3:A:108:MET:O	3:A:109:HIS:HB2	1.99	0.63
3:A:1444:MET:HE1	7:F:135:ARG:CZ	2.29	0.63
4:B:525:ALA:O	4:B:527:THR:HG22	1.98	0.63
4:B:604:ARG:HG2	4:B:604:ARG:O	1.98	0.63
4:B:666:TYR:C	4:B:668:ASP:H	2.06	0.63
8:H:31:THR:O	8:H:32:THR:CB	2.47	0.63
3:A:579:SER:OG	3:A:612:ILE:HG22	1.97	0.63
3:A:709:THR:HB	3:A:712:GLU:H	1.64	0.63
4:B:1104:HIS:HB2	4:B:1122:ARG:HD2	1.80	0.63
6:E:100:ILE:HG23	6:E:105:PHE:HB2	1.80	0.63
3:A:523:ILE:HD12	3:A:622:VAL:HG22	1.79	0.63
7:F:86:THR:OG1	7:F:89:GLU:HG3	1.98	0.63
2:T:1:DA:H1'	3:A:1386:ARG:HH12	1.64	0.63
4:B:914:LYS:HB3	4:B:937:ALA:O	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:1187:ASN:OD1	4:B:1190:ASP:HB3	1.99	0.63
1:R:5:A:C4	1:R:6:G:N7	2.67	0.63
14:R:3000:UTP:N3	2:T:4:DA:N1	2.46	0.63
3:A:871:ASP:OD2	6:E:204:THR:HG23	1.99	0.63
3:A:1364:ASN:ND2	3:A:1364:ASN:C	2.56	0.63
4:B:913:GLY:HA2	4:B:938:SER:HB3	1.81	0.63
6:E:50:MET:HE3	6:E:50:MET:O	1.98	0.63
6:E:93:MET:HE3	6:E:120:ALA:O	1.98	0.63
6:E:96:PHE:O	6:E:100:ILE:HG13	1.99	0.63
6:E:156:LEU:HD12	6:E:195:VAL:HG12	1.81	0.63
2:T:11:DC:H2'	2:T:12:DG:C8	2.34	0.62
4:B:496:ARG:HH11	4:B:539:LEU:HB2	1.62	0.62
9:I:7:CYS:HB2	9:I:29:CYS:HB2	1.81	0.62
3:A:418:SER:O	3:A:419:LYS:C	2.39	0.62
3:A:871:ASP:HB3	6:E:204:THR:HG22	1.82	0.62
12:L:55:ILE:HG13	12:L:56:LEU:H	1.63	0.62
3:A:629:LEU:HD13	3:A:645:LEU:HD21	1.79	0.62
4:B:39:ARG:HE	4:B:665:GLU:HG2	1.64	0.62
4:B:780:VAL:HG21	10:J:56:LEU:CD1	2.29	0.62
4:B:1106:ARG:HD2	4:B:1126:GLY:O	1.99	0.62
6:E:157:SER:C	6:E:159:ASP:H	2.07	0.62
7:F:111:LEU:C	7:F:113:GLY:H	2.07	0.62
3:A:73:GLY:O	3:A:75:ASN:N	2.32	0.62
3:A:418:SER:O	3:A:420:ARG:N	2.32	0.62
3:A:523:ILE:HD12	3:A:622:VAL:HG21	1.80	0.62
3:A:982:THR:HG22	3:A:984:LYS:H	1.64	0.62
3:A:1074:GLU:HB3	3:A:1075:PRO:CD	2.29	0.62
5:C:166:GLU:HA	11:K:6:ARG:HB3	1.82	0.62
7:F:97:ARG:O	7:F:101:ILE:HG13	1.99	0.62
3:A:871:ASP:HB3	6:E:204:THR:CG2	2.30	0.62
3:A:1212:VAL:O	3:A:1216:ILE:HG13	1.99	0.62
4:B:1002:THR:HG23	4:B:1004:GLU:H	1.64	0.62
5:C:235:VAL:HG21	10:J:6:ARG:HH21	1.65	0.62
3:A:33:ALA:O	3:A:83:HIS:HB3	1.99	0.62
3:A:268:ASP:HB3	3:A:299:HIS:ND1	2.14	0.62
4:B:208:SER:OG	4:B:210:LYS:HD3	1.99	0.62
4:B:373:ARG:NE	4:B:567:GLU:OE2	2.29	0.62
2:T:11:DC:H2''	2:T:12:DG:C5'	2.29	0.62
3:A:672:ASP:OD1	3:A:674:PRO:HD2	2.00	0.62
4:B:195:CYS:HB3	4:B:782:LEU:HD22	1.81	0.62
4:B:549:THR:HB	4:B:628:THR:CG2	2.30	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:616:ILE:HD12	4:B:616:ILE:N	2.15	0.62
7:F:135:ARG:HG2	7:F:137:TYR:CE1	2.34	0.62
12:L:34:CYS:SG	12:L:51:CYS:SG	2.98	0.62
4:B:25:ILE:HG22	4:B:26:THR:H	1.65	0.62
6:E:93:MET:O	6:E:97:VAL:HG23	2.00	0.62
7:F:111:LEU:H	7:F:111:LEU:CD1	2.13	0.62
10:J:3:VAL:HG21	10:J:18:TRP:CG	2.34	0.62
3:A:328:ARG:O	3:A:335:ARG:HG2	1.99	0.61
3:A:338:GLY:HA2	4:B:1129:ARG:NH2	2.10	0.61
3:A:590:ARG:HB3	3:A:605:MET:H	1.63	0.61
4:B:221:ASN:OD1	4:B:242:SER:HA	1.98	0.61
4:B:446:LEU:O	4:B:447:ALA:CB	2.48	0.61
7:F:109:VAL:HG23	7:F:124:GLU:HG2	1.82	0.61
8:H:49:VAL:HG12	8:H:50:ALA:H	1.62	0.61
11:K:63:VAL:CG2	11:K:63:VAL:O	2.48	0.61
3:A:689:LYS:O	3:A:693:VAL:HG23	1.99	0.61
3:A:855:THR:CG2	3:A:857:ARG:HG3	2.30	0.61
3:A:898:ARG:HB2	3:A:933:TYR:CE1	2.34	0.61
3:A:1054:LEU:O	3:A:1057:VAL:HG23	1.99	0.61
4:B:29:ASP:HB3	4:B:658:ILE:CD1	2.30	0.61
4:B:101:MET:HE3	4:B:169:ARG:NH2	2.15	0.61
4:B:211:VAL:O	4:B:480:SER:HA	2.01	0.61
4:B:1072:MET:HE3	4:B:1085:ILE:CD1	2.30	0.61
1:R:9:G:OP1	4:B:776:GLN:NE2	2.33	0.61
3:A:354:SER:HA	3:A:482:PHE:CD2	2.34	0.61
3:A:549:MET:SD	3:A:577:ILE:CD1	2.87	0.61
3:A:961:ARG:O	3:A:965:GLN:HG3	2.00	0.61
4:B:1169:MET:HE1	4:B:1201:LYS:O	2.00	0.61
10:J:64:ASN:HB3	10:J:65:PRO:CD	2.29	0.61
3:A:709:THR:OG1	3:A:712:GLU:HG3	2.00	0.61
6:E:5:ASN:ND2	6:E:52:ARG:HG2	2.12	0.61
6:E:178:ILE:HG23	6:E:214:CYS:HA	1.81	0.61
3:A:789:LYS:HG3	9:I:67:THR:HB	1.83	0.61
3:A:1021:LEU:O	3:A:1025:ARG:HG2	2.00	0.61
3:A:1437:GLY:HA3	7:F:88:TYR:CD2	2.36	0.61
4:B:803:LEU:H	4:B:822:ASN:HD21	1.48	0.61
9:I:8:ARG:HG3	9:I:9:ASP:N	2.16	0.61
3:A:821:ARG:HG3	3:A:825:ILE:HD11	1.82	0.61
5:C:49:VAL:HG21	5:C:67:LEU:HD12	1.82	0.61
3:A:915:SER:O	3:A:919:ILE:HG13	2.00	0.61
4:B:582:VAL:HG22	4:B:626:ILE:HB	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:148:CYS:O	3:A:168:GLY:HA2	1.99	0.61
5:C:173:ALA:O	5:C:174:ALA:HB3	2.00	0.61
12:L:51:CYS:HB2	12:L:53:HIS:CD2	2.35	0.61
3:A:506:ALA:HB1	3:A:508:PRO:HD2	1.83	0.61
3:A:1192:LEU:HD22	3:A:1239:ARG:NH2	2.16	0.61
4:B:185:THR:HG23	4:B:188:ASP:OD2	2.01	0.61
5:C:131:HIS:O	5:C:132:PRO:C	2.43	0.61
7:F:138:LEU:HB3	7:F:139:PRO:HD2	1.83	0.61
8:H:89:LEU:HD22	8:H:91:ASP:CG	2.25	0.61
3:A:565:ILE:CG2	3:A:567:LYS:HG2	2.31	0.61
3:A:1317:MET:HA	3:A:1322:ILE:HD11	1.81	0.61
4:B:57:TYR:CD1	4:B:57:TYR:N	2.68	0.61
4:B:1102:LYS:O	4:B:1104:HIS:N	2.32	0.61
5:C:46:ILE:HA	5:C:159:ALA:HA	1.82	0.61
5:C:123:ASN:HD22	5:C:125:MET:HG2	1.66	0.61
3:A:337:ARG:CZ	3:A:839:ARG:NH1	2.64	0.60
3:A:738:LYS:HZ1	5:C:194:GLU:HA	1.66	0.60
3:A:824:LEU:O	3:A:827:THR:HB	2.00	0.60
4:B:1039:GLY:HA2	10:J:51:LEU:CD2	2.31	0.60
4:B:1138:MET:HE2	4:B:1146:PHE:CD2	2.36	0.60
8:H:15:VAL:HG22	8:H:26:ILE:HG12	1.83	0.60
3:A:306:ASN:OD1	3:A:324:SER:HB3	2.01	0.60
3:A:1365:TYR:O	3:A:1366:ARG:C	2.43	0.60
4:B:809:MET:HE1	4:B:983:ARG:NH2	2.16	0.60
4:B:995:ARG:NH1	4:B:995:ARG:HB2	2.16	0.60
3:A:219:PHE:O	3:A:222:LEU:N	2.33	0.60
3:A:401:GLY:C	3:A:435:HIS:CD2	2.79	0.60
3:A:445:ASN:HB2	3:A:454:SER:O	2.00	0.60
3:A:1132:LYS:O	3:A:1135:ARG:HB3	2.01	0.60
4:B:429:PHE:HA	4:B:432:MET:HE3	1.82	0.60
3:A:528:LEU:O	3:A:531:ILE:HG22	2.01	0.60
3:A:1293:SER:OG	3:A:1294:PRO:HD2	2.01	0.60
4:B:839:MET:HE3	4:B:1010:LEU:CD1	2.30	0.60
4:B:999:MET:HE2	4:B:1011:ILE:CD1	2.30	0.60
3:A:322:VAL:O	3:A:323:LYS:HG3	2.01	0.60
3:A:1158:PRO:HB3	3:A:1241:ARG:NH1	2.17	0.60
4:B:913:GLY:HA2	4:B:938:SER:CB	2.31	0.60
6:E:78:LEU:HD23	6:E:79:TRP:N	2.16	0.60
9:I:5:ARG:HD3	9:I:36:GLU:OE2	2.01	0.60
3:A:50:ILE:C	3:A:52:GLY:H	2.09	0.60
3:A:86:LEU:HA	3:A:273:ASN:OD1	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:567:LYS:O	3:A:569:LYS:N	2.35	0.60
3:A:1208:THR:O	3:A:1212:VAL:HG23	2.01	0.60
4:B:114:PRO:HB3	4:B:174:LEU:HD11	1.82	0.60
11:K:90:ALA:O	11:K:94:ILE:HG13	2.01	0.60
2:T:1:DA:C6	2:T:2:DC:C4	2.90	0.60
3:A:896:ARG:NH2	3:A:1030:ARG:HH21	2.00	0.60
6:E:47:CYS:HA	6:E:53:PRO:HA	1.83	0.60
7:F:101:ILE:HD12	7:F:121:ALA:HB2	1.82	0.60
3:A:1223:ASP:HA	3:A:1243:VAL:CG1	2.32	0.60
4:B:794:ASN:C	4:B:795:ILE:HD12	2.26	0.60
9:I:7:CYS:C	9:I:8:ARG:O	2.43	0.60
3:A:1115:SER:O	3:A:1329:THR:HG23	2.02	0.60
4:B:299:GLU:OE1	4:B:571:PRO:HG2	2.01	0.60
4:B:778:MET:CE	4:B:1094:ARG:HD3	2.32	0.60
4:B:787:VAL:O	4:B:787:VAL:HG12	2.00	0.60
8:H:106:GLU:C	8:H:108:SER:N	2.57	0.60
3:A:31:SER:OG	3:A:83:HIS:HB2	2.02	0.60
3:A:567:LYS:CG	3:A:568:PRO:HD2	2.31	0.60
3:A:779:PHE:CZ	4:B:517:THR:HA	2.37	0.60
9:I:85:PHE:CD1	9:I:99:LEU:HD22	2.37	0.60
2:T:1:DA:C6	2:T:2:DC:N4	2.70	0.59
3:A:503:GLN:HE21	7:F:90:ARG:HH21	1.47	0.59
4:B:198:ASP:OD1	4:B:485:ARG:NH2	2.34	0.59
4:B:479:VAL:HG12	4:B:480:SER:N	2.17	0.59
4:B:1174:LYS:HB2	4:B:1179:GLN:O	2.02	0.59
5:C:244:VAL:O	5:C:248:ILE:HG13	2.03	0.59
2:T:11:DC:H2'	2:T:12:DG:H8	1.66	0.59
3:A:68:GLN:HE22	3:A:80:HIS:HB3	1.67	0.59
3:A:1402:PHE:CE2	3:A:1403:GLU:HG3	2.37	0.59
9:I:15:TYR:O	9:I:27:PHE:HA	2.02	0.59
3:A:76:GLU:HG3	3:A:76:GLU:O	2.02	0.59
3:A:239:LEU:HD12	3:A:240:PRO:HD2	1.83	0.59
4:B:975:GLN:HG2	4:B:976:ILE:H	1.67	0.59
3:A:567:LYS:CB	3:A:568:PRO:CD	2.67	0.59
4:B:463:THR:HG22	4:B:465:ASN:HD22	1.66	0.59
8:H:84:ALA:HA	8:H:87:ARG:CG	2.32	0.59
2:T:1:DA:C2'	2:T:2:DC:O5'	2.38	0.59
3:A:469:ARG:NH2	4:B:976:ILE:HD13	2.17	0.59
3:A:68:GLN:HE22	3:A:80:HIS:CB	2.15	0.59
3:A:151:ASP:HA	3:A:162:VAL:O	2.02	0.59
4:B:217:ARG:NH1	4:B:407:ASP:OD1	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:512:ARG:NH2	4:B:535:LEU:CD1	2.61	0.59
4:B:778:MET:HE3	4:B:1094:ARG:HD3	1.84	0.59
5:C:56:THR:CG2	5:C:57:VAL:H	2.09	0.59
5:C:166:GLU:CG	11:K:10:PHE:HZ	2.14	0.59
8:H:24:CYS:HB2	8:H:44:VAL:HG21	1.84	0.59
12:L:26:THR:O	12:L:27:LEU:HB3	2.01	0.59
3:A:44:THR:O	3:A:44:THR:HG22	2.02	0.59
3:A:57:ARG:O	3:A:68:GLN:HG3	2.03	0.59
3:A:233:TRP:C	3:A:235:ILE:N	2.60	0.59
3:A:704:ALA:HB2	3:A:710:LEU:CG	2.23	0.59
4:B:90:ILE:HD12	4:B:432:MET:SD	2.42	0.59
4:B:211:VAL:CG2	4:B:483:LEU:HD13	2.32	0.59
4:B:642:ASP:O	4:B:644:GLU:N	2.36	0.59
4:B:912:ILE:HD11	4:B:966:VAL:HG23	1.84	0.59
12:L:70:ARG:HG2	12:L:70:ARG:HH11	1.66	0.59
3:A:93:VAL:HG11	3:A:308:ILE:CD1	2.33	0.59
3:A:1018:PHE:O	3:A:1021:LEU:HB3	2.03	0.59
3:A:1336:MET:CE	3:A:1381:LEU:HG	2.33	0.59
3:A:1385:THR:HG22	3:A:1386:ARG:H	1.68	0.59
6:E:29:PHE:HB2	6:E:65:THR:HG22	1.83	0.59
8:H:109:LYS:HB2	8:H:109:LYS:NZ	2.18	0.59
3:A:596:THR:O	3:A:598:LEU:N	2.36	0.59
3:A:809:THR:O	3:A:810:PRO:C	2.46	0.59
3:A:1004:ASN:ND2	6:E:167:ARG:HD2	2.18	0.59
3:A:1394:THR:HG22	3:A:1395:GLY:N	2.17	0.59
4:B:46:GLN:O	4:B:408:LEU:HD23	2.03	0.59
4:B:642:ASP:HB3	4:B:649:LYS:HD2	1.85	0.59
4:B:848:ARG:NH1	10:J:8:PHE:O	2.35	0.59
4:B:1117:GLN:HG3	4:B:1156:ASP:OD1	2.02	0.59
11:K:49:GLU:HG3	11:K:94:ILE:CG1	2.33	0.59
11:K:49:GLU:HG3	11:K:94:ILE:HG12	1.83	0.59
11:K:55:LYS:HB3	11:K:81:TYR:CD1	2.35	0.59
3:A:399:HIS:C	3:A:401:GLY:H	2.10	0.59
3:A:821:ARG:O	3:A:822:GLU:C	2.46	0.59
3:A:896:ARG:HD3	3:A:897:TYR:HE1	1.67	0.59
3:A:1444:MET:HE1	7:F:135:ARG:NE	2.18	0.59
4:B:1159:ARG:CD	4:B:1193:GLN:HE21	2.15	0.59
4:B:1171:VAL:CG1	4:B:1191:ILE:HD13	2.32	0.59
5:C:18:VAL:HG23	5:C:240:VAL:CG1	2.33	0.59
6:E:61:GLN:HB2	6:E:79:TRP:CE3	2.38	0.59
3:A:90:VAL:HG11	3:A:297:GLN:HA	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:385:ILE:HG22	3:A:386:ASP:N	2.18	0.58
3:A:482:PHE:CD1	4:B:836:GLU:HB2	2.38	0.58
3:A:840:ARG:HB3	3:A:1384:VAL:HG12	1.85	0.58
4:B:758:PHE:C	4:B:760:ASP:H	2.11	0.58
6:E:156:LEU:HD12	6:E:195:VAL:CG1	2.33	0.58
9:I:111:THR:CG2	9:I:113:ASP:HB2	2.33	0.58
3:A:756:ILE:HG22	3:A:757:ASN:N	2.17	0.58
3:A:901:LEU:H	3:A:926:GLN:HE21	1.50	0.58
3:A:107:CYS:HB2	3:A:114:LEU:CD2	2.32	0.58
3:A:444:PHE:HB3	3:A:458:HIS:HD2	1.68	0.58
3:A:1325:THR:O	6:E:148:GLU:HB2	2.04	0.58
4:B:806:THR:HB	4:B:809:MET:HG3	1.85	0.58
4:B:958:GLN:O	4:B:960:GLY:N	2.33	0.58
4:B:1106:ARG:HH12	4:B:1118:PRO:HB3	1.67	0.58
12:L:51:CYS:C	12:L:53:HIS:H	2.12	0.58
3:A:97:ALA:HA	3:A:100:LYS:HE3	1.84	0.58
3:A:663:SER:OG	3:A:664:THR:N	2.34	0.58
3:A:1308:THR:HG21	3:A:1310:GLY:O	2.04	0.58
4:B:28:GLU:CD	4:B:807:ARG:HH22	2.10	0.58
4:B:405:ARG:NH1	4:B:632:ARG:HG2	2.17	0.58
3:A:225:ASN:C	3:A:227:VAL:H	2.10	0.58
4:B:1168:LEU:HD13	4:B:1208:MET:HE3	1.86	0.58
8:H:12:VAL:HA	8:H:28:ALA:HB2	1.85	0.58
3:A:1161:THR:HG22	3:A:1163:ILE:N	2.03	0.58
4:B:287:ARG:NH1	4:B:324:ILE:O	2.37	0.58
4:B:779:GLY:HA2	4:B:796:LEU:HB2	1.85	0.58
6:E:46:TYR:HA	6:E:57:MET:SD	2.43	0.58
7:F:85:MET:HE1	7:F:148:VAL:HG13	1.84	0.58
10:J:48:ARG:HE	10:J:49:MET:CE	2.16	0.58
11:K:47:ARG:HD3	11:K:59:ALA:O	2.04	0.58
3:A:742:ASN:CA	3:A:745:GLN:HB2	2.33	0.58
3:A:1155:ASP:OD2	3:A:1161:THR:HG23	2.04	0.58
4:B:205:ILE:N	4:B:205:ILE:HD12	2.19	0.58
4:B:744:HIS:CD2	4:B:746:SER:H	2.13	0.58
9:I:16:PRO:HB3	9:I:27:PHE:CE2	2.38	0.58
12:L:49:LYS:O	12:L:50:ASP:HB2	2.03	0.58
3:A:225:ASN:ND2	3:A:227:VAL:HB	2.18	0.58
3:A:260:ASP:OD1	3:A:261:ASP:N	2.37	0.58
4:B:589:VAL:HG12	4:B:590:HIS:N	2.18	0.58
4:B:1201:LYS:HE2	4:B:1205:GLN:NE2	2.18	0.58
3:A:28:ARG:HG2	3:A:83:HIS:CE1	2.39	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:63:ARG:HA	3:A:74:MET:HE2	1.86	0.58
3:A:1042:PHE:HE2	3:A:1046:LEU:HD11	1.66	0.58
3:A:1074:GLU:O	3:A:1076:ALA:N	2.37	0.58
3:A:1149:ALA:HB2	9:I:47:GLU:HA	1.84	0.58
4:B:101:MET:HB2	4:B:169:ARG:HH12	1.69	0.58
4:B:955:THR:OG1	12:L:55:ILE:HA	2.04	0.58
7:F:127:GLU:O	7:F:129:LYS:HG3	2.03	0.58
9:I:47:GLU:OE1	9:I:50:THR:HG23	2.04	0.58
3:A:524:VAL:HG12	3:A:525:GLN:H	1.69	0.58
4:B:93:GLY:N	4:B:131:ASP:O	2.37	0.58
4:B:860:MET:HG2	4:B:861:ASP:N	2.18	0.58
4:B:980:PHE:CE1	4:B:990:ILE:HD11	2.39	0.58
4:B:1077:THR:HG22	4:B:1079:LYS:N	2.13	0.58
5:C:148:ARG:HG3	10:J:61:LEU:O	2.03	0.58
3:A:1341:ILE:HD12	3:A:1379:GLY:C	2.28	0.57
3:A:1420:ASP:O	3:A:1421:CYS:HB2	2.04	0.57
4:B:973:ILE:HG23	4:B:974:PRO:HD2	1.86	0.57
8:H:81:PRO:CB	8:H:82:PRO:CD	2.81	0.57
11:K:65:HIS:CD2	11:K:67:PHE:HB2	2.39	0.57
1:R:9:G:N1	1:R:10:A:C6	2.71	0.57
3:A:225:ASN:HD22	3:A:227:VAL:HB	1.69	0.57
3:A:714:PHE:HB2	9:I:97:MET:HE1	1.86	0.57
3:A:1143:LEU:HD23	3:A:1267:MET:HB3	1.86	0.57
4:B:803:LEU:N	4:B:822:ASN:HD21	2.02	0.57
4:B:855:PHE:HZ	4:B:857:ARG:HH11	1.52	0.57
4:B:1072:MET:HE3	4:B:1085:ILE:HB	1.86	0.57
5:C:175:ALA:HB3	10:J:43:ARG:NH2	2.20	0.57
6:E:213:ILE:HG23	6:E:213:ILE:O	2.04	0.57
7:F:81:THR:HG22	7:F:82:THR:N	2.18	0.57
9:I:29:CYS:C	9:I:31:THR:H	2.13	0.57
3:A:41:MET:HB3	3:A:48:ALA:O	2.04	0.57
3:A:1400:CYS:SG	3:A:1409:LEU:HG	2.44	0.57
4:B:25:ILE:HG22	4:B:29:ASP:CB	2.34	0.57
4:B:653:VAL:HG22	4:B:689:LEU:HB3	1.85	0.57
4:B:701:ILE:HD11	4:B:703:ILE:HD11	1.86	0.57
4:B:1147:LEU:HD22	4:B:1151:LEU:CD2	2.34	0.57
7:F:147:SER:HG	7:F:150:GLU:HG3	1.70	0.57
11:K:33:ILE:HD13	11:K:87:LEU:HD22	1.85	0.57
2:T:1:DA:C4	2:T:2:DC:C6	2.92	0.57
3:A:353:ILE:HG22	3:A:468:PHE:HB2	1.85	0.57
3:A:1399:ARG:CB	3:A:1408:ILE:HD13	2.28	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:E:61:GLN:HB2	6:E:79:TRP:HE3	1.69	0.57
8:H:139:ASN:O	8:H:140:ALA:HB2	2.02	0.57
9:I:78:CYS:SG	9:I:106:CYS:SG	3.02	0.57
3:A:92:HIS:HD2	3:A:94:GLY:H	1.53	0.57
3:A:337:ARG:CD	3:A:839:ARG:HH22	2.17	0.57
3:A:399:HIS:O	3:A:435:HIS:HD2	1.87	0.57
4:B:23:ALA:O	4:B:654:ARG:HB3	2.04	0.57
4:B:547:VAL:H	4:B:612:GLU:CD	2.12	0.57
4:B:1077:THR:CG2	4:B:1079:LYS:HB2	2.34	0.57
4:B:1079:LYS:HA	5:C:27:LEU:HD21	1.87	0.57
7:F:111:LEU:N	7:F:111:LEU:CD1	2.67	0.57
11:K:65:HIS:HD2	11:K:67:PHE:N	2.02	0.57
2:T:1:DA:C5	2:T:2:DC:C5	2.93	0.57
3:A:76:GLU:O	3:A:76:GLU:CG	2.53	0.57
3:A:901:LEU:N	3:A:926:GLN:NE2	2.50	0.57
5:C:251:LEU:O	5:C:255:VAL:HG23	2.04	0.57
3:A:1332:PHE:CD2	3:A:1332:PHE:N	2.72	0.57
4:B:801:LYS:O	10:J:52:THR:CG2	2.52	0.57
4:B:979:LYS:HG2	4:B:1095:LEU:HD12	1.87	0.57
4:B:1116:ARG:HD2	4:B:1198:TYR:CG	2.40	0.57
5:C:258:ILE:O	5:C:261:ALA:HB3	2.04	0.57
7:F:97:ARG:NE	7:F:124:GLU:OE1	2.31	0.57
11:K:46:ILE:HG22	11:K:50:LEU:HD12	1.86	0.57
2:T:1:DA:N3	2:T:2:DC:C5	2.71	0.57
3:A:537:ARG:HB2	8:H:20:TYR:CE2	2.39	0.57
3:A:879:GLU:OE2	3:A:962:ARG:NH2	2.37	0.57
3:A:1281:ARG:HB2	3:A:1309:ASP:HB2	1.86	0.57
3:A:1295:THR:HG23	3:A:1297:GLU:OE1	2.03	0.57
3:A:1315:GLU:O	3:A:1318:THR:HG23	2.04	0.57
3:A:1329:THR:HG22	3:A:1331:SER:N	2.01	0.57
3:A:1342:GLU:HG2	6:E:212:ARG:NH1	2.20	0.57
4:B:118:ARG:NH2	4:B:194:GLU:CD	2.60	0.57
4:B:756:ILE:O	4:B:759:PRO:HD3	2.04	0.57
5:C:37:MET:HG2	5:C:243:VAL:CG1	2.34	0.57
1:R:5:A:C4	1:R:6:G:C8	2.93	0.57
3:A:69:THR:HB	4:B:1174:LYS:HE2	1.87	0.57
3:A:101:LYS:O	3:A:105:CYS:HB2	2.04	0.57
3:A:414:ASP:O	3:A:417:TYR:O	2.22	0.57
3:A:710:LEU:HD12	3:A:710:LEU:N	2.20	0.57
3:A:882:SER:HA	3:A:952:ALA:O	2.05	0.57
11:K:50:LEU:CD1	11:K:73:LEU:HD21	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:6:DC:C5	2:T:7:DC:C5	2.93	0.57
3:A:93:VAL:HG22	3:A:301:ALA:HA	1.85	0.57
3:A:166:GLY:O	3:A:167:CYS:HB3	2.03	0.57
3:A:1359:ASP:C	3:A:1361:SER:H	2.13	0.57
4:B:57:TYR:N	4:B:57:TYR:HD1	2.03	0.57
6:E:35:VAL:C	6:E:37:LEU:H	2.12	0.57
8:H:6:PHE:HE1	8:H:130:ARG:HE	1.53	0.57
8:H:89:LEU:HD22	8:H:91:ASP:OD2	2.05	0.57
1:R:10:A:H61	2:T:6:DC:N4	2.03	0.56
3:A:672:ASP:HB3	3:A:675:THR:OG1	2.05	0.56
3:A:886:ILE:CD1	3:A:943:LEU:HB3	2.31	0.56
3:A:1342:GLU:HG3	6:E:198:ILE:HG21	1.86	0.56
3:A:1364:ASN:ND2	3:A:1366:ARG:N	2.53	0.56
4:B:130:VAL:HG12	4:B:131:ASP:H	1.67	0.56
7:F:87:LYS:HE2	7:F:88:TYR:CZ	2.39	0.56
3:A:40:THR:HG21	3:A:259:GLU:OE2	2.04	0.56
3:A:98:LYS:O	3:A:102:VAL:HG23	2.05	0.56
3:A:577:ILE:O	3:A:580:VAL:HG23	2.04	0.56
3:A:596:THR:O	3:A:597:LEU:C	2.47	0.56
4:B:1051:THR:HG22	4:B:1052:VAL:N	2.17	0.56
1:R:5:A:C2	1:R:6:G:C4	2.93	0.56
3:A:401:GLY:O	3:A:435:HIS:CD2	2.58	0.56
3:A:452:LYS:HB3	4:B:1141:HIS:CE1	2.40	0.56
3:A:1389:PHE:O	3:A:1392:SER:HB3	2.05	0.56
4:B:23:ALA:HB1	4:B:24:PRO:HD2	1.85	0.56
4:B:243:ALA:HA	4:B:250:PHE:O	2.05	0.56
4:B:311:LEU:HB3	9:I:4:PHE:CE2	2.40	0.56
4:B:429:PHE:HA	4:B:432:MET:CE	2.35	0.56
4:B:522:VAL:HG11	4:B:537:LYS:HB3	1.86	0.56
4:B:640:VAL:O	4:B:641:GLU:C	2.46	0.56
4:B:704:ALA:HB1	4:B:710:LEU:HD12	1.87	0.56
4:B:806:THR:C	4:B:808:ALA:H	2.12	0.56
5:C:229:TYR:N	5:C:229:TYR:CD1	2.74	0.56
5:C:242:GLN:HE21	5:C:246:ARG:HE	1.54	0.56
6:E:46:TYR:CE2	6:E:58:MET:HA	2.40	0.56
8:H:5:LEU:CD1	8:H:135:LEU:HG	2.34	0.56
8:H:82:PRO:O	8:H:83:GLN:HB2	2.04	0.56
8:H:89:LEU:C	8:H:91:ASP:N	2.55	0.56
8:H:97:MET:CE	8:H:142:LEU:HD23	2.35	0.56
9:I:7:CYS:O	9:I:8:ARG:O	2.24	0.56
10:J:1:MET:HG3	10:J:60:PHE:HE2	1.69	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:62:LYS:C	12:L:64:LEU:H	2.13	0.56
3:A:665:GLY:HA3	4:B:1086:PHE:CD1	2.41	0.56
3:A:1193:LEU:CD2	3:A:1267:MET:HE2	2.35	0.56
3:A:885:THR:HG22	3:A:885:THR:O	2.05	0.56
4:B:984:HIS:HB3	4:B:1022:THR:OG1	2.05	0.56
8:H:24:CYS:SG	8:H:44:VAL:HG21	2.44	0.56
5:C:99:LEU:HD23	5:C:99:LEU:N	2.20	0.56
3:A:35:ILE:HG12	3:A:52:GLY:O	2.06	0.56
3:A:547:LEU:HD22	11:K:58:PHE:CD1	2.41	0.56
3:A:875:ALA:HB2	3:A:1366:ARG:HD2	1.88	0.56
3:A:1300:LYS:NZ	3:A:1300:LYS:HB3	2.20	0.56
4:B:864:LYS:HD3	4:B:871:THR:OG1	2.05	0.56
8:H:84:ALA:C	8:H:86:ASP:H	2.13	0.56
11:K:51:LEU:HD13	11:K:59:ALA:HB3	1.86	0.56
3:A:185:TRP:CZ3	3:A:200:ARG:HG2	2.40	0.56
3:A:567:LYS:HZ2	8:H:46:LEU:HB2	1.70	0.56
4:B:839:MET:CE	4:B:980:PHE:HB2	2.35	0.56
5:C:242:GLN:NE2	5:C:246:ARG:HE	2.02	0.56
5:C:248:ILE:CD1	11:K:101:LEU:HD22	2.35	0.56
6:E:22:MET:HE1	6:E:135:PHE:CE2	2.40	0.56
3:A:1328:TYR:CG	3:A:1329:THR:N	2.74	0.56
4:B:361:LEU:N	4:B:362:PRO:CD	2.69	0.56
4:B:566:LEU:HD22	4:B:586:TRP:O	2.06	0.56
4:B:983:ARG:HD2	4:B:1091:TYR:HB3	1.86	0.56
4:B:1084:GLN:H	4:B:1084:GLN:CD	2.14	0.56
4:B:1180:PHE:O	4:B:1181:GLU:HB2	2.05	0.56
5:C:145:CYS:SG	5:C:146:LYS:N	2.79	0.56
6:E:121:MET:C	6:E:123:LEU:H	2.13	0.56
7:F:99:LEU:HD12	7:F:99:LEU:O	2.06	0.56
9:I:111:THR:CG2	9:I:112:SER:N	2.69	0.56
1:R:8:G:N2	2:T:8:DT:C4	2.74	0.56
3:A:233:TRP:C	3:A:235:ILE:H	2.13	0.56
3:A:825:ILE:HD12	4:B:513:GLN:NE2	2.21	0.56
3:A:1261:LYS:HA	3:A:1264:GLU:HB3	1.88	0.56
4:B:1022:THR:HG23	4:B:1022:THR:O	2.05	0.56
4:B:1171:VAL:HG11	4:B:1191:ILE:HD13	1.88	0.56
3:A:1017:LEU:HD23	6:E:204:THR:O	2.06	0.55
4:B:515:HIS:H	4:B:518:HIS:CD2	2.24	0.55
6:E:61:GLN:NE2	6:E:105:PHE:CE2	2.71	0.55
3:A:1351:GLU:O	3:A:1352:VAL:C	2.49	0.55
3:A:1436:ILE:HG22	4:B:1142:GLY:HA2	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:34:ILE:O	4:B:37:PHE:HB3	2.06	0.55
4:B:120:ARG:NH1	12:L:54:ARG:NH1	2.54	0.55
4:B:63:ILE:HA	4:B:421:PHE:CE2	2.42	0.55
4:B:556:THR:HG22	4:B:557:PHE:N	2.20	0.55
4:B:566:LEU:HD13	4:B:588:GLY:CA	2.37	0.55
4:B:980:PHE:HE1	4:B:990:ILE:HD11	1.70	0.55
8:H:59:ILE:HG22	8:H:60:ALA:N	2.20	0.55
3:A:216:VAL:O	3:A:219:PHE:HB2	2.06	0.55
3:A:346:ASP:CG	4:B:1108:ARG:HA	2.31	0.55
3:A:843:LYS:HG3	3:A:1402:PHE:HD1	1.72	0.55
4:B:898:LEU:HD22	4:B:964:VAL:HG11	1.89	0.55
5:C:162:GLY:HA3	5:C:170:TRP:CE2	2.41	0.55
10:J:21:TYR:HA	10:J:39:LEU:HD11	1.89	0.55
3:A:548:ASN:HA	11:K:60:ALA:HB1	1.87	0.55
3:A:974:ASP:HB2	8:H:136:LYS:NZ	2.20	0.55
3:A:1096:SER:O	3:A:1099:PRO:HG2	2.06	0.55
3:A:1339:LEU:HD13	6:E:147:HIS:CD2	2.41	0.55
4:B:120:ARG:HE	4:B:955:THR:CG2	2.20	0.55
4:B:121:ASN:N	4:B:121:ASN:ND2	2.50	0.55
4:B:864:LYS:N	4:B:872:GLU:OE1	2.39	0.55
6:E:157:SER:C	6:E:159:ASP:N	2.64	0.55
6:E:195:VAL:HG22	6:E:213:ILE:CB	2.37	0.55
9:I:111:THR:HG22	9:I:112:SER:N	2.19	0.55
12:L:26:THR:HG22	12:L:27:LEU:N	2.21	0.55
3:A:463:ILE:HD11	3:A:469:ARG:HG3	1.89	0.55
3:A:556:TRP:CE3	3:A:558:GLY:HA2	2.40	0.55
3:A:754:SER:O	3:A:755:PHE:C	2.48	0.55
3:A:838:GLN:O	3:A:842:VAL:HG23	2.06	0.55
3:A:963:ILE:HD12	3:A:1049:ILE:HG12	1.88	0.55
3:A:1349:TYR:C	3:A:1349:TYR:CD2	2.84	0.55
5:C:238:ILE:HG23	5:C:242:GLN:HB2	1.89	0.55
3:A:384:ASN:O	3:A:385:ILE:C	2.48	0.55
3:A:829:VAL:C	3:A:831:THR:H	2.15	0.55
3:A:1364:ASN:HD21	3:A:1366:ARG:HG2	1.67	0.55
5:C:55:THR:HB	5:C:152:GLU:H	1.70	0.55
5:C:57:VAL:HG11	10:J:60:PHE:HB2	1.88	0.55
5:C:70:ILE:HD11	5:C:144:ILE:HG12	1.88	0.55
8:H:89:LEU:O	8:H:91:ASP:N	2.37	0.55
3:A:556:TRP:CD2	3:A:558:GLY:HA2	2.42	0.55
4:B:25:ILE:HD11	4:B:653:VAL:HB	1.89	0.55
8:H:17:PRO:HB3	8:H:24:CYS:SG	2.47	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:61:TYR:HA	11:K:72:LYS:O	2.06	0.55
12:L:63:ARG:O	12:L:64:LEU:O	2.25	0.55
3:A:23:SER:HB3	3:A:233:TRP:CE2	2.41	0.55
4:B:35:SER:O	4:B:36:ALA:C	2.50	0.55
9:I:75:CYS:C	9:I:77:LYS:N	2.59	0.55
10:J:32:GLU:O	10:J:36:LEU:HG	2.07	0.55
3:A:89:PRO:O	3:A:204:THR:HG21	2.07	0.55
3:A:451:HIS:CE1	3:A:1074:GLU:HG3	2.42	0.55
3:A:517:ASN:ND2	3:A:1362:TYR:HE2	2.05	0.55
3:A:710:LEU:H	3:A:710:LEU:CD1	2.19	0.55
3:A:849:MET:HE3	3:A:1061:GLY:CA	2.35	0.55
4:B:308:TRP:CH2	9:I:45:ARG:HG2	2.43	0.55
6:E:195:VAL:HG22	6:E:213:ILE:HB	1.88	0.55
3:A:356:ASP:OD2	11:K:65:HIS:HE1	1.90	0.54
3:A:399:HIS:O	3:A:435:HIS:CD2	2.60	0.54
3:A:533:LYS:O	3:A:535:THR:N	2.40	0.54
3:A:885:THR:O	3:A:940:ARG:HG3	2.07	0.54
3:A:1308:THR:CG2	3:A:1310:GLY:O	2.54	0.54
4:B:195:CYS:CB	4:B:782:LEU:HD22	2.37	0.54
4:B:864:LYS:HG3	4:B:865:LYS:N	2.21	0.54
6:E:16:PHE:CD1	6:E:58:MET:HE2	2.42	0.54
3:A:337:ARG:NE	3:A:839:ARG:NH2	2.55	0.54
3:A:902:LEU:HD21	3:A:923:LEU:HD23	1.90	0.54
3:A:1116:LEU:O	3:A:1308:THR:HB	2.07	0.54
4:B:756:ILE:HG21	4:B:759:PRO:HB3	1.90	0.54
4:B:780:VAL:HG21	10:J:56:LEU:HD13	1.88	0.54
4:B:911:ILE:HD11	4:B:941:LEU:CD1	2.37	0.54
6:E:46:TYR:CD2	6:E:58:MET:HG2	2.42	0.54
8:H:84:ALA:HA	8:H:87:ARG:HG3	1.88	0.54
3:A:350:ARG:HB2	3:A:488:ASN:OD1	2.08	0.54
3:A:515:GLN:HG3	3:A:516:SER:N	2.22	0.54
3:A:741:ASN:ND2	3:A:743:VAL:H	2.05	0.54
4:B:1051:THR:CG2	4:B:1052:VAL:N	2.70	0.54
5:C:101:LEU:HD13	5:C:118:LEU:HD23	1.88	0.54
5:C:183:TRP:CZ2	5:C:207:CYS:HB3	2.42	0.54
6:E:168:TYR:HB3	6:E:170:LEU:CD2	2.36	0.54
7:F:118:LEU:O	7:F:122:MET:HG3	2.08	0.54
8:H:83:GLN:C	8:H:85:GLY:H	2.14	0.54
8:H:84:ALA:C	8:H:86:ASP:N	2.64	0.54
1:R:9:G:H1	1:R:10:A:N6	2.04	0.54
2:T:1:DA:H1'	3:A:1386:ARG:NH1	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:563:PRO:HG3	3:A:572:TRP:CE2	2.42	0.54
4:B:179:CYS:SG	4:B:181:LEU:HB2	2.47	0.54
4:B:1034:VAL:HG12	4:B:1035:ALA:N	2.23	0.54
5:C:13:ALA:O	11:K:114:LEU:HD13	2.08	0.54
6:E:197:LYS:HG3	6:E:211:TYR:CE2	2.42	0.54
12:L:27:LEU:HD13	12:L:37:LYS:HB3	1.90	0.54
2:T:3:DG:C5'	3:A:836:TYR:CD1	2.87	0.54
3:A:619:LYS:O	3:A:623:GLY:N	2.38	0.54
3:A:898:ARG:HD2	3:A:899:VAL:H	1.73	0.54
3:A:1341:ILE:HD12	3:A:1379:GLY:O	2.07	0.54
3:A:1375:MET:HG2	3:A:1382:THR:O	2.08	0.54
4:B:102:VAL:HG22	4:B:112:LEU:HD22	1.88	0.54
6:E:153:HIS:CE1	6:E:184:VAL:HG11	2.43	0.54
12:L:70:ARG:HG2	12:L:70:ARG:NH1	2.22	0.54
3:A:38:PRO:N	3:A:270:LEU:HD23	2.22	0.54
3:A:92:HIS:CD2	3:A:94:GLY:H	2.26	0.54
3:A:154:SER:HB3	3:A:162:VAL:HG23	1.89	0.54
3:A:760:GLN:HB2	4:B:1021:MET:HE1	1.89	0.54
3:A:1116:LEU:H	3:A:1308:THR:HG22	1.72	0.54
4:B:172:ILE:HD13	4:B:178:ASN:CB	2.37	0.54
4:B:1106:ARG:HH21	4:B:1109:GLY:C	2.16	0.54
3:A:15:LYS:HD2	4:B:1220:ARG:HE	1.72	0.54
3:A:852:TYR:CE2	7:F:136:ARG:HG2	2.42	0.54
4:B:708:GLU:C	4:B:710:LEU:H	2.16	0.54
4:B:783:THR:HA	10:J:60:PHE:HE1	1.72	0.54
4:B:784:ASN:ND2	4:B:788:ARG:HD2	2.23	0.54
4:B:837:ASP:OD1	4:B:1020:ARG:NH2	2.41	0.54
4:B:839:MET:HE1	4:B:980:PHE:HB2	1.89	0.54
6:E:176:PRO:HD2	6:E:211:TYR:O	2.07	0.54
7:F:109:VAL:HG13	7:F:127:GLU:OE1	2.07	0.54
11:K:10:PHE:HD1	11:K:11:LEU:HD13	1.67	0.54
1:R:9:G:C4	1:R:10:A:N7	2.76	0.54
3:A:367:PRO:HB3	3:A:465:TYR:O	2.08	0.54
7:F:72:LYS:N	7:F:142:SER:HA	2.22	0.54
1:R:8:G:C2'	1:R:9:G:H5'	2.36	0.54
3:A:226:GLU:HG2	3:A:227:VAL:HG23	1.90	0.54
3:A:590:ARG:O	3:A:591:PHE:HB2	2.08	0.54
3:A:646:PHE:O	3:A:650:GLN:HG3	2.08	0.54
3:A:867:ILE:HG22	3:A:872:GLY:N	2.22	0.54
4:B:406:LEU:HD12	4:B:545:ILE:HD11	1.89	0.54
4:B:680:THR:HG22	4:B:681:TRP:H	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:906:SER:O	4:B:907:GLY:C	2.50	0.54
10:J:7:CYS:O	10:J:8:PHE:C	2.50	0.54
3:A:1366:ARG:O	3:A:1369:ALA:HB3	2.08	0.54
4:B:288:ALA:HB1	4:B:331:LEU:CD1	2.38	0.54
4:B:549:THR:HB	4:B:628:THR:HG23	1.89	0.54
5:C:248:ILE:HD13	11:K:101:LEU:HD22	1.89	0.54
7:F:107:VAL:HG12	7:F:109:VAL:H	1.72	0.54
8:H:32:THR:HG22	8:H:33:GLN:HG3	1.90	0.54
9:I:2:THR:HG22	9:I:2:THR:O	2.07	0.54
3:A:567:LYS:NZ	8:H:95:TYR:CE1	2.71	0.53
3:A:738:LYS:HB2	3:A:740:LEU:HG	1.89	0.53
3:A:845:LEU:N	3:A:845:LEU:HD23	2.22	0.53
3:A:1073:GLY:O	3:A:1076:ALA:HB3	2.07	0.53
3:A:1222:ASN:O	3:A:1223:ASP:HB3	2.06	0.53
4:B:515:HIS:H	4:B:518:HIS:HD2	1.55	0.53
6:E:23:VAL:HG12	6:E:28:TYR:HB2	1.89	0.53
3:A:122:MET:O	3:A:126:LEU:HG	2.07	0.53
3:A:418:SER:C	3:A:420:ARG:N	2.63	0.53
3:A:608:ILE:HD12	3:A:613:ILE:CD1	2.39	0.53
3:A:819:GLY:O	3:A:820:GLY:C	2.49	0.53
3:A:1326:ARG:O	3:A:1327:ILE:C	2.49	0.53
6:E:78:LEU:HD21	6:E:109:ILE:HD12	1.90	0.53
7:F:94:LEU:HD21	7:F:122:MET:HA	1.89	0.53
10:J:52:THR:O	10:J:52:THR:HG22	2.08	0.53
3:A:89:PRO:C	3:A:204:THR:HG21	2.33	0.53
3:A:90:VAL:HG13	3:A:297:GLN:HA	1.90	0.53
3:A:114:LEU:HD22	3:A:171:GLN:NE2	2.23	0.53
3:A:741:ASN:C	3:A:741:ASN:ND2	2.62	0.53
4:B:235:SER:OG	4:B:236:HIS:HD2	1.91	0.53
4:B:644:GLU:HG3	4:B:654:ARG:HH22	1.74	0.53
4:B:755:ILE:CG2	4:B:755:ILE:O	2.55	0.53
4:B:842:ASN:HD22	4:B:845:SER:CB	2.21	0.53
5:C:46:ILE:HD13	5:C:157:CYS:CB	2.38	0.53
9:I:46:HIS:CD2	9:I:48:LEU:HD21	2.44	0.53
3:A:557:ASP:OD2	3:A:559:VAL:HB	2.08	0.53
4:B:292:ILE:H	4:B:293:PRO:HD2	1.73	0.53
11:K:63:VAL:O	11:K:63:VAL:HG23	2.08	0.53
3:A:852:TYR:CZ	7:F:136:ARG:HG2	2.44	0.53
3:A:1205:LYS:O	3:A:1207:LEU:N	2.41	0.53
9:I:29:CYS:SG	9:I:29:CYS:O	2.66	0.53
3:A:768:GLN:HG2	3:A:816:HIS:CA	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:405:ARG:HA	4:B:631:GLY:O	2.09	0.53
4:B:479:VAL:HG12	4:B:480:SER:H	1.72	0.53
4:B:542:MET:HE1	4:B:743:ILE:CG2	2.37	0.53
4:B:1069:PHE:HA	4:B:1085:ILE:O	2.08	0.53
4:B:1106:ARG:NH2	4:B:1109:GLY:C	2.67	0.53
4:B:1177:HIS:HB3	4:B:1179:GLN:HE21	1.74	0.53
5:C:189:THR:HG22	5:C:190:ASP:N	2.24	0.53
6:E:191:LYS:O	6:E:192:ARG:C	2.50	0.53
1:R:10:A:OP1	1:R:10:A:O5'	2.19	0.53
3:A:134:ARG:HH12	3:A:220:THR:HG22	1.74	0.53
3:A:1161:THR:HG22	3:A:1162:VAL:N	2.24	0.53
3:A:1365:TYR:O	3:A:1367:HIS:N	2.42	0.53
3:A:1375:MET:HE3	3:A:1384:VAL:HG23	1.91	0.53
4:B:120:ARG:HB2	4:B:122:LEU:HG	1.91	0.53
4:B:205:ILE:HD11	4:B:461:LEU:HD23	1.90	0.53
5:C:241:ASP:O	5:C:245:VAL:HG23	2.08	0.53
3:A:339:ASN:O	3:A:343:LYS:HG2	2.07	0.53
3:A:384:ASN:OD1	3:A:385:ILE:N	2.42	0.53
3:A:387:ARG:O	3:A:391:LEU:HG	2.09	0.53
3:A:552:TRP:NE1	3:A:655:PHE:CD1	2.77	0.53
3:A:1094:VAL:HG13	3:A:1113:THR:CG2	2.37	0.53
3:A:1220:PHE:O	3:A:1222:ASN:N	2.42	0.53
3:A:1225:PHE:CE2	3:A:1227:ILE:HD11	2.43	0.53
3:A:1392:SER:O	3:A:1393:ASN:CG	2.51	0.53
4:B:875:GLU:O	4:B:877:PRO:HD3	2.09	0.53
4:B:916:THR:HG22	4:B:918:ILE:HG13	1.90	0.53
4:B:956:THR:CG2	4:B:960:GLY:HA2	2.38	0.53
6:E:28:TYR:CE1	6:E:78:LEU:HD12	2.44	0.53
3:A:407:ARG:HD2	3:A:413:ILE:HD11	1.91	0.53
4:B:234:ILE:HG21	4:B:257:LYS:HB3	1.91	0.53
4:B:332:ASP:C	4:B:334:ILE:H	2.17	0.53
4:B:484:ASN:ND2	4:B:486:TYR:CD1	2.76	0.53
6:E:7:ARG:C	6:E:9:ILE:H	2.17	0.53
6:E:17:ARG:O	6:E:21:GLU:HG3	2.09	0.53
8:H:38:LEU:CD1	8:H:125:LEU:HD13	2.38	0.53
9:I:62:ILE:HG23	9:I:63:GLY:N	2.22	0.53
12:L:38:LEU:O	12:L:39:SER:CB	2.56	0.53
2:T:3:DG:H5'	3:A:836:TYR:HD1	1.70	0.53
3:A:376:TYR:C	3:A:376:TYR:CD2	2.87	0.53
3:A:442:VAL:O	3:A:457:ALA:HA	2.09	0.53
3:A:444:PHE:HB3	3:A:458:HIS:CD2	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:696:GLU:OE2	3:A:702:LEU:HD23	2.08	0.53
3:A:928:LEU:O	3:A:931:GLU:N	2.43	0.53
4:B:43:LEU:HD13	4:B:812:LEU:CD2	2.38	0.53
4:B:287:ARG:HA	4:B:291:ILE:O	2.09	0.53
1:R:9:G:C5	1:R:10:A:N7	2.76	0.52
3:A:337:ARG:CZ	3:A:839:ARG:HH12	2.22	0.52
4:B:463:THR:HG21	4:B:465:ASN:HD22	1.74	0.52
4:B:898:LEU:CD2	4:B:964:VAL:HG11	2.38	0.52
5:C:93:ASP:OD1	5:C:122:SER:HB2	2.09	0.52
8:H:6:PHE:O	8:H:58:THR:HA	2.08	0.52
3:A:167:CYS:HB2	3:A:169:ASN:ND2	2.24	0.52
3:A:507:VAL:N	3:A:508:PRO:CD	2.72	0.52
3:A:1299:VAL:CG1	3:A:1300:LYS:H	2.20	0.52
4:B:43:LEU:HD13	4:B:812:LEU:HD23	1.90	0.52
4:B:120:ARG:NH2	12:L:54:ARG:HD2	2.24	0.52
4:B:248:SER:O	4:B:249:ARG:HB2	2.09	0.52
4:B:542:MET:CG	4:B:747:MET:HE3	2.36	0.52
4:B:911:ILE:HD11	4:B:941:LEU:HD12	1.91	0.52
7:F:114:GLU:OE1	7:F:119:ARG:HG3	2.08	0.52
10:J:36:LEU:HD12	10:J:47:ARG:NH1	2.23	0.52
11:K:46:ILE:O	11:K:50:LEU:HB2	2.09	0.52
1:R:5:A:H2'	1:R:6:G:H8	1.70	0.52
4:B:563:MET:HE2	4:B:588:GLY:HA3	1.92	0.52
4:B:707:PRO:CG	4:B:708:GLU:H	2.21	0.52
5:C:164:ALA:HA	5:C:167:HIS:O	2.10	0.52
3:A:261:ASP:OD2	3:A:323:LYS:HD2	2.10	0.52
3:A:675:THR:CG2	3:A:736:ASN:HD21	2.22	0.52
3:A:859:SER:OG	3:A:1398:MET:HE1	2.09	0.52
3:A:907:THR:HG22	3:A:908:LEU:N	2.25	0.52
3:A:1017:LEU:O	3:A:1018:PHE:C	2.53	0.52
3:A:1074:GLU:C	3:A:1076:ALA:H	2.18	0.52
4:B:98:THR:OG1	4:B:127:GLY:HA3	2.09	0.52
4:B:287:ARG:HG2	4:B:292:ILE:CA	2.27	0.52
4:B:484:ASN:ND2	4:B:486:TYR:CE1	2.77	0.52
4:B:899:ILE:HD11	4:B:910:VAL:O	2.09	0.52
6:E:12:LEU:HD22	6:E:55:ARG:CZ	2.39	0.52
6:E:124:VAL:HG22	6:E:132:ILE:CG2	2.39	0.52
7:F:132:LEU:O	7:F:148:VAL:HG23	2.09	0.52
8:H:95:TYR:HE2	8:H:97:MET:HG3	1.73	0.52
3:A:451:HIS:CD2	3:A:1074:GLU:HG3	2.45	0.52
3:A:529:CYS:HB2	4:B:1015:HIS:CE1	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:271:ALA:HB3	4:B:285:ILE:CD1	2.40	0.52
4:B:293:PRO:HA	9:I:12:ASN:HD21	1.75	0.52
4:B:857:ARG:HD2	4:B:945:GLU:OE1	2.08	0.52
4:B:1065:GLN:NE2	4:B:1067:ARG:HG2	2.24	0.52
1:R:10:A:N6	2:T:6:DC:H42	2.06	0.52
3:A:225:ASN:O	3:A:227:VAL:HG23	2.09	0.52
3:A:670:ILE:HD13	4:B:1067:ARG:CZ	2.39	0.52
3:A:714:PHE:CB	9:I:97:MET:HE1	2.40	0.52
3:A:1147:THR:HA	3:A:1197:LEU:HD23	1.90	0.52
4:B:31:TRP:CD1	4:B:807:ARG:NH1	2.78	0.52
4:B:90:ILE:CD1	4:B:432:MET:SD	2.97	0.52
4:B:100:PRO:HG3	4:B:172:ILE:HD12	1.92	0.52
4:B:284:ILE:HD13	4:B:324:ILE:HD12	1.91	0.52
4:B:428:ILE:O	4:B:431:TYR:HB3	2.10	0.52
4:B:428:ILE:HG22	4:B:432:MET:HE2	1.91	0.52
9:I:103:CYS:SG	9:I:106:CYS:SG	2.99	0.52
3:A:901:LEU:HD23	3:A:907:THR:HG23	1.92	0.52
3:A:1319:VAL:CG1	3:A:1320:PRO:HD2	2.39	0.52
4:B:59:LEU:HD11	4:B:417:PHE:CZ	2.44	0.52
4:B:559:SER:HA	4:B:563:MET:HB3	1.91	0.52
4:B:1053:GLU:O	4:B:1054:GLY:C	2.50	0.52
11:K:49:GLU:OE2	11:K:97:LYS:HE3	2.10	0.52
3:A:22:PHE:HB2	4:B:1211:ASN:CG	2.35	0.52
3:A:91:PHE:HB2	3:A:297:GLN:OE1	2.09	0.52
3:A:134:ARG:NH1	3:A:220:THR:O	2.42	0.52
3:A:443:LEU:HD11	4:B:1138:MET:SD	2.50	0.52
3:A:666:ILE:O	3:A:667:GLY:C	2.53	0.52
3:A:821:ARG:HG3	3:A:825:ILE:CD1	2.40	0.52
3:A:1029:ARG:HH11	3:A:1029:ARG:HG3	1.74	0.52
3:A:1299:VAL:CG1	3:A:1300:LYS:N	2.72	0.52
4:B:25:ILE:HG22	4:B:26:THR:N	2.24	0.52
4:B:614:SER:OG	4:B:627:PHE:HB2	2.09	0.52
4:B:750:GLY:O	4:B:751:VAL:C	2.52	0.52
4:B:1084:GLN:HG2	5:C:201:TRP:CZ2	2.45	0.52
9:I:73:ARG:O	9:I:81:ARG:HA	2.09	0.52
3:A:167:CYS:C	3:A:169:ASN:H	2.18	0.52
3:A:817:ALA:HA	4:B:764:SER:OG	2.10	0.52
3:A:1116:LEU:N	3:A:1308:THR:HG22	2.25	0.52
3:A:1152:ILE:CG2	3:A:1260:LEU:HD23	2.38	0.52
4:B:287:ARG:CG	4:B:292:ILE:HA	2.26	0.52
4:B:542:MET:HG3	4:B:747:MET:CE	2.38	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:552:MET:N	4:B:553:PRO:HD2	2.24	0.52
4:B:648:HIS:NE2	4:B:650:GLU:OE1	2.43	0.52
3:A:49:LYS:HB3	3:A:55:ASP:HB2	1.92	0.52
3:A:738:LYS:HZ1	5:C:194:GLU:CA	2.22	0.52
3:A:849:MET:CE	3:A:1061:GLY:HA2	2.36	0.52
3:A:1444:MET:HE2	7:F:135:ARG:HB2	1.92	0.52
4:B:230:ALA:C	4:B:232:SER:H	2.17	0.52
4:B:825:VAL:HG12	4:B:826:ALA:N	2.24	0.52
7:F:77:ASP:O	7:F:78:GLN:HB2	2.09	0.52
1:R:9:G:C6	1:R:10:A:N7	2.78	0.51
2:T:1:DA:N6	2:T:2:DC:N4	2.58	0.51
3:A:326:ARG:HG2	3:A:1406:VAL:CG2	2.39	0.51
3:A:365:GLY:HA3	3:A:469:ARG:HB2	1.91	0.51
3:A:836:TYR:CE2	3:A:840:ARG:HD2	2.45	0.51
3:A:1214:GLU:O	3:A:1218:GLN:HG2	2.10	0.51
4:B:25:ILE:CG2	4:B:29:ASP:HB3	2.40	0.51
4:B:46:GLN:NE2	4:B:496:ARG:HA	2.25	0.51
4:B:864:LYS:HD3	4:B:871:THR:HA	1.91	0.51
4:B:879:ARG:HD3	4:B:885:MET:HE2	1.92	0.51
4:B:1098:MET:O	4:B:1099:VAL:C	2.53	0.51
6:E:58:MET:O	6:E:59:SER:C	2.53	0.51
12:L:38:LEU:HG	12:L:39:SER:N	2.25	0.51
3:A:13:THR:HG23	3:A:1432:GLN:NE2	2.24	0.51
3:A:50:ILE:HG22	3:A:51:GLY:N	2.24	0.51
3:A:568:PRO:HB2	5:C:221:TYR:CE1	2.45	0.51
3:A:1074:GLU:C	3:A:1076:ALA:N	2.67	0.51
3:A:1392:SER:O	3:A:1393:ASN:CB	2.58	0.51
4:B:240:ILE:HG23	4:B:240:ILE:O	2.09	0.51
4:B:321:GLY:C	4:B:323:VAL:H	2.17	0.51
4:B:827:ILE:HG12	4:B:1012:ILE:HD11	1.93	0.51
6:E:102:GLU:C	6:E:104:ASN:N	2.67	0.51
6:E:155:ARG:HD2	6:E:194:GLU:OE2	2.09	0.51
8:H:40:LEU:CD2	8:H:42:ILE:HD11	2.39	0.51
1:R:5:A:N1	1:R:6:G:C5	2.74	0.51
3:A:41:MET:HG2	3:A:49:LYS:HG2	1.92	0.51
3:A:384:ASN:OD1	3:A:388:LEU:HD12	2.10	0.51
3:A:1269:GLU:OE2	4:B:263:GLY:HA3	2.10	0.51
4:B:834:ASN:O	4:B:1013:ASN:HB2	2.10	0.51
5:C:263:THR:C	5:C:265:MET:H	2.18	0.51
3:A:737:LEU:HD11	3:A:758:ILE:HG21	1.92	0.51
7:F:109:VAL:CG1	7:F:110:ASP:N	2.73	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:9:SER:CB	10:J:45:CYS:HB2	2.40	0.51
1:R:9:G:C2	1:R:10:A:N7	2.79	0.51
3:A:219:PHE:O	3:A:222:LEU:O	2.28	0.51
3:A:357:PRO:HG2	4:B:833:TYR:CE1	2.45	0.51
3:A:530:GLY:O	3:A:531:ILE:C	2.54	0.51
3:A:847:ASP:OD2	3:A:858:ASN:HB2	2.10	0.51
3:A:1410:PHE:C	3:A:1412:ALA:N	2.68	0.51
3:A:1436:ILE:CG2	3:A:1437:GLY:N	2.72	0.51
4:B:332:ASP:C	4:B:334:ILE:N	2.68	0.51
4:B:737:THR:CG2	9:I:66:PRO:HB2	2.40	0.51
4:B:846:ILE:HD13	4:B:974:PRO:HG2	1.91	0.51
5:C:62:PHE:C	5:C:62:PHE:CD2	2.89	0.51
11:K:65:HIS:HD2	11:K:67:PHE:HB2	1.74	0.51
3:A:535:THR:HG23	3:A:575:LYS:HE2	1.93	0.51
3:A:722:LEU:HD11	3:A:794:PRO:HB3	1.91	0.51
3:A:858:ASN:C	3:A:858:ASN:ND2	2.68	0.51
3:A:898:ARG:HD2	3:A:899:VAL:N	2.26	0.51
3:A:1410:PHE:CE2	4:B:1212:ILE:HD11	2.45	0.51
4:B:751:VAL:HG12	4:B:752:ALA:N	2.26	0.51
4:B:864:LYS:HG2	4:B:871:THR:HG23	1.93	0.51
4:B:1106:ARG:HH12	4:B:1118:PRO:CB	2.24	0.51
4:B:1169:MET:HE3	4:B:1205:GLN:HG2	1.93	0.51
9:I:50:THR:HG22	9:I:52:ILE:H	1.75	0.51
9:I:75:CYS:O	9:I:77:LYS:N	2.44	0.51
1:R:9:G:N1	1:R:10:A:C5	2.79	0.51
3:A:340:LEU:HD21	4:B:1200:ALA:CB	2.40	0.51
3:A:567:LYS:HD2	3:A:568:PRO:HD2	1.92	0.51
3:A:810:PRO:O	3:A:813:PHE:HB3	2.11	0.51
3:A:929:LEU:H	3:A:929:LEU:CD2	2.23	0.51
3:A:1166:ASP:CG	3:A:1194:ARG:HH21	2.19	0.51
3:A:1312:ASN:O	3:A:1316:VAL:HG23	2.11	0.51
3:A:1376:THR:HG23	6:E:212:ARG:NH2	2.26	0.51
5:C:5:GLY:O	5:C:6:PRO:C	2.54	0.51
6:E:23:VAL:HG13	6:E:28:TYR:CD1	2.45	0.51
7:F:101:ILE:HD13	7:F:120:ILE:HG22	1.92	0.51
3:A:96:ILE:O	3:A:100:LYS:HG3	2.10	0.51
3:A:649:ILE:O	3:A:653:VAL:HG23	2.11	0.51
3:A:715:GLU:OE2	3:A:774:ARG:NH1	2.43	0.51
3:A:751:SER:O	3:A:752:LYS:CG	2.59	0.51
3:A:753:GLY:HA2	3:A:757:ASN:HD22	1.74	0.51
4:B:130:VAL:CG2	4:B:167:ILE:HD12	2.33	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:563:MET:HG3	4:B:563:MET:O	2.10	0.51
10:J:7:CYS:SG	10:J:9:SER:HB2	2.50	0.51
12:L:32:ALA:HB3	12:L:55:ILE:CD1	2.26	0.51
12:L:40:LEU:HD13	12:L:44:ASP:OD1	2.11	0.51
3:A:329:LEU:HD22	4:B:1203:LEU:CD1	2.41	0.51
4:B:283:VAL:HG13	4:B:297:ILE:CD1	2.41	0.51
4:B:314:LEU:O	4:B:315:LYS:C	2.53	0.51
4:B:755:ILE:O	4:B:755:ILE:HG22	2.09	0.51
4:B:1163:CYS:SG	4:B:1182:CYS:SG	3.08	0.51
5:C:33:LEU:HG	5:C:37:MET:CE	2.41	0.51
5:C:177:GLU:HG3	5:C:231:ASN:HB3	1.93	0.51
6:E:205:SER:O	6:E:206:GLY:C	2.54	0.51
10:J:14:VAL:HG12	10:J:50:ILE:HD11	1.92	0.51
10:J:54:VAL:O	10:J:56:LEU:N	2.43	0.51
11:K:91:CYS:O	11:K:95:ILE:HG13	2.11	0.51
11:K:101:LEU:O	11:K:101:LEU:HD23	2.11	0.51
12:L:27:LEU:HD13	12:L:37:LYS:CG	2.41	0.51
3:A:675:THR:HG21	3:A:736:ASN:HD21	1.76	0.51
3:A:795:GLU:HG2	4:B:731:VAL:HG21	1.93	0.51
3:A:1384:VAL:HG12	3:A:1384:VAL:O	2.11	0.51
4:B:195:CYS:SG	4:B:197:PHE:HB2	2.51	0.51
4:B:271:ALA:O	4:B:279:ASP:HA	2.11	0.51
4:B:890:TYR:C	4:B:892:LYS:H	2.19	0.51
6:E:46:TYR:HE2	6:E:58:MET:HA	1.76	0.51
7:F:109:VAL:CG2	7:F:124:GLU:HG2	2.40	0.51
9:I:25:LEU:HD12	9:I:26:LEU:H	1.76	0.51
10:J:36:LEU:HD13	10:J:47:ARG:HG2	1.92	0.51
3:A:587:HIS:HA	3:A:607:ILE:O	2.11	0.50
3:A:1364:ASN:ND2	3:A:1366:ARG:HH11	2.09	0.50
4:B:130:VAL:CG1	4:B:131:ASP:N	2.74	0.50
4:B:234:ILE:H	4:B:234:ILE:CD1	2.16	0.50
4:B:1035:ALA:HB1	4:B:1040:ASN:O	2.10	0.50
4:B:1119:VAL:O	4:B:1126:GLY:HA3	2.11	0.50
4:B:1197:PRO:HG2	4:B:1200:ALA:CB	2.40	0.50
8:H:138:GLU:O	8:H:139:ASN:C	2.53	0.50
10:J:32:GLU:CD	10:J:32:GLU:H	2.19	0.50
11:K:24:ASP:HB3	11:K:30:ALA:HB3	1.93	0.50
11:K:61:TYR:CD1	11:K:61:TYR:C	2.89	0.50
1:R:5:A:C2'	1:R:6:G:O4'	2.60	0.50
3:A:107:CYS:HB2	3:A:114:LEU:HD23	1.93	0.50
3:A:540:PHE:C	3:A:541:ILE:HD12	2.35	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1376:THR:HG23	3:A:1376:THR:O	2.12	0.50
4:B:292:ILE:N	4:B:293:PRO:HD2	2.25	0.50
4:B:642:ASP:HB3	4:B:649:LYS:CD	2.41	0.50
4:B:756:ILE:CG2	4:B:759:PRO:HB3	2.42	0.50
4:B:975:GLN:O	4:B:990:ILE:HD12	2.12	0.50
4:B:1096:ARG:O	4:B:1097:HIS:CB	2.59	0.50
12:L:47:ARG:HG2	12:L:52:GLY:CA	2.39	0.50
3:A:105:CYS:SG	3:A:138:ILE:HG22	2.52	0.50
3:A:444:PHE:CB	3:A:458:HIS:HD2	2.24	0.50
3:A:1362:TYR:OH	3:A:1364:ASN:HA	2.11	0.50
4:B:653:VAL:C	4:B:654:ARG:HG2	2.36	0.50
5:C:62:PHE:C	5:C:62:PHE:HD2	2.20	0.50
6:E:5:ASN:O	6:E:9:ILE:HG13	2.11	0.50
10:J:16:ASP:OD1	10:J:17:LYS:HE3	2.12	0.50
3:A:32:VAL:HG21	3:A:68:GLN:HE22	1.74	0.50
3:A:852:TYR:OH	7:F:89:GLU:OE2	2.28	0.50
3:A:1116:LEU:HD12	3:A:1329:THR:HG1	1.72	0.50
4:B:185:THR:O	4:B:189:LEU:HG	2.11	0.50
4:B:514:LEU:HD12	4:B:515:HIS:H	1.74	0.50
4:B:577:ALA:HB1	4:B:589:VAL:HG11	1.91	0.50
4:B:758:PHE:C	4:B:760:ASP:N	2.68	0.50
4:B:1200:ALA:O	4:B:1201:LYS:C	2.54	0.50
5:C:254:LYS:HE2	11:K:42:LEU:HD13	1.94	0.50
3:A:27:VAL:HG13	3:A:240:PRO:HB3	1.92	0.50
3:A:167:CYS:O	3:A:169:ASN:N	2.45	0.50
3:A:893:PHE:CE1	3:A:940:ARG:HD2	2.46	0.50
3:A:1410:PHE:C	3:A:1412:ALA:H	2.19	0.50
4:B:542:MET:HE2	4:B:747:MET:HE2	1.93	0.50
4:B:581:PHE:HB2	4:B:625:LYS:HG2	1.93	0.50
4:B:911:ILE:HD11	4:B:941:LEU:HB2	1.94	0.50
5:C:66:ARG:NH2	10:J:2:ILE:CG2	2.74	0.50
6:E:168:TYR:HB3	6:E:170:LEU:CG	2.41	0.50
8:H:31:THR:O	8:H:32:THR:HB	2.11	0.50
9:I:75:CYS:O	9:I:76:PRO:C	2.52	0.50
3:A:500:GLU:OE1	4:B:1143:ALA:HB1	2.11	0.50
3:A:644:LYS:O	3:A:645:LEU:C	2.55	0.50
3:A:683:ILE:HD11	3:A:764:CYS:CB	2.36	0.50
3:A:1142:THR:O	3:A:1273:LEU:HD22	2.12	0.50
4:B:653:VAL:CG2	4:B:689:LEU:HB3	2.42	0.50
4:B:686:ASN:C	4:B:688:GLY:N	2.70	0.50
4:B:858:SER:HA	4:B:966:VAL:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:977:GLY:CA	4:B:1099:VAL:CG2	2.86	0.50
4:B:977:GLY:C	4:B:1099:VAL:HG23	2.37	0.50
9:I:8:ARG:HG3	9:I:9:ASP:CG	2.37	0.50
9:I:68:LEU:HB3	9:I:84:VAL:HG22	1.94	0.50
9:I:101:PHE:O	9:I:109:ILE:HA	2.12	0.50
3:A:306:ASN:HD21	3:A:324:SER:N	2.08	0.50
3:A:1134:ILE:O	3:A:1138:ILE:HG13	2.12	0.50
4:B:271:ALA:HB3	4:B:285:ILE:HD11	1.93	0.50
4:B:1177:HIS:CB	4:B:1179:GLN:HE21	2.24	0.50
5:C:77:ILE:HG23	5:C:161:LYS:HE3	1.94	0.50
8:H:47:PHE:HB2	8:H:95:TYR:HD1	1.76	0.50
1:R:8:G:C2	2:T:8:DT:N3	2.79	0.50
1:R:10:A:C3'	14:R:3000:UTP:O1A	2.60	0.50
3:A:100:LYS:NZ	3:A:176:LYS:HD2	2.27	0.50
3:A:542:GLU:C	3:A:546:VAL:HG23	2.36	0.50
3:A:573:SER:O	3:A:576:GLN:HB2	2.11	0.50
3:A:1046:LEU:O	3:A:1047:SER:C	2.55	0.50
4:B:365:THR:HG23	4:B:367:LEU:HG	1.93	0.50
4:B:800:GLN:OE1	4:B:822:ASN:HB2	2.12	0.50
8:H:128:ASN:O	8:H:131:ASN:ND2	2.45	0.50
9:I:99:LEU:HB2	9:I:112:SER:HB3	1.94	0.50
3:A:135:PHE:HD1	3:A:222:LEU:HD22	1.76	0.50
3:A:376:TYR:OH	3:A:498:ARG:HD2	2.11	0.50
3:A:612:ILE:HG23	3:A:612:ILE:O	2.12	0.50
3:A:709:THR:C	3:A:711:ARG:N	2.67	0.50
3:A:709:THR:CB	3:A:712:GLU:HG3	2.41	0.50
3:A:888:GLY:O	3:A:940:ARG:NH2	2.44	0.50
4:B:260:GLY:O	4:B:267:ARG:HD3	2.12	0.50
4:B:1159:ARG:CD	4:B:1193:GLN:HG3	2.31	0.50
5:C:11:ARG:NH2	5:C:229:TYR:CD2	2.68	0.50
6:E:54:GLN:O	6:E:57:MET:HB3	2.11	0.50
3:A:738:LYS:HZ1	5:C:194:GLU:C	2.20	0.49
3:A:738:LYS:NZ	5:C:194:GLU:HA	2.26	0.49
3:A:808:LEU:O	4:B:728:ARG:NH1	2.43	0.49
3:A:1405:THR:O	3:A:1406:VAL:C	2.54	0.49
4:B:737:THR:CG2	9:I:66:PRO:CB	2.89	0.49
5:C:18:VAL:HG12	5:C:20:PHE:HD2	1.76	0.49
6:E:80:VAL:HG22	6:E:109:ILE:HD12	1.94	0.49
6:E:98:ILE:O	6:E:102:GLU:HG3	2.12	0.49
6:E:102:GLU:C	6:E:104:ASN:H	2.20	0.49
6:E:177:ARG:O	6:E:212:ARG:HD3	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:F:82:THR:HG22	7:F:84:TYR:N	2.27	0.49
8:H:6:PHE:HE1	8:H:130:ARG:NE	2.10	0.49
9:I:15:TYR:N	9:I:15:TYR:CD1	2.79	0.49
3:A:394:ASN:OD1	3:A:398:GLU:OE1	2.30	0.49
3:A:1189:SER:OG	3:A:1190:PRO:HD2	2.12	0.49
3:A:1300:LYS:HB3	3:A:1300:LYS:HZ3	1.77	0.49
4:B:240:ILE:O	4:B:253:THR:HG23	2.11	0.49
4:B:269:ILE:CD1	4:B:386:LEU:HD21	2.39	0.49
4:B:579:ARG:HB2	4:B:586:TRP:NE1	2.27	0.49
4:B:844:SER:OG	4:B:996:ARG:N	2.33	0.49
4:B:873:THR:O	4:B:914:LYS:HA	2.13	0.49
4:B:896:ASP:OD2	12:L:58:LYS:HE3	2.13	0.49
5:C:22:LEU:CD1	5:C:230:MET:HE1	2.42	0.49
7:F:133:VAL:HG22	7:F:147:SER:HA	1.95	0.49
12:L:62:LYS:O	12:L:64:LEU:HG	2.11	0.49
3:A:74:MET:O	3:A:75:ASN:HB2	2.13	0.49
3:A:185:TRP:HZ3	3:A:200:ARG:HG2	1.74	0.49
3:A:332:LYS:HG3	3:A:333:GLU:HG2	1.94	0.49
3:A:567:LYS:NZ	8:H:46:LEU:CB	2.67	0.49
3:A:741:ASN:ND2	3:A:743:VAL:N	2.61	0.49
3:A:1150:SER:HB2	3:A:1195:LEU:HD23	1.92	0.49
3:A:1410:PHE:HD2	4:B:1212:ILE:HD11	1.70	0.49
4:B:25:ILE:CG2	4:B:29:ASP:CB	2.90	0.49
5:C:43:THR:CG2	5:C:44:LEU:N	2.75	0.49
8:H:88:SER:O	8:H:89:LEU:HG	2.12	0.49
9:I:75:CYS:C	9:I:77:LYS:H	2.20	0.49
11:K:97:LYS:O	11:K:100:ALA:HB3	2.12	0.49
3:A:15:LYS:CB	4:B:1220:ARG:HG2	2.33	0.49
3:A:538:ASP:OD1	8:H:22:LYS:HB2	2.13	0.49
3:A:1284:MET:HG2	3:A:1306:LEU:CD2	2.43	0.49
4:B:283:VAL:O	4:B:286:PHE:HB2	2.11	0.49
4:B:377:PHE:C	4:B:379:GLY:N	2.68	0.49
4:B:515:HIS:O	4:B:516:ASN:C	2.54	0.49
4:B:660:LYS:O	4:B:663:ALA:HB3	2.13	0.49
11:K:78:THR:O	11:K:79:GLU:C	2.56	0.49
12:L:52:GLY:O	12:L:54:ARG:HG3	2.12	0.49
3:A:418:SER:HB3	3:A:421:ALA:HB2	1.94	0.49
3:A:466:SER:HB3	11:K:2:ASN:ND2	2.27	0.49
3:A:545:GLN:O	3:A:548:ASN:N	2.44	0.49
3:A:589:GLN:OE1	3:A:591:PHE:HE1	1.96	0.49
3:A:606:LEU:HB2	3:A:614:PHE:CE2	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:783:THR:HG21	3:A:815:PHE:CE2	2.48	0.49
3:A:834:THR:HG21	3:A:1077:THR:CA	2.43	0.49
3:A:873:MET:HE3	3:A:957:PRO:HG3	1.94	0.49
3:A:1155:ASP:CG	3:A:1162:VAL:HG23	2.37	0.49
4:B:635:ARG:NH1	4:B:742:GLU:OE2	2.46	0.49
8:H:76:THR:O	8:H:76:THR:HG22	2.11	0.49
3:A:391:LEU:O	3:A:394:ASN:N	2.46	0.49
4:B:108:VAL:CG1	4:B:109:THR:N	2.76	0.49
4:B:485:ARG:NH2	4:B:782:LEU:HD11	2.27	0.49
4:B:734:HIS:O	4:B:735:ALA:HB2	2.12	0.49
4:B:957:ASN:O	4:B:958:GLN:C	2.55	0.49
8:H:49:VAL:CG1	8:H:50:ALA:N	2.74	0.49
9:I:55:THR:HG21	9:I:109:ILE:HD13	1.93	0.49
3:A:31:SER:HB2	3:A:83:HIS:HB2	1.91	0.49
3:A:474:VAL:HG13	3:A:478:TYR:CE1	2.48	0.49
3:A:491:VAL:O	3:A:493:GLN:NE2	2.46	0.49
3:A:857:ARG:HG2	3:A:863:VAL:HA	1.94	0.49
3:A:1001:ARG:HG2	3:A:1001:ARG:HH11	1.77	0.49
3:A:1153:TYR:HA	9:I:41:PRO:O	2.12	0.49
4:B:1043:ASP:O	4:B:1050:ILE:HD12	2.13	0.49
7:F:82:THR:HG22	7:F:84:TYR:H	1.77	0.49
8:H:84:ALA:HB1	8:H:87:ARG:HB2	1.94	0.49
2:T:5:DT:H2''	2:T:6:DC:H5'	1.95	0.49
2:T:6:DC:H4'	3:A:447:GLN:CD	2.37	0.49
3:A:54:ASN:HA	3:A:58:LEU:HD12	1.95	0.49
3:A:61:ILE:HA	3:A:74:MET:SD	2.53	0.49
3:A:78:PRO:O	3:A:79:GLY:C	2.56	0.49
3:A:1068:ALA:O	3:A:1069:ALA:C	2.55	0.49
3:A:1364:ASN:HD21	3:A:1366:ARG:HH11	1.61	0.49
3:A:1415:SER:O	3:A:1416:ALA:C	2.55	0.49
4:B:821:GLN:OE1	4:B:850:LEU:HD12	2.13	0.49
4:B:958:GLN:C	4:B:960:GLY:H	2.20	0.49
4:B:1208:MET:HA	4:B:1212:ILE:O	2.12	0.49
5:C:4:GLU:O	5:C:5:GLY:O	2.31	0.49
5:C:142:VAL:H	10:J:16:ASP:HB3	1.77	0.49
6:E:102:GLU:O	6:E:104:ASN:N	2.46	0.49
1:R:2:U:C4	1:R:3:C:C4	3.01	0.49
2:T:10:DT:H2''	2:T:11:DC:H5'	1.93	0.49
4:B:351:TYR:O	4:B:355:ILE:HG13	2.13	0.49
4:B:653:VAL:HG12	4:B:654:ARG:N	2.28	0.49
4:B:709:ASP:C	4:B:710:LEU:HD23	2.38	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:890:TYR:O	4:B:892:LYS:N	2.46	0.49
4:B:1077:THR:HG22	4:B:1079:LYS:HB2	1.94	0.49
4:B:1118:PRO:HD3	4:B:1155:SER:HA	1.95	0.49
5:C:67:LEU:HD11	5:C:155:LEU:HD13	1.95	0.49
8:H:59:ILE:O	8:H:60:ALA:HB3	2.12	0.49
10:J:44:TYR:HA	10:J:47:ARG:HB2	1.94	0.49
10:J:48:ARG:NH2	10:J:49:MET:HE1	2.20	0.49
3:A:13:THR:HG23	3:A:1432:GLN:CD	2.38	0.49
3:A:1066:VAL:O	3:A:1067:LEU:C	2.56	0.49
4:B:726:ALA:HB1	4:B:1051:THR:HG21	1.95	0.49
7:F:87:LYS:HE2	7:F:88:TYR:CE1	2.48	0.49
8:H:118:PHE:HB2	8:H:121:LEU:HB2	1.95	0.49
1:R:5:A:N1	2:T:10:DT:O4	2.46	0.48
3:A:666:ILE:CD1	4:B:1030:LEU:HD22	2.41	0.48
3:A:1100:ARG:NH2	3:A:1330:ASN:HB2	2.28	0.48
3:A:1406:VAL:CG1	3:A:1410:PHE:HE1	2.26	0.48
4:B:487:THR:O	4:B:488:TYR:C	2.56	0.48
4:B:526:GLU:CD	4:B:752:ALA:HB3	2.38	0.48
4:B:726:ALA:HB1	4:B:1051:THR:CG2	2.43	0.48
4:B:1160:VAL:HG11	4:B:1169:MET:SD	2.53	0.48
5:C:236:GLY:C	5:C:238:ILE:N	2.69	0.48
3:A:332:LYS:H	3:A:337:ARG:HD2	1.76	0.48
3:A:563:PRO:HG3	3:A:572:TRP:CH2	2.48	0.48
3:A:567:LYS:HZ2	8:H:46:LEU:CB	2.27	0.48
3:A:1066:VAL:O	3:A:1068:ALA:N	2.46	0.48
3:A:1099:PRO:O	3:A:1102:LYS:HB3	2.13	0.48
3:A:1394:THR:CG2	3:A:1398:MET:HE3	2.40	0.48
4:B:284:ILE:CD1	4:B:324:ILE:HD12	2.43	0.48
4:B:1054:GLY:O	4:B:1058:LEU:HG	2.13	0.48
7:F:81:THR:HG22	7:F:82:THR:H	1.78	0.48
8:H:36:CYS:HA	8:H:126:GLU:O	2.13	0.48
9:I:29:CYS:SG	9:I:31:THR:HG22	2.52	0.48
9:I:85:PHE:O	9:I:86:PHE:HB3	2.13	0.48
1:R:5:A:N3	1:R:6:G:C8	2.81	0.48
3:A:674:PRO:O	3:A:677:ARG:HB3	2.14	0.48
3:A:1121:GLU:O	3:A:1122:PRO:C	2.56	0.48
4:B:291:ILE:HD13	4:B:300:HIS:CD2	2.48	0.48
8:H:44:VAL:O	8:H:44:VAL:HG12	2.12	0.48
1:R:10:A:H2'	14:R:3000:UTP:O4'	2.13	0.48
3:A:614:PHE:CD1	3:A:614:PHE:C	2.92	0.48
3:A:890:ASP:H	3:A:1296:GLY:HA3	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:994:GLN:NE2	3:A:1019:CYS:HB3	2.27	0.48
3:A:1349:TYR:O	3:A:1350:LYS:C	2.56	0.48
4:B:225:VAL:HG11	4:B:388:CYS:HB3	1.95	0.48
4:B:570:VAL:HG11	4:B:573:GLN:OE1	2.13	0.48
4:B:781:PHE:O	4:B:782:LEU:HG	2.12	0.48
4:B:864:LYS:HB3	4:B:871:THR:HA	1.96	0.48
4:B:1053:GLU:O	4:B:1055:ILE:N	2.46	0.48
4:B:1156:ASP:HB3	4:B:1197:PRO:HA	1.95	0.48
5:C:135:GLN:C	5:C:136:ASP:O	2.56	0.48
5:C:254:LYS:O	5:C:258:ILE:HD13	2.13	0.48
6:E:78:LEU:HD21	6:E:80:VAL:HG22	1.95	0.48
3:A:18:GLN:O	4:B:1215:ARG:CG	2.62	0.48
3:A:68:GLN:NE2	3:A:80:HIS:CB	2.76	0.48
3:A:225:ASN:C	3:A:227:VAL:N	2.71	0.48
3:A:742:ASN:C	3:A:745:GLN:HB2	2.38	0.48
3:A:821:ARG:CG	3:A:825:ILE:HD11	2.41	0.48
3:A:918:GLU:HG3	3:A:918:GLU:O	2.12	0.48
3:A:994:GLN:HE21	3:A:1019:CYS:CB	2.26	0.48
4:B:227:LYS:HB2	4:B:395:GLN:OE1	2.14	0.48
4:B:488:TYR:CE2	4:B:813:LYS:HB2	2.48	0.48
4:B:825:VAL:CG1	4:B:826:ALA:N	2.76	0.48
4:B:1162:ILE:HD11	4:B:1194:ILE:CD1	2.41	0.48
7:F:111:LEU:C	7:F:113:GLY:N	2.71	0.48
8:H:33:GLN:OE1	8:H:129:TYR:CE2	2.67	0.48
11:K:83:PRO:HA	11:K:86:ALA:HB3	1.95	0.48
3:A:69:THR:O	3:A:69:THR:HG22	2.12	0.48
3:A:178:GLY:O	3:A:179:LEU:HD23	2.13	0.48
3:A:226:GLU:CG	3:A:227:VAL:N	2.75	0.48
3:A:829:VAL:C	3:A:831:THR:N	2.70	0.48
3:A:913:LEU:HD11	3:A:981:LEU:O	2.13	0.48
3:A:1049:ILE:O	3:A:1050:GLU:C	2.56	0.48
3:A:1097:GLY:C	3:A:1099:PRO:HD2	2.39	0.48
4:B:171:PRO:HD2	4:B:457:LEU:CD1	2.43	0.48
4:B:189:LEU:O	4:B:190:TYR:C	2.57	0.48
4:B:380:TYR:CE1	4:B:384:ARG:HD3	2.48	0.48
4:B:562:GLY:O	4:B:563:MET:C	2.56	0.48
4:B:1182:CYS:O	4:B:1183:LYS:O	2.31	0.48
5:C:75:MET:HG3	5:C:246:ARG:NH2	2.28	0.48
5:C:212:PRO:HB3	5:C:213:PRO:HD2	1.95	0.48
6:E:138:ALA:C	6:E:140:LEU:H	2.21	0.48
10:J:57:ILE:HG12	10:J:61:LEU:HD11	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:5:A:N1	1:R:6:G:O6	2.46	0.48
3:A:399:HIS:C	3:A:401:GLY:N	2.71	0.48
3:A:874:ASP:HA	3:A:1058:VAL:HG22	1.95	0.48
3:A:1386:ARG:HE	3:A:1387:HIS:CE1	2.32	0.48
4:B:806:THR:HG22	4:B:808:ALA:H	1.79	0.48
5:C:31:ASN:O	5:C:32:SER:C	2.56	0.48
5:C:62:PHE:O	5:C:66:ARG:HG3	2.13	0.48
9:I:74:GLU:OE1	9:I:79:HIS:ND1	2.47	0.48
11:K:27:ALA:HB1	11:K:28:PRO:HD2	1.95	0.48
11:K:43:GLY:HA2	11:K:71:PHE:CZ	2.49	0.48
12:L:31:CYS:SG	12:L:34:CYS:SG	3.11	0.48
3:A:5:GLN:O	4:B:1159:ARG:NH2	2.47	0.48
3:A:244:PRO:HG2	3:A:245:PRO:CD	2.33	0.48
3:A:378:GLU:HG2	3:A:388:LEU:HD11	1.94	0.48
3:A:774:ARG:O	3:A:775:ILE:C	2.57	0.48
3:A:845:LEU:O	3:A:846:GLU:C	2.57	0.48
3:A:929:LEU:HD21	3:A:983:ILE:HG21	1.94	0.48
4:B:55:VAL:HG12	4:B:56:ASP:N	2.27	0.48
4:B:108:VAL:CG1	4:B:109:THR:H	2.19	0.48
4:B:798:TYR:CD2	10:J:4:PRO:HG3	2.49	0.48
4:B:956:THR:HG21	4:B:960:GLY:HA2	1.96	0.48
11:K:10:PHE:CE1	11:K:11:LEU:HD13	2.49	0.48
2:T:9:DC:O2	2:T:9:DC:C2'	2.56	0.48
3:A:89:PRO:HG3	3:A:208:LEU:CD1	2.44	0.48
3:A:365:GLY:O	3:A:468:PHE:HA	2.14	0.48
3:A:1412:ALA:HA	3:A:1417:GLU:OE2	2.14	0.48
4:B:123:THR:O	4:B:125:SER:N	2.47	0.48
4:B:236:HIS:CE1	4:B:389:ALA:HA	2.49	0.48
4:B:745:PRO:C	4:B:747:MET:N	2.70	0.48
4:B:1177:HIS:C	4:B:1179:GLN:H	2.22	0.48
8:H:125:LEU:HG	8:H:130:ARG:CZ	2.43	0.48
1:R:10:A:H61	2:T:6:DC:H42	1.60	0.48
3:A:116:ASP:HB2	3:A:118:HIS:CD2	2.49	0.48
3:A:515:GLN:HA	3:A:1367:HIS:NE2	2.29	0.48
3:A:738:LYS:HB3	8:H:19:ARG:HH22	1.79	0.48
3:A:742:ASN:O	3:A:745:GLN:HB2	2.13	0.48
3:A:1356:ILE:HD12	3:A:1368:MET:SD	2.54	0.48
3:A:1436:ILE:CG2	3:A:1437:GLY:H	2.22	0.48
4:B:46:GLN:HE21	4:B:496:ARG:HG2	1.78	0.48
4:B:845:SER:HB2	10:J:8:PHE:HB3	1.96	0.48
4:B:1175:LEU:O	4:B:1176:ASN:CG	2.56	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:258:ILE:HG23	11:K:19:LEU:HD11	1.96	0.48
11:K:92:ASN:O	11:K:93:SER:C	2.56	0.48
3:A:351:THR:CG2	4:B:1103:ILE:HA	2.36	0.47
3:A:545:GLN:O	3:A:546:VAL:C	2.55	0.47
3:A:954:TRP:O	3:A:956:LEU:HG	2.14	0.47
4:B:174:LEU:O	4:B:175:ARG:CB	2.48	0.47
4:B:642:ASP:O	4:B:643:ASP:C	2.56	0.47
4:B:1103:ILE:O	4:B:1104:HIS:C	2.56	0.47
4:B:1124:ARG:O	4:B:1125:ASP:HB3	2.14	0.47
4:B:1177:HIS:C	4:B:1179:GLN:N	2.68	0.47
5:C:43:THR:HG22	5:C:44:LEU:N	2.29	0.47
6:E:9:ILE:C	6:E:11:ARG:N	2.71	0.47
6:E:135:PHE:HD2	6:E:140:LEU:HD21	1.79	0.47
9:I:50:THR:HG22	9:I:51:ASN:N	2.28	0.47
9:I:54:GLU:O	9:I:89:GLN:HG2	2.14	0.47
3:A:226:GLU:HG2	3:A:227:VAL:N	2.29	0.47
3:A:545:GLN:OE1	3:A:549:MET:HE2	2.14	0.47
3:A:869:GLY:O	6:E:204:THR:HG21	2.14	0.47
4:B:773:MET:SD	4:B:987:LYS:HD2	2.54	0.47
6:E:7:ARG:C	6:E:9:ILE:N	2.71	0.47
7:F:98:ALA:O	7:F:117:PRO:HB2	2.14	0.47
8:H:47:PHE:CD1	8:H:95:TYR:HB2	2.49	0.47
3:A:783:THR:CG2	3:A:815:PHE:CE2	2.97	0.47
3:A:960:ILE:O	3:A:961:ARG:C	2.57	0.47
3:A:1134:ILE:HD11	3:A:1321:GLY:HA3	1.96	0.47
3:A:1392:SER:O	3:A:1393:ASN:ND2	2.48	0.47
4:B:51:PHE:CD2	4:B:173:MET:HB3	2.49	0.47
5:C:66:ARG:CZ	10:J:2:ILE:HG21	2.44	0.47
8:H:39:THR:O	8:H:123:MET:HA	2.14	0.47
8:H:49:VAL:CG1	8:H:50:ALA:H	2.27	0.47
3:A:332:LYS:N	3:A:337:ARG:HD2	2.29	0.47
6:E:56:LYS:HG3	6:E:84:ASP:CB	2.42	0.47
7:F:101:ILE:HD13	7:F:120:ILE:CG2	2.45	0.47
9:I:62:ILE:CG2	9:I:63:GLY:N	2.77	0.47
3:A:12:ARG:HD3	4:B:1218:THR:HB	1.97	0.47
3:A:14:VAL:H	3:A:1432:GLN:HE22	1.61	0.47
3:A:222:LEU:O	3:A:224:PHE:N	2.46	0.47
3:A:897:TYR:HD2	3:A:936:LEU:HD13	1.78	0.47
3:A:962:ARG:O	3:A:963:ILE:C	2.57	0.47
3:A:1336:MET:HE1	3:A:1380:GLY:C	2.40	0.47
4:B:708:GLU:C	4:B:710:LEU:N	2.72	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:75:MET:HG3	5:C:246:ARG:HH22	1.77	0.47
6:E:100:ILE:CG2	6:E:105:PHE:HB2	2.42	0.47
6:E:137:GLU:O	6:E:138:ALA:C	2.57	0.47
12:L:30:ILE:CD1	12:L:59:ALA:HA	2.44	0.47
3:A:61:ILE:HG22	3:A:62:ASP:N	2.16	0.47
3:A:443:LEU:CD2	3:A:455:MET:HB3	2.42	0.47
3:A:890:ASP:N	3:A:1296:GLY:HA3	2.30	0.47
4:B:210:LYS:HE2	4:B:461:LEU:O	2.14	0.47
4:B:294:ASP:H	9:I:12:ASN:ND2	2.12	0.47
4:B:363:HIS:CD2	4:B:585:VAL:HG22	2.49	0.47
4:B:892:LYS:NZ	4:B:909:ASP:OD2	2.47	0.47
4:B:1169:MET:SD	4:B:1201:LYS:HG2	2.54	0.47
5:C:142:VAL:H	10:J:16:ASP:CB	2.26	0.47
7:F:79:ARG:HG2	7:F:146:TRP:CZ2	2.49	0.47
11:K:59:ALA:HA	11:K:74:ARG:O	2.15	0.47
3:A:90:VAL:HG21	3:A:296:LEU:HG	1.96	0.47
3:A:112:LYS:HG2	3:A:113:LEU:H	1.79	0.47
3:A:154:SER:HB3	3:A:162:VAL:HG21	1.92	0.47
3:A:531:ILE:CD1	3:A:617:VAL:HG11	2.44	0.47
3:A:568:PRO:HB2	5:C:221:TYR:CZ	2.50	0.47
3:A:923:LEU:O	3:A:927:VAL:HG23	2.14	0.47
3:A:1074:GLU:HB3	3:A:1075:PRO:HD3	1.97	0.47
3:A:1237:ILE:CG2	3:A:1238:ILE:N	2.78	0.47
4:B:566:LEU:CD1	4:B:588:GLY:HA2	2.43	0.47
4:B:726:ALA:CB	4:B:1051:THR:HG21	2.45	0.47
4:B:763:GLN:CG	4:B:765:PRO:HD2	2.40	0.47
4:B:800:GLN:HB3	10:J:52:THR:HG22	1.96	0.47
4:B:806:THR:C	4:B:808:ALA:N	2.70	0.47
4:B:1013:ASN:OD1	4:B:1015:HIS:HB2	2.15	0.47
4:B:1065:GLN:HE22	4:B:1067:ARG:HG2	1.79	0.47
4:B:1104:HIS:HB2	4:B:1122:ARG:CD	2.44	0.47
4:B:1117:GLN:NE2	4:B:1156:ASP:OD2	2.48	0.47
4:B:1158:PHE:HE2	4:B:1201:LYS:HE3	1.80	0.47
5:C:35:ARG:O	5:C:38:ILE:N	2.47	0.47
5:C:38:ILE:HG13	5:C:176:ILE:HD12	1.97	0.47
9:I:7:CYS:CB	9:I:14:LEU:HD21	2.32	0.47
3:A:533:LYS:C	3:A:535:THR:H	2.23	0.47
3:A:1327:ILE:O	6:E:147:HIS:HE1	1.98	0.47
4:B:284:ILE:HD13	4:B:333:PHE:CD2	2.49	0.47
4:B:802:PRO:HA	4:B:822:ASN:HD21	1.79	0.47
7:F:101:ILE:HD11	7:F:124:GLU:OE1	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:113:LEU:C	3:A:115:LEU:H	2.23	0.47
3:A:873:MET:C	3:A:1058:VAL:HG23	2.40	0.47
4:B:100:PRO:O	4:B:180:TYR:OH	2.31	0.47
4:B:100:PRO:HD2	4:B:180:TYR:CE1	2.50	0.47
4:B:280:ILE:HD13	4:B:334:ILE:HG12	1.95	0.47
4:B:487:THR:HG22	4:B:489:SER:N	2.24	0.47
4:B:640:VAL:HG23	4:B:740:HIS:HA	1.97	0.47
5:C:258:ILE:HD12	5:C:258:ILE:N	2.30	0.47
6:E:100:ILE:O	6:E:101:GLN:C	2.58	0.47
9:I:2:THR:OG1	9:I:45:ARG:HB3	2.15	0.47
10:J:27:GLU:C	10:J:29:GLU:H	2.23	0.47
3:A:294:SER:HA	3:A:297:GLN:HB3	1.96	0.47
3:A:908:LEU:O	3:A:909:ASP:C	2.58	0.47
3:A:964:ILE:HD13	3:A:1035:TYR:CZ	2.50	0.47
3:A:1227:ILE:HG22	3:A:1228:TRP:N	2.30	0.47
3:A:1237:ILE:HG22	3:A:1238:ILE:N	2.29	0.47
4:B:291:ILE:HD13	4:B:300:HIS:NE2	2.30	0.47
4:B:346:GLU:O	4:B:347:LYS:C	2.58	0.47
4:B:484:ASN:CG	4:B:486:TYR:HE1	2.23	0.47
4:B:666:TYR:C	4:B:668:ASP:N	2.72	0.47
4:B:780:VAL:HG21	10:J:56:LEU:HD11	1.97	0.47
4:B:1116:ARG:NH1	4:B:1198:TYR:CD1	2.83	0.47
6:E:179:GLN:HA	6:E:179:GLN:OE1	2.16	0.47
10:J:1:MET:O	10:J:2:ILE:O	2.33	0.47
11:K:83:PRO:O	11:K:87:LEU:N	2.46	0.47
3:A:1192:LEU:HD11	3:A:1239:ARG:CB	2.37	0.46
4:B:96:TYR:N	4:B:96:TYR:CD1	2.83	0.46
4:B:324:ILE:HG23	4:B:329:THR:HB	1.96	0.46
4:B:851:PHE:O	4:B:974:PRO:HD3	2.15	0.46
5:C:18:VAL:HG12	5:C:18:VAL:O	2.15	0.46
7:F:109:VAL:HG11	7:F:123:LYS:HG2	1.96	0.46
1:R:8:G:C2	2:T:8:DT:C4	3.04	0.46
3:A:68:GLN:C	3:A:70:CYS:N	2.73	0.46
3:A:693:VAL:HG21	3:A:721:PHE:CE1	2.38	0.46
3:A:829:VAL:O	3:A:831:THR:N	2.48	0.46
3:A:881:GLN:OE1	3:A:959:ASN:HA	2.15	0.46
3:A:1173:HIS:CD2	3:A:1227:ILE:HG23	2.51	0.46
3:A:1347:ALA:O	3:A:1348:LEU:C	2.55	0.46
3:A:1436:ILE:O	3:A:1437:GLY:C	2.56	0.46
4:B:298:LEU:N	4:B:298:LEU:HD23	2.29	0.46
4:B:821:GLN:HB2	4:B:851:PHE:CE2	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:1106:ARG:CD	4:B:1126:GLY:O	2.62	0.46
3:A:341:MET:CE	3:A:1401:SER:HB2	2.41	0.46
3:A:343:LYS:NZ	4:B:1156:ASP:OD2	2.49	0.46
3:A:352:VAL:HG12	3:A:353:ILE:N	2.29	0.46
3:A:475:THR:CG2	3:A:476:SER:N	2.76	0.46
3:A:679:ILE:HG23	3:A:729:ALA:CB	2.39	0.46
3:A:893:PHE:CD1	3:A:940:ARG:HD2	2.51	0.46
3:A:975:HIS:ND1	3:A:1036:ARG:HG3	2.30	0.46
4:B:300:HIS:ND1	4:B:376:PHE:CD2	2.81	0.46
4:B:315:LYS:O	4:B:318:VAL:N	2.46	0.46
4:B:842:ASN:HD22	4:B:845:SER:HB3	1.80	0.46
4:B:871:THR:HG22	4:B:872:GLU:O	2.14	0.46
4:B:906:SER:CB	4:B:946:ASN:HB2	2.46	0.46
4:B:1072:MET:O	4:B:1081:LEU:HB2	2.15	0.46
4:B:1182:CYS:O	4:B:1183:LYS:HD2	2.15	0.46
6:E:96:PHE:CE1	6:E:100:ILE:HD11	2.50	0.46
9:I:34:TYR:O	9:I:35:VAL:HG23	2.16	0.46
11:K:71:PHE:CD1	11:K:71:PHE:C	2.93	0.46
3:A:20:GLY:HA2	3:A:1413:GLY:O	2.14	0.46
3:A:112:LYS:HG2	3:A:113:LEU:N	2.31	0.46
3:A:381:THR:CG2	3:A:383:TYR:CD1	2.98	0.46
3:A:517:ASN:ND2	3:A:1362:TYR:CE2	2.83	0.46
3:A:848:ILE:CD1	3:A:1374:VAL:HG21	2.45	0.46
3:A:982:THR:HB	3:A:985:ASP:CG	2.40	0.46
3:A:1140:HIS:HB2	3:A:1276:VAL:O	2.16	0.46
3:A:1394:THR:HG21	3:A:1398:MET:SD	2.56	0.46
4:B:167:ILE:O	4:B:167:ILE:HG22	2.14	0.46
4:B:350:GLN:O	4:B:351:TYR:C	2.58	0.46
4:B:830:TYR:CE2	4:B:1000:PRO:HD3	2.50	0.46
4:B:1051:THR:HG21	4:B:1053:GLU:HB2	1.97	0.46
12:L:34:CYS:HG	12:L:51:CYS:HG	1.62	0.46
3:A:533:LYS:C	3:A:535:THR:N	2.72	0.46
3:A:849:MET:HB2	3:A:1063:MET:SD	2.55	0.46
3:A:1037:LEU:HD13	3:A:1042:PHE:HA	1.98	0.46
3:A:1209:MET:CG	3:A:1236:LEU:HD22	2.45	0.46
3:A:1277:GLU:O	3:A:1278:ASN:HB2	2.14	0.46
4:B:282:ILE:HG13	4:B:283:VAL:N	2.31	0.46
3:A:50:ILE:HG22	3:A:51:GLY:H	1.81	0.46
3:A:446:ARG:HG2	3:A:446:ARG:NH1	2.28	0.46
3:A:535:THR:HG22	3:A:616:VAL:HA	1.97	0.46
3:A:567:LYS:CD	3:A:568:PRO:HD2	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:666:ILE:H	3:A:666:ILE:HG13	1.33	0.46
3:A:1111:MET:CE	3:A:1330:ASN:OD1	2.57	0.46
4:B:31:TRP:CE3	4:B:34:ILE:HD12	2.50	0.46
4:B:50:SER:O	4:B:53:GLN:HB3	2.16	0.46
4:B:574:SER:HB3	4:B:577:ALA:HB2	1.98	0.46
4:B:707:PRO:O	4:B:708:GLU:C	2.59	0.46
5:C:180:TYR:O	5:C:181:ASP:HB3	2.15	0.46
6:E:96:PHE:CE2	6:E:110:PHE:HB2	2.50	0.46
10:J:34:THR:O	10:J:35:ALA:C	2.58	0.46
3:A:87:ALA:HB3	3:A:276:LEU:CD2	2.45	0.46
3:A:223:GLY:HA3	3:A:1415:SER:HB3	1.98	0.46
3:A:573:SER:OG	3:A:576:GLN:HG3	2.15	0.46
3:A:658:LEU:HD13	4:B:831:SER:HA	1.98	0.46
3:A:928:LEU:O	3:A:929:LEU:C	2.59	0.46
3:A:1208:THR:HG22	3:A:1210:GLY:H	1.81	0.46
4:B:62:ILE:HG21	4:B:417:PHE:HD2	1.80	0.46
4:B:240:ILE:C	4:B:253:THR:HG23	2.41	0.46
4:B:260:GLY:HA3	4:B:267:ARG:HG2	1.98	0.46
4:B:307:ASP:O	4:B:308:TRP:C	2.59	0.46
4:B:519:TRP:HE1	4:B:635:ARG:HH22	1.64	0.46
4:B:737:THR:HG23	9:I:66:PRO:HB2	1.94	0.46
4:B:1013:ASN:OD1	4:B:1015:HIS:N	2.44	0.46
4:B:1020:ARG:O	4:B:1021:MET:C	2.58	0.46
5:C:262:LEU:O	5:C:265:MET:HB3	2.15	0.46
8:H:26:ILE:HD13	8:H:49:VAL:HG11	1.97	0.46
8:H:113:ALA:HA	8:H:125:LEU:O	2.15	0.46
3:A:79:GLY:C	3:A:243:PRO:HG3	2.41	0.46
3:A:83:HIS:CE1	3:A:238:CYS:SG	3.08	0.46
3:A:244:PRO:O	3:A:245:PRO:C	2.59	0.46
3:A:1242:VAL:CG1	3:A:1243:VAL:H	2.22	0.46
4:B:295:GLY:O	4:B:299:GLU:HG3	2.16	0.46
4:B:316:PRO:HA	4:B:319:GLU:HG2	1.98	0.46
4:B:605:ARG:CZ	4:B:639:ILE:HD13	2.46	0.46
4:B:704:ALA:HB2	4:B:738:PHE:CE1	2.51	0.46
4:B:800:GLN:CB	10:J:52:THR:CG2	2.89	0.46
5:C:252:GLN:CG	11:K:95:ILE:HG23	2.46	0.46
8:H:83:GLN:C	8:H:85:GLY:N	2.73	0.46
3:A:35:ILE:HD12	3:A:241:VAL:HG21	1.98	0.46
3:A:47:ARG:O	3:A:48:ALA:HB2	2.16	0.46
3:A:53:LEU:HD13	3:A:263:THR:HG23	1.97	0.46
3:A:1041:ALA:O	3:A:1044:TRP:HB3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:230:ALA:N	4:B:231:PRO:HD2	2.31	0.46
4:B:702:LEU:HD21	4:B:735:ALA:HB1	1.98	0.46
4:B:893:LEU:HD22	4:B:897:GLY:O	2.16	0.46
4:B:1017:ILE:HB	4:B:1018:PRO:HD3	1.98	0.46
4:B:1060:ARG:C	4:B:1062:HIS:N	2.69	0.46
4:B:1085:ILE:CG2	4:B:1086:PHE:N	2.78	0.46
6:E:71:LYS:C	6:E:73:PRO:HD3	2.40	0.46
6:E:94:LYS:O	6:E:98:ILE:HG13	2.16	0.46
11:K:12:LEU:H	11:K:12:LEU:CD1	2.23	0.46
3:A:481:ASP:C	3:A:481:ASP:OD1	2.58	0.46
3:A:645:LEU:O	3:A:649:ILE:HG13	2.15	0.46
3:A:648:ASN:O	3:A:649:ILE:C	2.59	0.46
3:A:1433:MET:HE1	7:F:92:ARG:CZ	2.46	0.46
4:B:300:HIS:ND1	4:B:376:PHE:CE2	2.83	0.46
4:B:515:HIS:CD2	4:B:517:THR:OG1	2.66	0.46
4:B:860:MET:HB2	4:B:965:LYS:HG2	1.97	0.46
4:B:864:LYS:H	4:B:872:GLU:CG	2.28	0.46
4:B:914:LYS:H	4:B:938:SER:HB3	1.81	0.46
4:B:1154:ALA:O	4:B:1155:SER:CB	2.64	0.46
5:C:80:LEU:CD2	5:C:129:ILE:HD11	2.28	0.46
5:C:166:GLU:CG	11:K:10:PHE:CZ	2.96	0.46
7:F:117:PRO:O	7:F:120:ILE:HB	2.16	0.46
8:H:40:LEU:HG	8:H:42:ILE:HG13	1.98	0.46
8:H:81:PRO:HD2	8:H:82:PRO:HD2	1.98	0.46
8:H:114:VAL:O	8:H:124:ARG:HA	2.16	0.46
12:L:45:ALA:O	12:L:46:VAL:CG2	2.64	0.46
3:A:477:PRO:HG2	3:A:521:MET:HG2	1.97	0.45
3:A:556:TRP:CZ3	3:A:558:GLY:HA2	2.51	0.45
3:A:573:SER:H	3:A:576:GLN:HG3	1.81	0.45
3:A:848:ILE:HD13	3:A:864:ILE:HD13	1.98	0.45
3:A:866:PHE:C	3:A:867:ILE:HG13	2.40	0.45
3:A:1208:THR:HG22	3:A:1210:GLY:N	2.32	0.45
4:B:1120:GLU:HG2	4:B:1121:GLY:N	2.31	0.45
9:I:100:PHE:HZ	9:I:118:ARG:HH12	1.62	0.45
11:K:73:LEU:CD2	11:K:75:ILE:HD11	2.46	0.45
3:A:265:LYS:HZ1	3:A:323:LYS:H	1.62	0.45
3:A:598:LEU:O	3:A:599:SER:C	2.59	0.45
3:A:1225:PHE:O	3:A:1240:CYS:HA	2.14	0.45
4:B:345:LYS:O	4:B:347:LYS:N	2.49	0.45
5:C:73:GLN:NE2	5:C:75:MET:H	1.97	0.45
6:E:10:SER:O	6:E:14:ARG:HG3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:E:112:TYR:CE2	6:E:134:THR:HB	2.51	0.45
8:H:26:ILE:CD1	8:H:49:VAL:HG11	2.46	0.45
8:H:116:TYR:HE2	8:H:140:ALA:CB	2.30	0.45
11:K:91:CYS:O	11:K:94:ILE:HB	2.16	0.45
2:T:4:DA:H2'	2:T:5:DT:H72	1.98	0.45
3:A:103:CYS:O	3:A:106:VAL:O	2.35	0.45
3:A:152:VAL:CG1	3:A:153:PRO:HD2	2.45	0.45
3:A:388:LEU:O	3:A:392:VAL:HG23	2.17	0.45
3:A:535:THR:O	3:A:536:LEU:C	2.59	0.45
3:A:567:LYS:NZ	8:H:95:TYR:CD1	2.80	0.45
3:A:650:GLN:O	3:A:651:LYS:C	2.58	0.45
3:A:889:SER:HB3	3:A:1297:GLU:HG3	1.97	0.45
4:B:201:GLY:H	4:B:202:TYR:HD2	1.63	0.45
4:B:321:GLY:C	4:B:323:VAL:N	2.74	0.45
4:B:361:LEU:N	4:B:362:PRO:HD2	2.31	0.45
4:B:578:THR:HG23	4:B:622:LYS:C	2.42	0.45
4:B:589:VAL:HG12	4:B:590:HIS:H	1.81	0.45
4:B:824:ILE:CG2	4:B:1087:PHE:CE2	3.00	0.45
6:E:78:LEU:C	6:E:78:LEU:CD2	2.89	0.45
11:K:55:LYS:CD	11:K:78:THR:HB	2.41	0.45
3:A:418:SER:O	3:A:421:ALA:N	2.49	0.45
3:A:571:LEU:HD22	8:H:46:LEU:HD11	1.99	0.45
3:A:786:HIS:CE1	4:B:742:GLU:OE1	2.64	0.45
3:A:1149:ALA:CB	9:I:47:GLU:HA	2.45	0.45
3:A:1155:ASP:OD1	3:A:1162:VAL:HG23	2.17	0.45
4:B:100:PRO:HA	4:B:125:SER:O	2.17	0.45
4:B:215:GLN:HB2	4:B:407:ASP:HB2	1.98	0.45
4:B:1106:ARG:HG2	4:B:1107:ALA:N	2.31	0.45
5:C:17:ASN:OD1	5:C:233:GLU:HG2	2.16	0.45
5:C:29:MET:O	5:C:30:ALA:C	2.59	0.45
5:C:242:GLN:OE1	5:C:242:GLN:HA	2.16	0.45
8:H:40:LEU:HD13	8:H:123:MET:HB2	1.99	0.45
10:J:5:VAL:O	10:J:6:ARG:HB2	2.15	0.45
1:R:9:G:C2	1:R:10:A:C5	3.05	0.45
14:R:3000:UTP:C3'	14:R:3000:UTP:C6	3.00	0.45
3:A:771:GLU:H	3:A:822:GLU:CD	2.25	0.45
3:A:1209:MET:CE	3:A:1236:LEU:HB3	2.47	0.45
4:B:640:VAL:O	4:B:640:VAL:HG12	2.15	0.45
4:B:806:THR:OG1	4:B:809:MET:HE3	2.15	0.45
4:B:1020:ARG:H	4:B:1020:ARG:HG2	1.51	0.45
9:I:34:TYR:O	9:I:35:VAL:CG2	2.65	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:34:TYR:C	9:I:35:VAL:HG23	2.41	0.45
3:A:738:LYS:NZ	5:C:194:GLU:C	2.74	0.45
3:A:1114:PRO:O	3:A:1330:ASN:OD1	2.35	0.45
4:B:247:GLY:O	4:B:248:SER:HB3	2.17	0.45
4:B:549:THR:H	4:B:628:THR:HG22	1.81	0.45
4:B:1158:PHE:CD2	4:B:1198:TYR:HD1	2.35	0.45
8:H:101:ALA:HB2	8:H:116:TYR:CD2	2.51	0.45
3:A:55:ASP:HB3	3:A:56:PRO:HD3	1.98	0.45
3:A:210:ILE:O	3:A:214:ILE:HG13	2.17	0.45
3:A:420:ARG:O	3:A:424:ILE:HG13	2.16	0.45
3:A:592:ASP:N	3:A:595:THR:OG1	2.48	0.45
3:A:1336:MET:HE1	3:A:1381:LEU:N	2.31	0.45
4:B:25:ILE:HD11	4:B:653:VAL:CB	2.46	0.45
4:B:56:ASP:HB3	4:B:57:TYR:CD1	2.52	0.45
4:B:185:THR:H	4:B:188:ASP:HB2	1.81	0.45
4:B:322:PHE:CG	4:B:322:PHE:O	2.69	0.45
4:B:332:ASP:O	4:B:334:ILE:N	2.50	0.45
6:E:117:THR:C	6:E:119:SER:N	2.73	0.45
2:T:1:DA:N3	2:T:1:DA:C2'	2.77	0.45
3:A:69:THR:O	4:B:1174:LYS:HG2	2.17	0.45
3:A:511:ILE:HG12	3:A:521:MET:CE	2.42	0.45
3:A:738:LYS:NZ	5:C:194:GLU:CA	2.79	0.45
3:A:958:VAL:HG22	3:A:1052:GLN:HB3	1.98	0.45
3:A:1220:PHE:O	3:A:1221:LYS:C	2.60	0.45
4:B:371:GLU:OE1	4:B:371:GLU:N	2.49	0.45
4:B:702:LEU:HD12	4:B:702:LEU:HA	1.76	0.45
4:B:744:HIS:CD2	4:B:746:SER:OG	2.70	0.45
4:B:963:PHE:HE2	4:B:965:LYS:HE3	1.81	0.45
4:B:980:PHE:HE1	4:B:990:ILE:CD1	2.30	0.45
4:B:1100:ASP:HA	4:B:1103:ILE:CG1	2.46	0.45
9:I:29:CYS:O	9:I:31:THR:N	2.49	0.45
12:L:55:ILE:H	12:L:55:ILE:HG12	1.53	0.45
3:A:80:HIS:O	3:A:243:PRO:HB3	2.17	0.45
3:A:329:LEU:HA	3:A:335:ARG:HB2	1.98	0.45
3:A:974:ASP:CB	8:H:136:LYS:NZ	2.80	0.45
3:A:1377:THR:C	3:A:1379:GLY:H	2.25	0.45
4:B:276:ILE:HD13	4:B:334:ILE:CG2	2.47	0.45
4:B:680:THR:O	4:B:683:SER:OG	2.34	0.45
4:B:1072:MET:HE2	4:B:1085:ILE:HB	1.96	0.45
5:C:249:ASP:O	5:C:252:GLN:HB3	2.16	0.45
7:F:109:VAL:HG12	7:F:110:ASP:H	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:11:GLN:C	8:H:28:ALA:HB1	2.42	0.45
8:H:111:LEU:HA	8:H:127:GLY:O	2.17	0.45
10:J:1:MET:N	10:J:56:LEU:HB2	2.17	0.45
11:K:24:ASP:HB3	11:K:30:ALA:CB	2.47	0.45
1:R:2:U:C5	1:R:3:C:C4	3.05	0.45
3:A:219:PHE:CE2	3:A:231:PRO:HD2	2.52	0.45
3:A:517:ASN:OD1	3:A:517:ASN:O	2.34	0.45
4:B:238:ALA:HB3	4:B:256:VAL:HB	1.98	0.45
4:B:986:GLN:OE1	4:B:986:GLN:CA	2.64	0.45
5:C:39:ALA:HA	5:C:164:ALA:CB	2.46	0.45
5:C:120:ILE:HD11	5:C:130:GLY:O	2.17	0.45
6:E:117:THR:C	6:E:119:SER:H	2.25	0.45
9:I:92:ARG:CG	9:I:93:LYS:H	2.30	0.45
11:K:98:LEU:O	11:K:99:GLY:C	2.58	0.45
3:A:1207:LEU:HA	3:A:1211:GLN:OE1	2.17	0.44
3:A:1336:MET:SD	3:A:1381:LEU:HG	2.56	0.44
4:B:426:LYS:O	4:B:430:ARG:HG3	2.17	0.44
4:B:864:LYS:HD3	4:B:871:THR:CA	2.47	0.44
4:B:1038:SER:HB3	4:B:1062:HIS:NE2	2.33	0.44
6:E:136:ASN:C	6:E:136:ASN:OD1	2.60	0.44
6:E:147:HIS:CD2	6:E:149:LEU:H	2.35	0.44
8:H:24:CYS:CB	8:H:44:VAL:HG21	2.47	0.44
8:H:84:ALA:HA	8:H:87:ARG:HB2	1.98	0.44
11:K:92:ASN:C	11:K:94:ILE:N	2.75	0.44
3:A:152:VAL:HG13	3:A:153:PRO:HD2	1.99	0.44
3:A:340:LEU:HD21	4:B:1200:ALA:CA	2.47	0.44
3:A:815:PHE:C	3:A:817:ALA:N	2.72	0.44
3:A:921:GLY:O	3:A:922:ASP:C	2.59	0.44
4:B:200:GLY:HA2	4:B:202:TYR:CD2	2.50	0.44
4:B:229:ALA:HB1	4:B:231:PRO:HD2	1.98	0.44
5:C:9:LYS:HB2	5:C:21:ILE:HB	1.98	0.44
6:E:190:LEU:HD11	6:E:196:VAL:HG11	1.98	0.44
8:H:5:LEU:O	8:H:133:ASN:HB3	2.17	0.44
9:I:7:CYS:HB2	9:I:14:LEU:CD2	2.34	0.44
9:I:99:LEU:HB2	9:I:112:SER:CB	2.46	0.44
12:L:62:LYS:O	12:L:64:LEU:N	2.37	0.44
3:A:67:CYS:SG	3:A:77:CYS:SG	3.11	0.44
3:A:701:LEU:HA	9:I:115:LYS:HE3	1.98	0.44
4:B:130:VAL:CG1	4:B:131:ASP:H	2.29	0.44
4:B:800:GLN:CB	10:J:52:THR:HG22	2.47	0.44
4:B:1085:ILE:HG22	4:B:1086:PHE:N	2.31	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:31:ASN:O	5:C:35:ARG:HG3	2.17	0.44
3:A:21:LEU:HD21	3:A:95:PHE:CZ	2.53	0.44
3:A:456:MET:HB2	3:A:478:TYR:OH	2.17	0.44
3:A:1098:VAL:O	3:A:1099:PRO:C	2.59	0.44
3:A:1441:PHE:HB2	7:F:134:ILE:CG2	2.47	0.44
4:B:216:GLU:OE1	4:B:537:LYS:CE	2.66	0.44
4:B:276:ILE:HD13	4:B:334:ILE:HG23	1.99	0.44
4:B:288:ALA:HA	4:B:331:LEU:HD13	1.99	0.44
4:B:365:THR:CG2	4:B:367:LEU:H	2.30	0.44
4:B:408:LEU:HD12	4:B:408:LEU:HA	1.71	0.44
4:B:446:LEU:N	4:B:446:LEU:HD23	2.33	0.44
4:B:707:PRO:O	4:B:708:GLU:O	2.35	0.44
4:B:781:PHE:CE2	4:B:795:ILE:HD11	2.53	0.44
4:B:915:THR:HG21	4:B:934:LYS:HG2	1.99	0.44
4:B:1033:LYS:NZ	4:B:1070:GLU:OE1	2.46	0.44
5:C:22:LEU:HD12	5:C:230:MET:HE1	1.99	0.44
5:C:69:LEU:HD12	5:C:69:LEU:HA	1.76	0.44
6:E:16:PHE:O	6:E:17:ARG:C	2.60	0.44
8:H:98:TYR:O	8:H:118:PHE:HD2	1.99	0.44
3:A:233:TRP:O	3:A:235:ILE:N	2.50	0.44
3:A:525:GLN:HB2	4:B:835:GLN:HG2	2.00	0.44
3:A:741:ASN:HD22	3:A:743:VAL:N	2.16	0.44
3:A:815:PHE:O	3:A:818:MET:N	2.50	0.44
4:B:361:LEU:O	4:B:363:HIS:O	2.35	0.44
4:B:563:MET:HE1	4:B:580:VAL:HB	2.00	0.44
4:B:737:THR:O	4:B:738:PHE:C	2.60	0.44
4:B:995:ARG:NH1	4:B:997:GLU:OE1	2.49	0.44
4:B:1002:THR:CG2	4:B:1004:GLU:HB2	2.47	0.44
4:B:1060:ARG:O	4:B:1063:GLY:N	2.45	0.44
6:E:28:TYR:CE2	6:E:64:PRO:HG3	2.53	0.44
8:H:93:TYR:HA	8:H:145:ARG:CB	2.41	0.44
11:K:24:ASP:OD1	11:K:26:LYS:N	2.51	0.44
3:A:92:HIS:CD2	3:A:92:HIS:C	2.96	0.44
3:A:243:PRO:HB2	3:A:245:PRO:HD2	1.99	0.44
3:A:388:LEU:HD23	3:A:388:LEU:HA	1.88	0.44
3:A:591:PHE:HD2	3:A:595:THR:HB	1.83	0.44
3:A:595:THR:HG22	3:A:596:THR:N	2.33	0.44
3:A:1384:VAL:O	3:A:1389:PHE:HE2	2.01	0.44
4:B:65:GLU:HG3	4:B:66:ASP:N	2.27	0.44
4:B:168:GLY:H	4:B:450:ALA:HB1	1.82	0.44
4:B:214:ALA:HB2	4:B:408:LEU:CD1	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:640:VAL:HG23	4:B:740:HIS:CA	2.48	0.44
4:B:864:LYS:HD3	4:B:871:THR:CB	2.47	0.44
4:B:995:ARG:HB2	4:B:995:ARG:HH11	1.81	0.44
6:E:185:ALA:CB	6:E:190:LEU:HD12	2.47	0.44
12:L:51:CYS:C	12:L:53:HIS:N	2.75	0.44
3:A:494:SER:HB2	3:A:497:THR:OG1	2.18	0.44
3:A:679:ILE:O	3:A:682:THR:HB	2.18	0.44
3:A:960:ILE:HD12	3:A:1021:LEU:HD21	1.99	0.44
4:B:56:ASP:HB3	4:B:57:TYR:CE1	2.53	0.44
4:B:293:PRO:C	4:B:294:ASP:O	2.57	0.44
4:B:973:ILE:CG2	4:B:974:PRO:HD2	2.47	0.44
4:B:1163:CYS:C	4:B:1165:ILE:H	2.25	0.44
6:E:138:ALA:O	6:E:140:LEU:N	2.50	0.44
12:L:38:LEU:HG	12:L:39:SER:H	1.82	0.44
3:A:381:THR:O	3:A:384:ASN:N	2.41	0.44
3:A:458:HIS:ND1	3:A:507:VAL:HG21	2.33	0.44
3:A:845:LEU:O	3:A:848:ILE:HG13	2.17	0.44
3:A:1118:VAL:O	3:A:1305:VAL:HG13	2.17	0.44
4:B:102:VAL:HG21	4:B:112:LEU:HD13	1.99	0.44
4:B:370:PHE:N	4:B:371:GLU:OE1	2.50	0.44
4:B:847:ASP:O	5:C:65:HIS:HE1	2.01	0.44
4:B:872:GLU:CD	4:B:914:LYS:HE2	2.43	0.44
4:B:912:ILE:O	4:B:938:SER:CB	2.59	0.44
9:I:50:THR:HG22	9:I:52:ILE:N	2.33	0.44
3:A:84:ILE:CG2	3:A:239:LEU:HB3	2.48	0.44
3:A:99:ILE:O	3:A:100:LYS:C	2.61	0.44
3:A:366:VAL:HA	3:A:367:PRO:HD2	1.81	0.44
3:A:567:LYS:HZ3	8:H:95:TYR:HE1	1.52	0.44
3:A:1046:LEU:C	3:A:1048:ASN:N	2.75	0.44
3:A:1094:VAL:HG12	3:A:1095:THR:N	2.32	0.44
3:A:1097:GLY:O	3:A:1098:VAL:C	2.60	0.44
3:A:1364:ASN:HD22	3:A:1365:TYR:N	2.13	0.44
4:B:57:TYR:O	4:B:58:THR:C	2.60	0.44
4:B:203:PHE:HE1	4:B:212:LEU:CD1	2.31	0.44
4:B:205:ILE:HG12	4:B:461:LEU:HB3	1.99	0.44
4:B:1185:CYS:O	4:B:1186:ASP:HB2	2.17	0.44
5:C:8:VAL:CG1	5:C:9:LYS:N	2.80	0.44
5:C:143:LEU:HD21	5:C:146:LYS:HE3	1.99	0.44
6:E:137:GLU:O	6:E:140:LEU:N	2.43	0.44
10:J:16:ASP:OD1	10:J:17:LYS:HG3	2.17	0.44
11:K:24:ASP:OD2	11:K:74:ARG:NH1	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:54:ASN:O	3:A:55:ASP:HB2	2.18	0.43
3:A:326:ARG:HE	3:A:1406:VAL:HG11	1.82	0.43
3:A:404:TYR:HA	3:A:413:ILE:O	2.18	0.43
3:A:496:GLU:O	3:A:497:THR:C	2.60	0.43
3:A:562:THR:HA	3:A:563:PRO:HD3	1.92	0.43
3:A:922:ASP:CG	3:A:925:LEU:HG	2.43	0.43
3:A:1364:ASN:HD22	3:A:1366:ARG:N	2.16	0.43
3:A:1441:PHE:HB2	7:F:134:ILE:HG23	2.00	0.43
4:B:310:MET:O	4:B:313:MET:HB2	2.18	0.43
4:B:650:GLU:HG2	4:B:654:ARG:NH1	2.33	0.43
4:B:690:VAL:HG12	4:B:691:GLU:N	2.33	0.43
4:B:806:THR:N	4:B:809:MET:HE3	2.33	0.43
5:C:46:ILE:HG23	5:C:157:CYS:HB3	2.00	0.43
5:C:77:ILE:CG2	5:C:161:LYS:HE3	2.48	0.43
8:H:5:LEU:O	8:H:6:PHE:HB2	2.18	0.43
9:I:91:ARG:HA	9:I:91:ARG:HD3	1.75	0.43
9:I:98:VAL:CG1	9:I:99:LEU:N	2.81	0.43
11:K:40:HIS:O	11:K:41:THR:C	2.60	0.43
11:K:47:ARG:C	11:K:47:ARG:HD2	2.43	0.43
11:K:55:LYS:HD3	11:K:78:THR:OG1	2.18	0.43
12:L:26:THR:C	12:L:27:LEU:HD23	2.43	0.43
1:R:2:U:H3'	1:R:3:C:C6	2.54	0.43
3:A:31:SER:HB2	3:A:82:GLY:C	2.43	0.43
3:A:535:THR:HG21	3:A:616:VAL:CA	2.43	0.43
3:A:825:ILE:C	3:A:827:THR:N	2.70	0.43
3:A:1015:VAL:HG12	3:A:1015:VAL:O	2.18	0.43
3:A:1343:ALA:O	3:A:1344:GLY:C	2.61	0.43
4:B:315:LYS:N	4:B:316:PRO:HD2	2.32	0.43
4:B:972:LYS:CD	4:B:1098:MET:HE1	2.48	0.43
4:B:1002:THR:HG21	4:B:1006:ILE:HB	2.00	0.43
6:E:82:PHE:CD1	6:E:82:PHE:N	2.85	0.43
6:E:133:GLU:HB3	6:E:135:PHE:HE1	1.83	0.43
8:H:84:ALA:CA	8:H:87:ARG:HB2	2.48	0.43
8:H:84:ALA:CB	8:H:87:ARG:HB2	2.49	0.43
12:L:61:THR:HG22	12:L:62:LYS:N	2.33	0.43
2:T:8:DT:H2'	2:T:9:DC:C6	2.53	0.43
3:A:42:ASP:OD1	3:A:45:GLN:O	2.36	0.43
3:A:53:LEU:O	3:A:54:ASN:C	2.60	0.43
3:A:367:PRO:CB	3:A:466:SER:HA	2.47	0.43
3:A:629:LEU:CD1	3:A:645:LEU:HD21	2.48	0.43
3:A:850:VAL:O	3:A:1060:PRO:HA	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:212:LEU:HD13	4:B:409:ALA:HA	2.00	0.43
4:B:358:LYS:O	4:B:359:GLU:OE1	2.36	0.43
4:B:781:PHE:HE2	4:B:795:ILE:HD11	1.83	0.43
4:B:850:LEU:CD2	4:B:1009:ASP:HB3	2.48	0.43
5:C:173:ALA:O	5:C:174:ALA:CB	2.64	0.43
6:E:113:GLN:HG2	6:E:137:GLU:OE1	2.19	0.43
9:I:84:VAL:O	9:I:84:VAL:CG1	2.65	0.43
2:T:1:DA:N3	2:T:2:DC:C6	2.86	0.43
3:A:373:THR:HG21	4:B:1105:ALA:O	2.17	0.43
3:A:412:ARG:CZ	4:B:1108:ARG:NH2	2.81	0.43
3:A:778:GLY:HA3	4:B:516:ASN:CB	2.46	0.43
3:A:879:GLU:CD	3:A:962:ARG:HH22	2.26	0.43
3:A:1129:GLU:O	3:A:1130:GLN:C	2.61	0.43
3:A:1148:ILE:HD12	3:A:1196:GLU:HG2	2.01	0.43
3:A:1385:THR:HG22	3:A:1386:ARG:N	2.33	0.43
4:B:366:GLN:O	4:B:367:LEU:O	2.36	0.43
4:B:556:THR:O	4:B:557:PHE:C	2.61	0.43
4:B:784:ASN:HB3	10:J:63:TYR:OH	2.18	0.43
5:C:52:GLU:HB3	5:C:154:LYS:HB3	1.99	0.43
5:C:56:THR:CG2	5:C:57:VAL:N	2.69	0.43
5:C:123:ASN:ND2	5:C:125:MET:HG2	2.31	0.43
5:C:251:LEU:HG	11:K:98:LEU:HD11	2.01	0.43
5:C:264:GLN:HG3	5:C:264:GLN:H	1.61	0.43
8:H:57:VAL:HG12	8:H:58:THR:N	2.32	0.43
12:L:27:LEU:HD13	12:L:37:LYS:CB	2.48	0.43
12:L:43:THR:HG22	12:L:43:THR:O	2.18	0.43
3:A:55:ASP:O	3:A:56:PRO:C	2.61	0.43
3:A:84:ILE:HG23	3:A:84:ILE:O	2.17	0.43
3:A:148:CYS:HB3	3:A:167:CYS:O	2.18	0.43
3:A:901:LEU:HD13	3:A:919:ILE:CG2	2.48	0.43
4:B:194:GLU:OE1	4:B:194:GLU:HA	2.18	0.43
4:B:202:TYR:CD2	4:B:202:TYR:N	2.87	0.43
4:B:831:SER:CB	4:B:994:TYR:OH	2.67	0.43
4:B:904:ARG:CZ	4:B:948:ILE:HD11	2.48	0.43
4:B:1171:VAL:HG13	4:B:1191:ILE:HD13	1.99	0.43
6:E:114:ASN:O	6:E:115:ASN:HB3	2.18	0.43
11:K:47:ARG:HH11	11:K:47:ARG:CB	2.23	0.43
1:R:6:G:H2'	1:R:7:A:O5'	2.19	0.43
14:R:3000:UTP:C2	2:T:4:DA:N1	2.86	0.43
3:A:99:ILE:O	3:A:102:VAL:HB	2.19	0.43
3:A:344:ARG:O	4:B:1118:PRO:HG2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:565:ILE:HD13	3:A:567:LYS:HE2	2.01	0.43
3:A:751:SER:OG	4:B:1015:HIS:CE1	2.71	0.43
3:A:968:GLN:NE2	3:A:1035:TYR:HB2	2.33	0.43
3:A:1424:VAL:HG11	4:B:1139:ILE:HD13	2.00	0.43
4:B:280:ILE:CG2	4:B:285:ILE:HG13	2.47	0.43
4:B:295:GLY:H	4:B:298:LEU:HG	1.84	0.43
4:B:345:LYS:N	4:B:348:ARG:HE	2.15	0.43
4:B:758:PHE:CZ	4:B:1044:ALA:HA	2.53	0.43
4:B:955:THR:HA	12:L:54:ARG:O	2.19	0.43
4:B:1116:ARG:CZ	4:B:1198:TYR:CE1	3.01	0.43
4:B:1117:GLN:HG3	4:B:1156:ASP:CG	2.43	0.43
5:C:39:ALA:CA	5:C:164:ALA:HB3	2.47	0.43
5:C:148:ARG:HD3	5:C:149:LYS:H	1.83	0.43
6:E:138:ALA:C	6:E:140:LEU:N	2.76	0.43
3:A:50:ILE:C	3:A:52:GLY:N	2.69	0.43
3:A:381:THR:O	3:A:382:PRO:C	2.60	0.43
3:A:645:LEU:HD11	3:A:649:ILE:HD11	2.01	0.43
3:A:672:ASP:O	3:A:675:THR:HB	2.19	0.43
3:A:673:GLY:N	3:A:674:PRO:HD2	2.33	0.43
3:A:852:TYR:CE2	7:F:136:ARG:NE	2.86	0.43
3:A:1048:ASN:O	3:A:1049:ILE:C	2.61	0.43
3:A:1409:LEU:HD23	3:A:1409:LEU:HA	1.83	0.43
4:B:204:ILE:C	4:B:205:ILE:HD12	2.43	0.43
4:B:648:HIS:HB2	4:B:649:LYS:H	1.61	0.43
4:B:745:PRO:C	4:B:747:MET:H	2.26	0.43
5:C:135:GLN:O	5:C:136:ASP:O	2.37	0.43
6:E:145:THR:HG21	6:E:187:TYR:CE2	2.53	0.43
10:J:31:ASP:O	10:J:32:GLU:C	2.61	0.43
12:L:40:LEU:HD23	12:L:40:LEU:HA	1.77	0.43
3:A:89:PRO:HG3	3:A:208:LEU:HD12	2.00	0.43
3:A:367:PRO:O	3:A:368:LYS:C	2.61	0.43
3:A:457:ALA:O	3:A:507:VAL:HG23	2.19	0.43
3:A:466:SER:HB3	11:K:2:ASN:HD22	1.83	0.43
3:A:601:LYS:O	3:A:602:ASP:C	2.62	0.43
3:A:709:THR:O	3:A:712:GLU:N	2.52	0.43
3:A:709:THR:HG23	9:I:94:ASP:HA	2.00	0.43
3:A:1194:ARG:HH22	3:A:1237:ILE:HD13	1.73	0.43
4:B:126:SER:OG	4:B:172:ILE:HD11	2.18	0.43
4:B:128:LEU:HD12	4:B:128:LEU:HA	1.82	0.43
4:B:705:MET:H	4:B:710:LEU:CD1	2.32	0.43
4:B:784:ASN:HD21	4:B:788:ARG:HD2	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:839:MET:HE1	4:B:980:PHE:CB	2.48	0.43
4:B:878:GLN:O	4:B:879:ARG:C	2.61	0.43
4:B:1108:ARG:O	4:B:1108:ARG:CG	2.67	0.43
8:H:47:PHE:CB	8:H:95:TYR:HD1	2.31	0.43
9:I:106:CYS:O	9:I:107:SER:HB2	2.18	0.43
3:A:63:ARG:CA	3:A:74:MET:HE2	2.49	0.43
3:A:114:LEU:HD12	3:A:142:CYS:O	2.19	0.43
3:A:396:PRO:HG3	3:A:416:ARG:HB3	2.00	0.43
3:A:547:LEU:HD22	11:K:58:PHE:HD1	1.84	0.43
3:A:1004:ASN:O	3:A:1008:GLN:HB2	2.19	0.43
3:A:1394:THR:HG22	3:A:1395:GLY:O	2.19	0.43
4:B:113:TYR:CD2	4:B:192:LEU:HD22	2.53	0.43
4:B:436:VAL:O	4:B:437:GLU:C	2.61	0.43
4:B:702:LEU:HD22	4:B:737:THR:CG2	2.49	0.43
4:B:809:MET:HE1	4:B:983:ARG:HH22	1.82	0.43
6:E:16:PHE:CZ	6:E:20:LYS:HE2	2.54	0.43
6:E:69:ILE:O	6:E:73:PRO:HG3	2.19	0.43
7:F:140:ASP:OD1	7:F:141:GLY:N	2.52	0.43
8:H:111:LEU:HD23	8:H:127:GLY:O	2.18	0.43
3:A:306:ASN:OD1	3:A:313:GLN:NE2	2.51	0.43
3:A:337:ARG:CZ	3:A:839:ARG:CZ	2.97	0.43
3:A:907:THR:HG22	3:A:908:LEU:H	1.82	0.43
3:A:1368:MET:O	3:A:1369:ALA:C	2.62	0.43
4:B:274:PRO:O	4:B:276:ILE:N	2.51	0.43
4:B:1023:VAL:O	4:B:1024:ALA:C	2.62	0.43
5:C:249:ASP:OD1	5:C:253:LYS:HE3	2.19	0.43
6:E:168:TYR:O	6:E:170:LEU:HD23	2.19	0.43
9:I:46:HIS:O	9:I:47:GLU:HB2	2.18	0.43
9:I:59:VAL:HG12	9:I:60:GLN:N	2.34	0.43
3:A:134:ARG:O	3:A:137:ALA:N	2.52	0.42
3:A:289:ILE:C	3:A:291:GLU:H	2.27	0.42
3:A:362:ASP:OD1	3:A:459:ARG:HD3	2.18	0.42
3:A:518:LYS:HB2	3:A:519:PRO:HD2	2.01	0.42
3:A:1428:VAL:HG13	4:B:1151:LEU:HD23	2.00	0.42
4:B:34:ILE:HG12	4:B:542:MET:CE	2.49	0.42
4:B:794:ASN:O	4:B:795:ILE:HD12	2.19	0.42
4:B:1070:GLU:O	4:B:1071:VAL:C	2.60	0.42
5:C:148:ARG:H	5:C:151:GLN:HG3	1.84	0.42
3:A:86:LEU:HB3	3:A:296:LEU:HD21	2.00	0.42
3:A:574:GLY:O	3:A:575:LYS:C	2.61	0.42
3:A:868:TYR:C	3:A:870:GLU:N	2.76	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1366:ARG:HG2	3:A:1366:ARG:HH11	1.84	0.42
4:B:329:THR:O	4:B:332:ASP:HB3	2.19	0.42
4:B:416:LEU:O	4:B:417:PHE:C	2.61	0.42
4:B:482:VAL:O	4:B:483:LEU:C	2.63	0.42
4:B:601:ARG:O	4:B:605:ARG:HG3	2.19	0.42
4:B:806:THR:O	4:B:808:ALA:N	2.52	0.42
5:C:59:ALA:O	5:C:63:ILE:HG13	2.18	0.42
5:C:76:ASP:OD2	5:C:128:ASN:N	2.47	0.42
5:C:263:THR:C	5:C:265:MET:N	2.76	0.42
6:E:98:ILE:O	6:E:99:HIS:C	2.62	0.42
2:T:1:DA:H2''	2:T:2:DC:C5'	2.41	0.42
2:T:6:DC:C2'	2:T:7:DC:O5'	2.67	0.42
3:A:30:ILE:O	3:A:31:SER:O	2.37	0.42
3:A:80:HIS:N	3:A:243:PRO:HB3	2.34	0.42
3:A:131:SER:OG	3:A:132:LYS:N	2.51	0.42
3:A:451:HIS:HB2	3:A:454:SER:OG	2.19	0.42
3:A:753:GLY:HA2	3:A:757:ASN:ND2	2.34	0.42
3:A:811:GLN:O	3:A:812:GLU:C	2.62	0.42
3:A:1027:ALA:O	3:A:1030:ARG:HB2	2.20	0.42
4:B:281:PRO:HG2	4:B:284:ILE:CD1	2.45	0.42
4:B:880:THR:O	4:B:881:ASN:HB2	2.20	0.42
4:B:955:THR:CG2	12:L:54:ARG:O	2.65	0.42
4:B:1060:ARG:C	4:B:1062:HIS:H	2.26	0.42
4:B:1073:TYR:CD1	4:B:1073:TYR:N	2.87	0.42
4:B:1148:LYS:O	4:B:1152:MET:HB2	2.19	0.42
4:B:1177:HIS:O	4:B:1179:GLN:HG3	2.19	0.42
5:C:8:VAL:HA	5:C:21:ILE:O	2.19	0.42
5:C:242:GLN:O	5:C:246:ARG:N	2.52	0.42
6:E:134:THR:C	6:E:135:PHE:HD1	2.28	0.42
6:E:168:TYR:CB	6:E:170:LEU:HG	2.49	0.42
9:I:84:VAL:O	9:I:84:VAL:HG13	2.19	0.42
10:J:9:SER:HB2	10:J:45:CYS:HB2	2.00	0.42
11:K:95:ILE:O	11:K:98:LEU:HB2	2.19	0.42
3:A:7:SER:OG	4:B:1193:GLN:NE2	2.51	0.42
3:A:35:ILE:HD13	3:A:53:LEU:HD23	2.00	0.42
3:A:68:GLN:O	3:A:70:CYS:N	2.52	0.42
3:A:151:ASP:OD1	3:A:163:SER:HA	2.19	0.42
3:A:166:GLY:O	3:A:167:CYS:CB	2.67	0.42
3:A:223:GLY:O	3:A:1415:SER:CA	2.64	0.42
3:A:447:GLN:HA	3:A:448:PRO:C	2.44	0.42
3:A:751:SER:O	3:A:752:LYS:CB	2.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1152:ILE:HG23	3:A:1260:LEU:CD2	2.43	0.42
4:B:55:VAL:O	4:B:59:LEU:HB3	2.19	0.42
4:B:348:ARG:O	4:B:349:ILE:C	2.60	0.42
4:B:757:PRO:HG2	4:B:984:HIS:CE1	2.54	0.42
4:B:969:ARG:HG2	4:B:970:THR:N	2.33	0.42
8:H:143:LEU:HD12	8:H:143:LEU:N	2.34	0.42
9:I:55:THR:HG21	9:I:109:ILE:CD1	2.49	0.42
10:J:21:TYR:CA	10:J:39:LEU:HD11	2.49	0.42
10:J:53:HIS:CE1	10:J:55:ASP:HA	2.54	0.42
12:L:58:LYS:O	12:L:59:ALA:C	2.63	0.42
4:B:39:ARG:HG2	4:B:39:ARG:HH11	1.85	0.42
4:B:115:GLN:HG2	4:B:193:LYS:HB2	2.01	0.42
4:B:1197:PRO:O	4:B:1200:ALA:HB3	2.19	0.42
4:B:1204:PHE:O	4:B:1207:LEU:HB2	2.19	0.42
5:C:20:PHE:CD1	5:C:20:PHE:C	2.97	0.42
6:E:72:PHE:CD2	6:E:155:ARG:NH2	2.83	0.42
2:T:4:DA:C6	3:A:831:THR:HG21	2.54	0.42
3:A:113:LEU:C	3:A:115:LEU:N	2.77	0.42
3:A:441:PRO:O	3:A:441:PRO:HG2	2.20	0.42
3:A:530:GLY:O	3:A:532:ARG:N	2.53	0.42
3:A:894:GLU:C	3:A:896:ARG:N	2.74	0.42
3:A:984:LYS:O	3:A:988:LEU:HB2	2.19	0.42
3:A:1161:THR:OG1	3:A:1170:ILE:HD11	2.20	0.42
4:B:28:GLU:OE1	4:B:807:ARG:NH2	2.44	0.42
4:B:121:ASN:HA	4:B:207:GLY:CA	2.46	0.42
4:B:234:ILE:HD12	4:B:234:ILE:N	2.30	0.42
4:B:405:ARG:CZ	4:B:632:ARG:HG2	2.49	0.42
4:B:1026:LEU:O	4:B:1027:ILE:C	2.63	0.42
4:B:1106:ARG:HH12	4:B:1118:PRO:CA	2.33	0.42
5:C:214:ASN:CB	5:C:217:ASP:OD2	2.68	0.42
5:C:261:ALA:O	5:C:262:LEU:C	2.61	0.42
6:E:59:SER:HA	6:E:80:VAL:O	2.19	0.42
3:A:76:GLU:O	3:A:78:PRO:CD	2.68	0.42
3:A:1150:SER:HB2	3:A:1195:LEU:CD2	2.49	0.42
3:A:1187:GLN:HA	3:A:1243:VAL:HG23	2.02	0.42
4:B:331:LEU:HD12	4:B:331:LEU:HA	1.87	0.42
4:B:640:VAL:HG22	4:B:651:LEU:HD23	2.01	0.42
4:B:758:PHE:CE2	4:B:1044:ALA:HA	2.53	0.42
4:B:834:ASN:HB2	4:B:838:SER:O	2.19	0.42
4:B:995:ARG:HH11	4:B:995:ARG:CB	2.33	0.42
4:B:1182:CYS:SG	4:B:1185:CYS:HB2	2.60	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:252:GLN:NE2	11:K:99:GLY:N	2.68	0.42
9:I:87:GLN:O	9:I:88:SER:C	2.62	0.42
3:A:113:LEU:HG	3:A:218:ASP:OD1	2.19	0.42
3:A:401:GLY:H	3:A:435:HIS:HD2	1.66	0.42
3:A:427:GLN:O	3:A:428:TYR:C	2.62	0.42
3:A:639:PRO:HG2	3:A:640:GLN:H	1.84	0.42
3:A:683:ILE:CD1	3:A:764:CYS:HB2	2.42	0.42
3:A:760:GLN:CB	4:B:1021:MET:HE1	2.50	0.42
4:B:105:SER:O	4:B:106:ASP:HB2	2.20	0.42
4:B:203:PHE:HE1	4:B:212:LEU:HD12	1.85	0.42
4:B:435:THR:O	4:B:435:THR:HG22	2.20	0.42
4:B:640:VAL:HG22	4:B:651:LEU:CD2	2.50	0.42
4:B:835:GLN:O	4:B:836:GLU:C	2.62	0.42
4:B:849:GLY:O	4:B:850:LEU:C	2.59	0.42
7:F:89:GLU:HB3	7:F:134:ILE:HD13	2.00	0.42
9:I:101:PHE:HD1	9:I:110:PHE:O	2.02	0.42
3:A:383:TYR:HB3	7:F:115:THR:CG2	2.44	0.42
3:A:534:LEU:HD13	3:A:656:TRP:CD1	2.54	0.42
3:A:637:LYS:HA	3:A:637:LYS:HD3	1.93	0.42
3:A:834:THR:HG21	3:A:1077:THR:HA	2.00	0.42
3:A:1168:GLU:O	3:A:1172:LEU:HG	2.19	0.42
3:A:1390:ASN:HD21	3:A:1399:ARG:HA	1.78	0.42
4:B:634:TYR:CD1	4:B:692:TYR:HB3	2.55	0.42
4:B:705:MET:N	4:B:710:LEU:HD12	2.34	0.42
4:B:749:LEU:HD22	4:B:753:ALA:CB	2.50	0.42
4:B:855:PHE:HZ	4:B:857:ARG:HH12	1.64	0.42
4:B:877:PRO:O	4:B:878:GLN:HG2	2.19	0.42
4:B:1152:MET:SD	4:B:1197:PRO:HD3	2.59	0.42
8:H:12:VAL:HG13	8:H:26:ILE:HG23	2.01	0.42
8:H:111:LEU:C	8:H:112:ILE:HG13	2.45	0.42
9:I:29:CYS:C	9:I:31:THR:N	2.77	0.42
3:A:84:ILE:HG21	3:A:239:LEU:HD23	2.01	0.42
3:A:407:ARG:HG2	3:A:430:TRP:CE2	2.54	0.42
3:A:474:VAL:HG13	3:A:474:VAL:O	2.20	0.42
3:A:633:VAL:HG11	3:A:645:LEU:HD22	2.01	0.42
3:A:725:ALA:HA	3:A:728:LYS:HE2	2.02	0.42
3:A:1342:GLU:HG2	6:E:212:ARG:HH11	1.83	0.42
4:B:313:MET:HE1	4:B:386:LEU:HD22	1.99	0.42
4:B:546:SER:OG	4:B:631:GLY:N	2.52	0.42
4:B:1106:ARG:HH12	4:B:1118:PRO:HA	1.85	0.42
5:C:5:GLY:O	5:C:6:PRO:O	2.37	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:214:ASN:O	5:C:215:GLU:C	2.62	0.42
6:E:19:VAL:O	6:E:19:VAL:HG12	2.20	0.42
8:H:31:THR:O	8:H:32:THR:OG1	2.37	0.42
11:K:93:SER:O	11:K:97:LYS:HG3	2.20	0.42
3:A:38:PRO:CA	3:A:270:LEU:HD23	2.50	0.41
3:A:59:GLY:HA2	3:A:67:CYS:SG	2.60	0.41
3:A:101:LYS:HG2	3:A:139:TRP:CZ2	2.55	0.41
3:A:399:HIS:CB	3:A:400:PRO:HD3	2.45	0.41
3:A:782:ARG:NH2	9:I:67:THR:HG22	2.35	0.41
3:A:1343:ALA:O	3:A:1346:ALA:HB3	2.20	0.41
3:A:1406:VAL:CG1	3:A:1410:PHE:CE1	3.03	0.41
4:B:230:ALA:O	4:B:232:SER:N	2.47	0.41
5:C:14:SER:HA	11:K:114:LEU:HD22	2.02	0.41
6:E:178:ILE:CG2	6:E:214:CYS:HA	2.48	0.41
8:H:57:VAL:CG1	8:H:58:THR:N	2.83	0.41
12:L:29:TYR:C	12:L:30:ILE:HG13	2.45	0.41
1:R:2:U:C4	1:R:3:C:N4	2.88	0.41
3:A:474:VAL:HG13	3:A:478:TYR:HE1	1.85	0.41
3:A:515:GLN:CG	3:A:516:SER:N	2.84	0.41
3:A:1223:ASP:C	3:A:1243:VAL:HG12	2.45	0.41
3:A:1329:THR:HG22	3:A:1330:ASN:N	2.35	0.41
4:B:56:ASP:CB	4:B:57:TYR:HD1	2.34	0.41
4:B:368:GLU:O	4:B:371:GLU:OE1	2.37	0.41
5:C:27:LEU:O	5:C:27:LEU:HD12	2.20	0.41
6:E:79:TRP:HD1	6:E:96:PHE:HE1	1.67	0.41
8:H:139:ASN:O	8:H:140:ALA:CB	2.68	0.41
3:A:88:LYS:HD2	3:A:293:GLU:OE1	2.20	0.41
3:A:683:ILE:O	3:A:686:ALA:N	2.53	0.41
3:A:881:GLN:NE2	3:A:958:VAL:O	2.46	0.41
3:A:1139:GLU:HG3	3:A:1280:GLU:O	2.20	0.41
3:A:1173:HIS:NE2	3:A:1227:ILE:HG23	2.35	0.41
3:A:1205:LYS:O	3:A:1206:ASP:C	2.63	0.41
3:A:1364:ASN:HD21	3:A:1366:ARG:NH1	2.19	0.41
4:B:315:LYS:O	4:B:317:CYS:N	2.53	0.41
4:B:797:TYR:HB3	4:B:798:TYR:CD1	2.55	0.41
4:B:879:ARG:O	4:B:880:THR:HB	2.20	0.41
4:B:1114:LEU:O	4:B:1198:TYR:HE2	2.04	0.41
4:B:1162:ILE:HG22	4:B:1163:CYS:N	2.34	0.41
4:B:1177:HIS:O	4:B:1179:GLN:N	2.52	0.41
5:C:17:ASN:C	5:C:18:VAL:HG23	2.45	0.41
8:H:4:THR:O	8:H:5:LEU:HD23	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:25:LEU:HD12	9:I:26:LEU:N	2.35	0.41
10:J:53:HIS:CD2	10:J:54:VAL:N	2.88	0.41
11:K:35:PHE:O	11:K:70:ARG:HB2	2.21	0.41
3:A:49:LYS:NZ	3:A:60:SER:HA	2.34	0.41
3:A:542:GLU:OE1	3:A:569:LYS:HE2	2.20	0.41
3:A:568:PRO:CB	5:C:221:TYR:CZ	3.03	0.41
3:A:783:THR:CG2	3:A:815:PHE:CZ	2.98	0.41
3:A:871:ASP:CB	6:E:204:THR:CG2	2.98	0.41
3:A:1064:VAL:O	3:A:1065:GLY:C	2.63	0.41
3:A:1378:GLN:C	3:A:1380:GLY:H	2.29	0.41
5:C:204:SER:O	5:C:205:LYS:C	2.63	0.41
11:K:82:ASP:O	11:K:85:ASP:HB2	2.20	0.41
12:L:41:SER:O	12:L:44:ASP:HB2	2.21	0.41
3:A:172:PRO:HB3	3:A:185:TRP:CZ2	2.55	0.41
3:A:339:ASN:HB3	4:B:1117:GLN:HE22	1.85	0.41
3:A:383:TYR:O	7:F:115:THR:HG22	2.20	0.41
3:A:401:GLY:N	3:A:435:HIS:HD2	2.19	0.41
3:A:885:THR:HG23	3:A:893:PHE:CE1	2.36	0.41
3:A:1126:ALA:O	3:A:1128:GLN:N	2.53	0.41
3:A:1254:ALA:O	3:A:1255:GLU:HB2	2.20	0.41
3:A:1317:MET:CA	3:A:1322:ILE:HD11	2.46	0.41
3:A:1359:ASP:C	3:A:1361:SER:N	2.78	0.41
3:A:1402:PHE:O	3:A:1404:GLU:N	2.51	0.41
4:B:54:PHE:HA	4:B:58:THR:CB	2.47	0.41
4:B:171:PRO:HD2	4:B:457:LEU:HD12	2.03	0.41
4:B:310:MET:O	4:B:311:LEU:C	2.62	0.41
4:B:362:PRO:C	4:B:363:HIS:O	2.58	0.41
4:B:499:ASN:OD1	4:B:500:THR:N	2.53	0.41
4:B:872:GLU:CD	4:B:914:LYS:CE	2.94	0.41
4:B:1033:LYS:NZ	4:B:1087:PHE:O	2.51	0.41
6:E:13:TRP:O	6:E:16:PHE:HB3	2.21	0.41
6:E:35:VAL:C	6:E:37:LEU:N	2.78	0.41
6:E:121:MET:C	6:E:123:LEU:N	2.75	0.41
11:K:107:THR:O	11:K:108:GLU:C	2.63	0.41
3:A:71:GLN:HB2	3:A:72:GLU:H	1.62	0.41
3:A:553:VAL:HG22	3:A:652:VAL:CG2	2.51	0.41
3:A:568:PRO:HB3	5:C:221:TYR:OH	2.21	0.41
3:A:980:ASP:OD2	3:A:1039:LYS:HB3	2.21	0.41
4:B:92:PHE:HD2	4:B:130:VAL:HG11	1.85	0.41
4:B:167:ILE:O	4:B:168:GLY:O	2.38	0.41
4:B:841:MET:HE3	4:B:1010:LEU:HD13	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:911:ILE:HD11	4:B:941:LEU:CB	2.50	0.41
5:C:175:ALA:HB3	10:J:43:ARG:CZ	2.51	0.41
5:C:178:PHE:C	5:C:178:PHE:CD2	2.99	0.41
5:C:252:GLN:HG3	11:K:95:ILE:HG23	2.03	0.41
6:E:72:PHE:N	6:E:72:PHE:CD1	2.89	0.41
6:E:116:ILE:CG2	6:E:117:THR:N	2.84	0.41
9:I:63:GLY:O	9:I:70:ARG:NH2	2.53	0.41
9:I:85:PHE:HD1	9:I:99:LEU:HD22	1.83	0.41
10:J:3:VAL:CG2	10:J:18:TRP:CG	3.02	0.41
10:J:12:LYS:O	10:J:13:VAL:C	2.64	0.41
3:A:45:GLN:O	3:A:46:THR:C	2.64	0.41
3:A:514:PRO:HB2	3:A:875:ALA:HB3	2.01	0.41
3:A:541:ILE:HD12	3:A:541:ILE:N	2.34	0.41
3:A:577:ILE:O	3:A:578:LEU:C	2.62	0.41
3:A:808:LEU:HD12	3:A:808:LEU:N	2.35	0.41
3:A:815:PHE:O	3:A:816:HIS:C	2.63	0.41
3:A:1155:ASP:O	3:A:1190:PRO:O	2.37	0.41
4:B:53:GLN:HG2	4:B:547:VAL:HG13	2.02	0.41
4:B:120:ARG:HH12	12:L:54:ARG:NH1	2.18	0.41
4:B:269:ILE:HB	4:B:317:CYS:SG	2.60	0.41
4:B:530:GLY:O	4:B:531:GLN:C	2.64	0.41
4:B:591:ARG:O	4:B:592:ASN:C	2.63	0.41
4:B:850:LEU:HD22	4:B:1009:ASP:HB3	2.02	0.41
4:B:1106:ARG:HH11	4:B:1118:PRO:HB3	1.82	0.41
5:C:186:LEU:HD12	5:C:186:LEU:HA	1.86	0.41
6:E:131:THR:HG21	6:E:191:LYS:HE2	2.02	0.41
8:H:109:LYS:HB2	8:H:109:LYS:HZ2	1.86	0.41
3:A:14:VAL:HB	3:A:1430:LEU:HD13	2.02	0.41
3:A:332:LYS:H	3:A:337:ARG:CB	2.33	0.41
3:A:407:ARG:HG2	3:A:430:TRP:CZ2	2.56	0.41
3:A:556:TRP:CE2	3:A:558:GLY:HA2	2.56	0.41
3:A:971:PHE:O	3:A:972:HIS:C	2.63	0.41
3:A:1107:VAL:CG2	3:A:1383:SER:HA	2.51	0.41
4:B:205:ILE:HG21	4:B:462:ALA:HB2	2.03	0.41
4:B:244:LEU:HB2	4:B:249:ARG:HA	2.03	0.41
4:B:387:LEU:HD23	4:B:393:LYS:HD2	2.03	0.41
4:B:702:LEU:CD2	4:B:735:ALA:HB1	2.51	0.41
4:B:952:VAL:HG13	4:B:966:VAL:HG22	2.03	0.41
9:I:40:SER:HB2	9:I:41:PRO:HD2	2.03	0.41
11:K:106:GLU:O	11:K:110:ASN:ND2	2.54	0.41
1:R:5:A:C5	1:R:6:G:N7	2.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:9:DC:OP1	4:B:1123:SER:CB	2.61	0.41
3:A:14:VAL:O	3:A:15:LYS:HD3	2.20	0.41
3:A:134:ARG:O	3:A:136:ALA:N	2.54	0.41
3:A:384:ASN:CG	3:A:388:LEU:HD12	2.45	0.41
3:A:432:VAL:O	3:A:434:ARG:N	2.54	0.41
3:A:574:GLY:O	3:A:577:ILE:HG12	2.21	0.41
3:A:843:LYS:HG3	3:A:1402:PHE:CD1	2.54	0.41
3:A:878:ILE:C	3:A:879:GLU:CG	2.94	0.41
3:A:894:GLU:C	3:A:896:ARG:H	2.29	0.41
3:A:1006:ILE:HG22	3:A:1007:ILE:N	2.36	0.41
3:A:1039:LYS:NZ	3:A:1043:ASP:OD1	2.47	0.41
3:A:1074:GLU:O	3:A:1075:PRO:C	2.63	0.41
3:A:1116:LEU:CD2	3:A:1316:VAL:HG21	2.51	0.41
3:A:1208:THR:O	3:A:1209:MET:C	2.62	0.41
4:B:51:PHE:O	4:B:54:PHE:N	2.54	0.41
4:B:188:ASP:O	4:B:192:LEU:HG	2.21	0.41
4:B:205:ILE:N	4:B:205:ILE:CD1	2.84	0.41
4:B:293:PRO:O	4:B:294:ASP:C	2.64	0.41
4:B:418:LYS:O	4:B:420:LEU:N	2.54	0.41
4:B:577:ALA:HB1	4:B:589:VAL:HG12	2.00	0.41
4:B:579:ARG:HB2	4:B:586:TRP:HE1	1.84	0.41
4:B:589:VAL:CG1	4:B:590:HIS:N	2.84	0.41
4:B:737:THR:HG23	9:I:66:PRO:HB3	2.01	0.41
4:B:843:GLN:HB2	4:B:993:THR:OG1	2.20	0.41
4:B:1115:THR:CG2	4:B:1199:ALA:HB2	2.50	0.41
4:B:1152:MET:O	4:B:1156:ASP:O	2.39	0.41
4:B:1177:HIS:HB2	4:B:1179:GLN:HG3	2.03	0.41
5:C:114:TYR:CG	5:C:140:ASN:HB3	2.56	0.41
6:E:3:GLN:HG3	6:E:5:ASN:H	1.85	0.41
6:E:7:ARG:HG3	6:E:8:ASN:N	2.36	0.41
6:E:116:ILE:HG22	6:E:117:THR:N	2.36	0.41
7:F:75:PRO:C	7:F:77:ASP:N	2.78	0.41
7:F:109:VAL:CG1	7:F:110:ASP:H	2.34	0.41
8:H:38:LEU:HD13	8:H:125:LEU:CD1	2.46	0.41
9:I:6:PHE:HD2	9:I:13:MET:HA	1.86	0.41
9:I:98:VAL:HG12	9:I:99:LEU:N	2.36	0.41
9:I:99:LEU:HB2	9:I:112:SER:OG	2.21	0.41
11:K:65:HIS:HD2	11:K:67:PHE:CB	2.33	0.41
11:K:103:THR:O	11:K:106:GLU:N	2.53	0.41
3:A:321:PRO:O	3:A:322:VAL:CB	2.63	0.41
3:A:336:ILE:CD1	3:A:1405:THR:HG21	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1017:LEU:HB3	6:E:205:SER:HA	2.03	0.41
4:B:121:ASN:HD21	4:B:965:LYS:HE3	1.86	0.41
4:B:233:PRO:HG2	4:B:234:ILE:HG13	2.03	0.41
4:B:280:ILE:O	4:B:281:PRO:C	2.64	0.41
4:B:369:GLY:C	4:B:370:PHE:CD1	2.99	0.41
4:B:381:MET:HE3	4:B:381:MET:HB2	1.97	0.41
4:B:704:ALA:HB2	4:B:738:PHE:CD1	2.56	0.41
4:B:846:ILE:CG2	4:B:974:PRO:HG2	2.51	0.41
4:B:864:LYS:CG	4:B:865:LYS:N	2.80	0.41
4:B:992:ILE:CD1	4:B:994:TYR:CE2	3.04	0.41
4:B:995:ARG:O	4:B:996:ARG:C	2.63	0.41
4:B:1149:GLU:HG3	4:B:1153:GLU:OE1	2.20	0.41
8:H:84:ALA:HA	8:H:87:ARG:CB	2.51	0.41
9:I:16:PRO:HA	9:I:26:LEU:O	2.20	0.41
9:I:26:LEU:HD23	9:I:37:GLU:HA	2.03	0.41
10:J:27:GLU:C	10:J:29:GLU:N	2.77	0.41
3:A:130:ASP:O	3:A:131:SER:C	2.64	0.40
3:A:205:GLU:O	3:A:208:LEU:HB2	2.22	0.40
3:A:530:GLY:O	3:A:533:LYS:N	2.53	0.40
3:A:909:ASP:OD1	3:A:910:PRO:HD2	2.22	0.40
3:A:960:ILE:HD12	3:A:1021:LEU:CD2	2.50	0.40
3:A:992:ASP:O	3:A:993:LEU:C	2.64	0.40
3:A:1038:THR:O	3:A:1039:LYS:C	2.62	0.40
3:A:1107:VAL:HG23	3:A:1383:SER:HA	2.03	0.40
3:A:1345:ARG:HH11	3:A:1373:ASP:CG	2.29	0.40
4:B:627:PHE:O	4:B:632:ARG:NH1	2.54	0.40
4:B:737:THR:HG21	9:I:66:PRO:C	2.39	0.40
4:B:941:LEU:HD21	4:B:946:ASN:HA	2.02	0.40
5:C:46:ILE:CG2	5:C:157:CYS:HB3	2.51	0.40
5:C:51:VAL:HG22	5:C:155:LEU:CD2	2.47	0.40
6:E:28:TYR:CE1	6:E:78:LEU:CD1	3.03	0.40
6:E:63:ASN:HA	6:E:64:PRO:HD3	1.92	0.40
7:F:138:LEU:HD23	7:F:138:LEU:HA	1.83	0.40
8:H:126:GLU:N	8:H:130:ARG:HH12	2.19	0.40
10:J:48:ARG:HG2	10:J:48:ARG:HH11	1.86	0.40
11:K:47:ARG:HH11	11:K:48:ALA:N	2.19	0.40
2:T:7:DC:C5'	2:T:7:DC:P	3.05	0.40
3:A:30:ILE:O	3:A:31:SER:C	2.64	0.40
3:A:203:SER:O	3:A:207:ILE:HG12	2.21	0.40
3:A:399:HIS:NE2	3:A:462:VAL:HG21	2.36	0.40
3:A:1102:LYS:HG2	3:A:1106:ASN:ND2	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1166:ASP:OD1	3:A:1194:ARG:NH2	2.49	0.40
4:B:175:ARG:HG2	4:B:175:ARG:HH11	1.87	0.40
4:B:624:LEU:C	4:B:624:LEU:HD12	2.46	0.40
4:B:803:LEU:CD1	4:B:1036:ALA:HB2	2.52	0.40
4:B:846:ILE:HG23	4:B:974:PRO:HG2	2.04	0.40
4:B:901:PRO:O	4:B:949:VAL:O	2.38	0.40
4:B:911:ILE:HG21	4:B:966:VAL:HG11	2.01	0.40
4:B:958:GLN:C	4:B:960:GLY:N	2.79	0.40
4:B:1197:PRO:O	4:B:1200:ALA:N	2.52	0.40
5:C:146:LYS:O	5:C:147:LEU:HD23	2.20	0.40
8:H:33:GLN:OE1	8:H:129:TYR:HE2	2.05	0.40
8:H:96:VAL:HG13	8:H:143:LEU:HG	2.02	0.40
9:I:99:LEU:O	9:I:111:THR:HG23	2.21	0.40
1:R:10:A:O3'	14:R:3000:UTP:O1A	2.37	0.40
3:A:18:GLN:O	4:B:1215:ARG:HG3	2.21	0.40
3:A:19:PHE:HA	4:B:1213:THR:O	2.22	0.40
3:A:209:ASN:O	3:A:210:ILE:C	2.64	0.40
3:A:331:GLY:O	3:A:332:LYS:O	2.39	0.40
3:A:445:ASN:HB3	3:A:455:MET:HG2	2.03	0.40
3:A:463:ILE:CD1	3:A:469:ARG:HG3	2.50	0.40
3:A:679:ILE:CG2	3:A:729:ALA:HB1	2.44	0.40
3:A:719:VAL:HG22	3:A:774:ARG:HD2	2.03	0.40
3:A:738:LYS:HA	8:H:19:ARG:NH2	2.36	0.40
3:A:751:SER:OG	4:B:1015:HIS:HE1	2.03	0.40
3:A:901:LEU:O	3:A:920:LEU:HD23	2.22	0.40
3:A:913:LEU:CD1	3:A:981:LEU:O	2.69	0.40
3:A:1224:LEU:HD11	3:A:1240:CYS:HB3	2.03	0.40
3:A:1322:ILE:HD12	3:A:1327:ILE:HD12	2.03	0.40
4:B:61:ASP:OD1	4:B:61:ASP:N	2.54	0.40
4:B:175:ARG:HH11	4:B:175:ARG:CG	2.34	0.40
4:B:276:ILE:HD11	4:B:355:ILE:CD1	2.50	0.40
4:B:330:ALA:C	4:B:332:ASP:N	2.78	0.40
4:B:380:TYR:O	4:B:384:ARG:HG2	2.21	0.40
4:B:658:ILE:HG22	4:B:662:MET:HE2	2.03	0.40
4:B:758:PHE:HB2	4:B:1024:ALA:HB1	2.03	0.40
4:B:840:ILE:HB	4:B:1011:ILE:HB	2.03	0.40
4:B:972:LYS:HD3	4:B:1098:MET:HE1	2.03	0.40
4:B:1104:HIS:HB2	4:B:1122:ARG:CB	2.51	0.40
6:E:11:ARG:NH2	6:E:141:VAL:HG21	2.37	0.40
8:H:138:GLU:HG2	8:H:139:ASN:N	2.35	0.40
3:A:270:LEU:O	3:A:274:ILE:HG13	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1240:CYS:C	3:A:1241:ARG:HG3	2.47	0.40
4:B:283:VAL:HG13	4:B:297:ILE:HD12	2.04	0.40
4:B:319:GLU:O	4:B:320:ASP:C	2.65	0.40
4:B:363:HIS:O	4:B:364:ILE:CG1	2.70	0.40
4:B:409:ALA:O	4:B:410:GLY:C	2.65	0.40
4:B:458:LYS:O	4:B:459:TYR:C	2.65	0.40
4:B:801:LYS:HE2	10:J:51:LEU:O	2.22	0.40
4:B:1156:ASP:HB3	4:B:1197:PRO:CA	2.52	0.40
5:C:182:PRO:HB2	5:C:207:CYS:SG	2.61	0.40
6:E:182:ASP:O	6:E:186:LEU:HG	2.21	0.40
11:K:7:PHE:C	11:K:9:LEU:H	2.29	0.40
11:K:49:GLU:C	11:K:51:LEU:N	2.79	0.40
11:K:51:LEU:CD1	11:K:59:ALA:HB3	2.51	0.40
12:L:28:LYS:O	12:L:29:TYR:CG	2.74	0.40
3:A:19:PHE:HB3	3:A:1413:GLY:HA2	2.03	0.40
3:A:48:ALA:O	3:A:49:LYS:CG	2.65	0.40
3:A:302:THR:O	3:A:313:GLN:NE2	2.54	0.40
3:A:379:VAL:HG22	3:A:431:LYS:HG2	2.03	0.40
3:A:1116:LEU:H	3:A:1308:THR:CG2	2.34	0.40
4:B:120:ARG:HH22	12:L:54:ARG:HD2	1.86	0.40
4:B:230:ALA:C	4:B:232:SER:N	2.79	0.40
4:B:288:ALA:O	4:B:331:LEU:CD1	2.69	0.40
4:B:484:ASN:ND2	4:B:486:TYR:HD1	2.19	0.40
4:B:616:ILE:HG12	4:B:696:GLU:HG3	2.03	0.40
4:B:839:MET:HE2	4:B:980:PHE:CD1	2.56	0.40
4:B:1084:GLN:NE2	5:C:192:TRP:HB2	2.37	0.40
4:B:1120:GLU:CG	4:B:1121:GLY:N	2.84	0.40
4:B:1159:ARG:NE	4:B:1193:GLN:NE2	2.33	0.40
4:B:1180:PHE:O	4:B:1181:GLU:CB	2.70	0.40
5:C:66:ARG:HB3	10:J:5:VAL:HG21	2.04	0.40
5:C:180:TYR:CD1	5:C:180:TYR:C	3.00	0.40
6:E:90:VAL:HA	6:E:120:ALA:HB2	2.04	0.40
7:F:130:ILE:HA	7:F:131:PRO:HD2	1.94	0.40
7:F:138:LEU:HB3	7:F:139:PRO:CD	2.51	0.40
8:H:117:SER:HA	8:H:122:LEU:HD23	2.02	0.40
9:I:92:ARG:CG	9:I:93:LYS:N	2.84	0.40
12:L:45:ALA:C	12:L:46:VAL:HG23	2.45	0.40

All (59) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:736:THR:CB	9:I:79:HIS:CD2[2_556]	0.78	1.42
4:B:736:THR:OG1	9:I:79:HIS:NE2[2_556]	0.83	1.37
9:I:81:ARG:O	9:I:81:ARG:CB[2_556]	1.01	1.19
4:B:736:THR:OG1	9:I:79:HIS:CD2[2_556]	1.02	1.18
3:A:923:LEU:CD1	9:I:35:VAL:C[4_546]	1.06	1.14
3:A:918:GLU:CB	9:I:21:GLU:OE1[4_546]	1.09	1.11
9:I:81:ARG:CA	9:I:81:ARG:O[2_556]	1.16	1.04
4:B:736:THR:OG1	9:I:79:HIS:CE1[2_556]	1.24	0.96
9:I:81:ARG:CA	9:I:81:ARG:C[2_556]	1.27	0.93
9:I:81:ARG:C	9:I:81:ARG:CB[2_556]	1.30	0.90
4:B:736:THR:CB	9:I:79:HIS:NE2[2_556]	1.35	0.85
9:I:71:SER:O	9:I:81:ARG:NE[2_556]	1.40	0.80
4:B:736:THR:OG1	9:I:79:HIS:CG[2_556]	1.42	0.78
3:A:923:LEU:CD1	9:I:36:GLU:N[4_546]	1.50	0.70
4:B:736:THR:OG1	9:I:79:HIS:ND1[2_556]	1.51	0.69
3:A:923:LEU:CD2	9:I:35:VAL:CB[4_546]	1.54	0.66
9:I:80:SER:OG	9:I:82:GLU:OE1[2_556]	1.56	0.64
9:I:81:ARG:N	9:I:81:ARG:O[2_556]	1.57	0.63
3:A:918:GLU:CB	9:I:21:GLU:CD[4_546]	1.62	0.58
9:I:81:ARG:O	9:I:81:ARG:CG[2_556]	1.66	0.54
3:A:923:LEU:CG	9:I:35:VAL:CB[4_546]	1.73	0.47
9:I:81:ARG:N	9:I:81:ARG:C[2_556]	1.73	0.47
3:A:923:LEU:CD1	9:I:35:VAL:O[4_546]	1.74	0.46
9:I:71:SER:N	9:I:81:ARG:NH2[2_556]	1.75	0.45
9:I:70:ARG:CA	9:I:81:ARG:NH2[2_556]	1.76	0.44
4:B:736:THR:CA	9:I:79:HIS:NE2[2_556]	1.77	0.43
9:I:80:SER:CB	9:I:82:GLU:CG[2_556]	1.79	0.41
9:I:70:ARG:C	9:I:81:ARG:NH2[2_556]	1.80	0.40
9:I:81:ARG:NH1	9:I:83:ASN:CB[2_556]	1.83	0.37
9:I:81:ARG:CA	9:I:81:ARG:CA[2_556]	1.83	0.37
3:A:918:GLU:CB	9:I:21:GLU:OE2[4_546]	1.85	0.35
9:I:81:ARG:NH1	9:I:83:ASN:CA[2_556]	1.89	0.31
9:I:81:ARG:NH1	9:I:83:ASN:C[2_556]	1.89	0.31
3:A:918:GLU:CA	9:I:21:GLU:OE1[4_546]	1.91	0.29
9:I:81:ARG:CA	9:I:81:ARG:CB[2_556]	1.91	0.29
9:I:81:ARG:C	9:I:81:ARG:C[2_556]	1.91	0.29
3:A:923:LEU:CD1	9:I:35:VAL:CA[4_546]	1.92	0.28
3:A:923:LEU:CD1	9:I:35:VAL:CG1[4_546]	1.92	0.28
3:A:923:LEU:CD2	9:I:35:VAL:CA[4_546]	1.93	0.27
4:B:736:THR:CG2	9:I:79:HIS:CD2[2_556]	1.96	0.24
9:I:71:SER:O	9:I:81:ARG:CD[2_556]	2.01	0.19
9:I:72:ASP:O	9:I:72:ASP:CB[2_556]	2.02	0.18

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:923:LEU:CD2	9:I:35:VAL:N[4_546]	2.04	0.16
3:A:923:LEU:CG	9:I:35:VAL:O[4_546]	2.07	0.13
3:A:923:LEU:CG	9:I:35:VAL:CG1[4_546]	2.07	0.13
3:A:923:LEU:CG	9:I:35:VAL:C[4_546]	2.07	0.13
3:A:923:LEU:CB	9:I:35:VAL:O[4_546]	2.09	0.11
9:I:80:SER:CB	9:I:82:GLU:CD[2_556]	2.09	0.11
9:I:81:ARG:NH1	9:I:83:ASN:O[2_556]	2.09	0.11
3:A:923:LEU:CD1	9:I:35:VAL:CB[4_546]	2.11	0.09
4:B:736:THR:CB	9:I:79:HIS:CG[2_556]	2.13	0.07
4:B:736:THR:CA	9:I:79:HIS:CD2[2_556]	2.15	0.05
4:B:736:THR:N	9:I:79:HIS:NE2[2_556]	2.15	0.05
9:I:72:ASP:O	9:I:72:ASP:O[2_556]	2.15	0.05
9:I:82:GLU:OE2	9:I:105:SER:OG[2_556]	2.15	0.05
4:B:715:ALA:CB	9:I:117:LYS:CD[2_556]	2.17	0.03
9:I:71:SER:C	9:I:81:ARG:NE[2_556]	2.19	0.01
9:I:80:SER:CB	9:I:82:GLU:OE1[2_556]	2.19	0.01
9:I:81:ARG:CD	9:I:83:ASN:ND2[2_556]	2.19	0.01

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	A	1365/1733 (79%)	1023 (75%)	252 (18%)	90 (7%)	1	12
4	B	1077/1224 (88%)	839 (78%)	169 (16%)	69 (6%)	1	13
5	C	264/318 (83%)	208 (79%)	40 (15%)	16 (6%)	1	14
6	E	212/215 (99%)	170 (80%)	33 (16%)	9 (4%)	2	18
7	F	82/155 (53%)	64 (78%)	15 (18%)	3 (4%)	2	20
8	H	129/146 (88%)	93 (72%)	21 (16%)	15 (12%)	0	5
9	I	117/122 (96%)	93 (80%)	15 (13%)	9 (8%)	1	10
10	J	63/70 (90%)	48 (76%)	11 (18%)	4 (6%)	1	13

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	K	112/120 (93%)	96 (86%)	15 (13%)	1 (1%)	14	49
12	L	44/70 (63%)	22 (50%)	12 (27%)	10 (23%)	0	1
All	All	3465/4173 (83%)	2656 (77%)	583 (17%)	226 (6%)	1	13

All (226) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	31	SER
3	A	48	ALA
3	A	55	ASP
3	A	56	PRO
3	A	74	MET
3	A	75	ASN
3	A	167	CYS
3	A	322	VAL
3	A	404	TYR
3	A	418	SER
3	A	543	LEU
3	A	567	LYS
3	A	597	LEU
3	A	598	LEU
3	A	628	GLY
3	A	752	LYS
3	A	846	GLU
3	A	998	LEU
3	A	1036	ARG
3	A	1127	ASP
3	A	1206	ASP
3	A	1221	LYS
3	A	1223	ASP
3	A	1392	SER
3	A	1393	ASN
3	A	1403	GLU
3	A	1406	VAL
3	A	1416	ALA
4	B	65	GLU
4	B	124	TYR
4	B	174	LEU
4	B	175	ARG
4	B	200	GLY
4	B	229	ALA

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Mol	Chain	Res	Type
4	B	364	ILE
4	B	367	LEU
4	B	531	GLN
4	B	708	GLU
4	B	709	ASP
4	B	731	VAL
4	B	751	VAL
4	B	958	GLN
4	B	959	ASP
4	B	1046	PRO
4	B	1103	ILE
4	B	1167	GLY
4	B	1176	ASN
4	B	1183	LYS
5	C	4	GLU
5	C	5	GLY
5	C	6	PRO
5	C	110	THR
5	C	142	VAL
5	C	215	GLU
7	F	73	ALA
8	H	32	THR
8	H	81	PRO
8	H	140	ALA
9	I	8	ARG
10	J	2	ILE
10	J	55	ASP
12	L	27	LEU
12	L	38	LEU
12	L	64	LEU
3	A	35	ILE
3	A	54	ASN
3	A	62	ASP
3	A	87	ALA
3	A	109	HIS
3	A	135	PHE
3	A	168	GLY
3	A	332	LYS
3	A	385	ILE
3	A	419	LYS
3	A	534	LEU
3	A	568	PRO

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Mol	Chain	Res	Type
3	A	790	ASP
3	A	986	ILE
3	A	1114	PRO
3	A	1365	TYR
3	A	1366	ARG
3	A	1379	GLY
4	B	55	VAL
4	B	168	GLY
4	B	275	TYR
4	B	346	GLU
4	B	410	GLY
4	B	480	SER
4	B	641	GLU
4	B	643	ASP
4	B	792	MET
4	B	864	LYS
4	B	866	TYR
4	B	884	ARG
4	B	891	ASP
4	B	992	ILE
4	B	1066	SER
4	B	1155	SER
5	C	136	ASP
7	F	142	SER
8	H	61	SER
8	H	77	ARG
8	H	88	SER
8	H	128	ASN
9	I	30	ARG
9	I	79	HIS
12	L	39	SER
12	L	52	GLY
3	A	6	TYR
3	A	45	GLN
3	A	59	GLY
3	A	67	CYS
3	A	69	THR
3	A	335	ARG
3	A	433	GLU
3	A	596	THR
3	A	737	LEU
3	A	775	ILE

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Mol	Chain	Res	Type
3	A	830	LYS
3	A	920	LEU
4	B	28	GLU
4	B	249	ARG
4	B	277	LYS
4	B	447	ALA
4	B	629	ASP
4	B	735	ALA
4	B	807	ARG
4	B	880	THR
4	B	1017	ILE
4	B	1099	VAL
4	B	1104	HIS
4	B	1178	ASN
5	C	48	SER
5	C	149	LYS
5	C	212	PRO
5	C	227	THR
6	E	31	THR
6	E	102	GLU
6	E	103	LYS
6	E	122	LYS
6	E	139	ALA
6	E	206	GLY
7	F	128	LYS
8	H	8	ASP
8	H	17	PRO
8	H	82	PRO
8	H	135	LEU
8	H	139	ASN
9	I	9	ASP
9	I	33	SER
9	I	86	PHE
10	J	9	SER
12	L	63	ARG
3	A	101	LYS
3	A	134	ARG
3	A	139	TRP
3	A	223	GLY
3	A	424	ILE
3	A	599	SER
3	A	1067	LEU

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Mol	Chain	Res	Type
3	A	1097	GLY
3	A	1115	SER
3	A	1122	PRO
3	A	1405	THR
4	B	304	ASP
4	B	436	VAL
4	B	501	PRO
4	B	667	GLN
4	B	791	THR
4	B	1054	GLY
4	B	1097	HIS
5	C	18	VAL
5	C	174	ALA
6	E	59	SER
10	J	6	ARG
12	L	50	ASP
12	L	56	LEU
3	A	58	LEU
3	A	399	HIS
3	A	400	PRO
3	A	958	VAL
3	A	972	HIS
3	A	1098	VAL
3	A	1130	GLN
3	A	1282	VAL
3	A	1351	GLU
3	A	1378	GLN
4	B	248	SER
4	B	419	THR
4	B	619	ILE
4	B	648	HIS
4	B	687	GLU
4	B	707	PRO
4	B	712	PRO
4	B	764	SER
4	B	907	GLY
4	B	982	SER
4	B	1108	ARG
6	E	36	GLU
8	H	62	SER
8	H	89	LEU
9	I	47	GLU

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Mol	Chain	Res	Type
9	I	88	SER
3	A	226	GLU
3	A	368	LYS
3	A	531	ILE
3	A	1014	ALA
3	A	1352	VAL
4	B	27	ALA
6	E	167	ARG
8	H	138	GLU
9	I	98	VAL
11	K	107	THR
12	L	59	ALA
4	B	247	GLY
3	A	336	ILE
3	A	1104	ILE
12	L	55	ILE
3	A	810	PRO
3	A	1075	PRO
3	A	1242	VAL
5	C	172	PRO
5	C	216	GLY
3	A	78	PRO
4	B	511	PRO
5	C	218	PRO

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	A	1206/1520 (79%)	1124 (93%)	82 (7%)	14	37
4	B	952/1061 (90%)	873 (92%)	79 (8%)	10	31
5	C	234/274 (85%)	218 (93%)	16 (7%)	14	37
6	E	196/197 (100%)	192 (98%)	4 (2%)	48	66
7	F	74/137 (54%)	68 (92%)	6 (8%)	11	32

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	H	117/128 (91%)	113 (97%)	4 (3%)	32	54
9	I	113/116 (97%)	105 (93%)	8 (7%)	13	36
10	J	60/65 (92%)	54 (90%)	6 (10%)	7	24
11	K	99/102 (97%)	88 (89%)	11 (11%)	6	21
12	L	40/57 (70%)	34 (85%)	6 (15%)	3	14
All	All	3091/3657 (84%)	2869 (93%)	222 (7%)	13	35

All (222) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	18	GLN
3	A	22	PHE
3	A	31	SER
3	A	56	PRO
3	A	70	CYS
3	A	93	VAL
3	A	247	ARG
3	A	269	ILE
3	A	302	THR
3	A	322	VAL
3	A	326	ARG
3	A	351	THR
3	A	375	THR
3	A	381	THR
3	A	385	ILE
3	A	397	ASN
3	A	434	ARG
3	A	443	LEU
3	A	445	ASN
3	A	450	LEU
3	A	451	HIS
3	A	461	LYS
3	A	466	SER
3	A	474	VAL
3	A	475	THR
3	A	493	GLN
3	A	503	GLN
3	A	504	LEU
3	A	524	VAL
3	A	535	THR

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Mol	Chain	Res	Type
3	A	590	ARG
3	A	596	THR
3	A	597	LEU
3	A	598	LEU
3	A	618	GLU
3	A	629	LEU
3	A	666	ILE
3	A	682	THR
3	A	740	LEU
3	A	741	ASN
3	A	745	GLN
3	A	756	ILE
3	A	768	GLN
3	A	821	ARG
3	A	845	LEU
3	A	849	MET
3	A	854	ASN
3	A	855	THR
3	A	858	ASN
3	A	913	LEU
3	A	920	LEU
3	A	929	LEU
3	A	948	VAL
3	A	979	SER
3	A	1029	ARG
3	A	1035	TYR
3	A	1043	ASP
3	A	1055	ARG
3	A	1057	VAL
3	A	1077	THR
3	A	1122	PRO
3	A	1136	SER
3	A	1208	THR
3	A	1212	VAL
3	A	1222	ASN
3	A	1232	ASN
3	A	1258	HIS
3	A	1264	GLU
3	A	1295	THR
3	A	1308	THR
3	A	1311	VAL
3	A	1318	THR

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Mol	Chain	Res	Type
3	A	1332	PHE
3	A	1335	ILE
3	A	1351	GLU
3	A	1355	VAL
3	A	1359	ASP
3	A	1364	ASN
3	A	1375	MET
3	A	1376	THR
3	A	1425	SER
3	A	1442	ASP
4	B	43	LEU
4	B	57	TYR
4	B	63	ILE
4	B	98	THR
4	B	109	THR
4	B	121	ASN
4	B	175	ARG
4	B	185	THR
4	B	194	GLU
4	B	232	SER
4	B	234	ILE
4	B	254	LEU
4	B	261	ARG
4	B	268	THR
4	B	309	GLN
4	B	313	MET
4	B	317	CYS
4	B	320	ASP
4	B	331	LEU
4	B	361	LEU
4	B	387	LEU
4	B	396	ASP
4	B	408	LEU
4	B	453	ILE
4	B	484	ASN
4	B	485	ARG
4	B	498	THR
4	B	513	GLN
4	B	514	LEU
4	B	538	ASN
4	B	542	MET
4	B	547	VAL

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Mol	Chain	Res	Type
4	B	556	THR
4	B	563	MET
4	B	570	VAL
4	B	576	ASP
4	B	624	LEU
4	B	644	GLU
4	B	680	THR
4	B	723	VAL
4	B	732	SER
4	B	737	THR
4	B	762	ASN
4	B	764	SER
4	B	780	VAL
4	B	791	THR
4	B	835	GLN
4	B	839	MET
4	B	860	MET
4	B	901	PRO
4	B	915	THR
4	B	944	THR
4	B	951	GLN
4	B	953	LEU
4	B	954	VAL
4	B	976	ILE
4	B	986	GLN
4	B	987	LYS
4	B	996	ARG
4	B	997	GLU
4	B	999	MET
4	B	1002	THR
4	B	1007	VAL
4	B	1017	ILE
4	B	1021	MET
4	B	1034	VAL
4	B	1049	ASP
4	B	1065	GLN
4	B	1073	TYR
4	B	1103	ILE
4	B	1110	PRO
4	B	1111	MET
4	B	1118	PRO
4	B	1132	GLU

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Mol	Chain	Res	Type
4	B	1133	MET
4	B	1147	LEU
4	B	1150	ARG
4	B	1151	LEU
4	B	1185	CYS
5	C	22	LEU
5	C	25	VAL
5	C	26	ASP
5	C	58	LEU
5	C	62	PHE
5	C	69	LEU
5	C	77	ILE
5	C	99	LEU
5	C	133	ILE
5	C	195	GLN
5	C	229	TYR
5	C	233	GLU
5	C	238	ILE
5	C	240	VAL
5	C	259	LEU
5	C	264	GLN
6	E	40	GLU
6	E	84	ASP
6	E	92	THR
6	E	183	PRO
7	F	79	ARG
7	F	90	ARG
7	F	103	MET
7	F	111	LEU
7	F	115	THR
7	F	133	VAL
8	H	21	ASN
8	H	27	GLU
8	H	109	LYS
8	H	110	ASP
9	I	12	ASN
9	I	29	CYS
9	I	31	THR
9	I	52	ILE
9	I	75	CYS
9	I	76	PRO
9	I	87	GLN

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Mol	Chain	Res	Type
9	I	97	MET
10	J	1	MET
10	J	2	ILE
10	J	7	CYS
10	J	22	LEU
10	J	47	ARG
10	J	48	ARG
11	K	11	LEU
11	K	20	LYS
11	K	25	THR
11	K	29	ASN
11	K	31	VAL
11	K	47	ARG
11	K	50	LEU
11	K	51	LEU
11	K	63	VAL
11	K	77	THR
11	K	114	LEU
12	L	50	ASP
12	L	54	ARG
12	L	55	ILE
12	L	65	VAL
12	L	68	GLU
12	L	70	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (96) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	68	GLN
3	A	92	HIS
3	A	118	HIS
3	A	169	ASN
3	A	225	ASN
3	A	281	HIS
3	A	339	ASN
3	A	425	GLN
3	A	435	HIS
3	A	445	ASN
3	A	447	GLN
3	A	493	GLN
3	A	503	GLN
3	A	517	ASN

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Mol	Chain	Res	Type
3	A	631	HIS
3	A	698	GLN
3	A	736	ASN
3	A	741	ASN
3	A	757	ASN
3	A	760	GLN
3	A	768	GLN
3	A	786	HIS
3	A	858	ASN
3	A	877	HIS
3	A	926	GLN
3	A	953	ASN
3	A	965	GLN
3	A	968	GLN
3	A	994	GLN
3	A	1011	GLN
3	A	1033	GLN
3	A	1070	GLN
3	A	1124	HIS
3	A	1130	GLN
3	A	1188	GLN
3	A	1364	ASN
3	A	1387	HIS
3	A	1390	ASN
3	A	1393	ASN
3	A	1432	GLN
4	B	46	GLN
4	B	47	GLN
4	B	53	GLN
4	B	121	ASN
4	B	215	GLN
4	B	224	GLN
4	B	236	HIS
4	B	309	GLN
4	B	325	GLN
4	B	363	HIS
4	B	366	GLN
4	B	415	GLN
4	B	465	ASN
4	B	484	ASN
4	B	513	GLN
4	B	515	HIS

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Mol	Chain	Res	Type
4	B	516	ASN
4	B	518	HIS
4	B	538	ASN
4	B	744	HIS
4	B	770	GLN
4	B	822	ASN
4	B	842	ASN
4	B	862	GLN
4	B	957	ASN
4	B	975	GLN
4	B	1065	GLN
4	B	1093	GLN
4	B	1117	GLN
4	B	1141	HIS
4	B	1178	ASN
4	B	1179	GLN
4	B	1193	GLN
5	C	65	HIS
5	C	73	GLN
5	C	112	ASN
5	C	123	ASN
5	C	131	HIS
5	C	140	ASN
5	C	167	HIS
5	C	242	GLN
5	C	252	GLN
6	E	5	ASN
6	E	101	GLN
6	E	104	ASN
6	E	114	ASN
6	E	115	ASN
6	E	147	HIS
7	F	78	GLN
8	H	33	GLN
9	I	12	ASN
10	J	53	HIS
11	K	44	ASN
11	K	65	HIS
11	K	76	GLN
11	K	110	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	R	10/10 (100%)	3 (30%)	3 (30%)

All (3) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	R	2	U
1	R	5	A
1	R	6	G

All (3) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	R	1	A
1	R	4	G
1	R	5	A

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	UTP	R	3000	1,13	29,30,30	2.41	9 (31%)	43,47,47	3.09	11 (25%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	UTP	R	3000	1,13	1/1/7/7	4/22/38/38	0/2/2/2

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	R	3000	UTP	C3'-C4'	-5.54	1.38	1.53
14	R	3000	UTP	C5'-C4'	5.47	1.68	1.51
14	R	3000	UTP	O2'-C2'	4.93	1.55	1.43
14	R	3000	UTP	C1'-N1	4.78	1.61	1.47
14	R	3000	UTP	O4'-C4'	-4.31	1.35	1.45
14	R	3000	UTP	O3'-C3'	-4.12	1.32	1.43
14	R	3000	UTP	PA-O3A	2.85	1.62	1.59
14	R	3000	UTP	PB-O1B	-2.04	1.45	1.55
14	R	3000	UTP	C2'-C1'	-2.00	1.47	1.53

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	R	3000	UTP	O4'-C4'-C5'	13.48	152.51	109.33
14	R	3000	UTP	C5'-C4'-C3'	-6.87	90.48	115.21
14	R	3000	UTP	O5'-C5'-C4'	6.85	132.33	108.99
14	R	3000	UTP	C2'-C1'-N1	-6.35	95.58	113.25
14	R	3000	UTP	O3'-C3'-C2'	-4.60	97.06	111.82
14	R	3000	UTP	O4'-C4'-C3'	4.30	113.69	105.15
14	R	3000	UTP	O1B-PB-O3A	3.27	116.10	107.27
14	R	3000	UTP	O2'-C2'-C1'	-2.74	100.68	110.10
14	R	3000	UTP	O2'-C2'-C3'	-2.11	105.06	111.82
14	R	3000	UTP	C1'-N1-C2	2.09	121.35	117.59
14	R	3000	UTP	C4'-O4'-C1'	-2.02	105.00	109.47

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
14	R	3000	UTP	C4'

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	R	3000	UTP	C5'-O5'-PA-O2A

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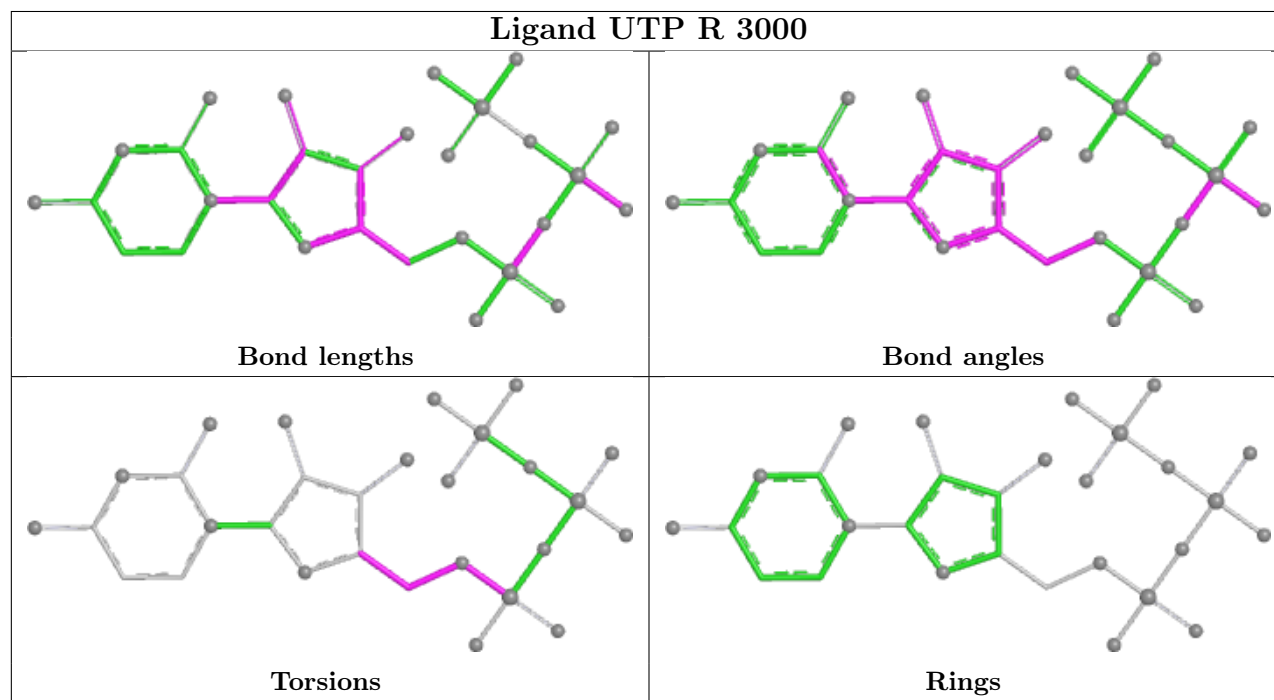
Mol	Chain	Res	Type	Atoms
14	R	3000	UTP	C5'-O5'-PA-O3A
14	R	3000	UTP	C4'-C5'-O5'-PA
14	R	3000	UTP	O4'-C4'-C5'-O5'

There are no ring outliers.

1 monomer is involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	R	3000	UTP	8	0

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	T	3
1	R	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	T	7:DC	O3'	8:DT	P	1.39
1	R	5:A	O3'	6:G	P	1.33
1	T	4:DA	O3'	5:DT	P	1.24
1	T	3:DG	O3'	4:DA	P	1.18

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	R	10/10 (100%)	0.93	0 100 100	79, 137, 196, 199	0
2	T	14/14 (100%)	1.73	5 (35%) 1 3	91, 150, 197, 202	0
3	A	1381/1733 (79%)	1.09	226 (16%) 4 8	12, 134, 202, 202	0
4	B	1097/1224 (89%)	1.11	177 (16%) 4 8	12, 121, 202, 202	0
5	C	266/318 (83%)	0.93	32 (12%) 9 12	20, 115, 194, 202	0
6	E	214/215 (99%)	1.27	36 (16%) 4 8	29, 156, 202, 202	0
7	F	84/155 (54%)	0.76	6 (7%) 22 23	17, 130, 196, 202	0
8	H	133/146 (91%)	1.21	26 (19%) 3 7	56, 150, 202, 202	0
9	I	119/122 (97%)	1.19	28 (23%) 2 5	25, 159, 202, 202	0
10	J	65/70 (92%)	0.99	5 (7%) 19 21	40, 110, 179, 202	0
11	K	114/120 (95%)	0.62	5 (4%) 39 33	12, 118, 178, 199	0
12	L	46/70 (65%)	1.32	9 (19%) 3 6	36, 163, 202, 202	0
All	All	3543/4197 (84%)	1.08	555 (15%) 5 9	12, 131, 202, 202	0

All (555) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	B	791	THR	7.2
6	E	83	CYS	7.2
6	E	35	VAL	6.8
4	B	467	GLY	6.6
3	A	313	GLN	6.5
4	B	273	LEU	5.8
4	B	530	GLY	5.7
3	A	105	CYS	5.2
3	A	1317	MET	5.1
4	B	486	TYR	5.1
4	B	532	ALA	5.1

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Mol	Chain	Res	Type	RSRZ
3	A	1080	THR	5.0
3	A	300	VAL	5.0
3	A	1165	GLU	4.9
3	A	1169	ILE	4.9
10	J	44	TYR	4.9
4	B	950	ASP	4.8
4	B	315	LYS	4.7
4	B	1132	GLU	4.7
3	A	998	LEU	4.7
4	B	1097	HIS	4.7
6	E	96	PHE	4.6
4	B	276	ILE	4.6
8	H	119	GLY	4.6
4	B	529	GLU	4.5
3	A	488	ASN	4.5
3	A	1131	ALA	4.4
3	A	1261	LYS	4.4
4	B	823	ALA	4.3
6	E	97	VAL	4.3
6	E	144	ILE	4.3
4	B	268	THR	4.3
4	B	25	ILE	4.2
4	B	977	GLY	4.2
3	A	339	ASN	4.2
3	A	1153	TYR	4.2
4	B	985	GLY	4.1
3	A	680	THR	4.1
6	E	121	MET	4.1
8	H	102	TYR	4.0
6	E	118	PRO	4.0
9	I	16	PRO	4.0
3	A	1349	TYR	3.9
3	A	952	ALA	3.9
4	B	1112	GLN	3.9
4	B	548	GLY	3.9
12	L	57	LEU	3.9
5	C	81	GLU	3.9
3	A	68	GLN	3.8
3	A	323	LYS	3.8
4	B	1139	ILE	3.8
4	B	937	ALA	3.8
3	A	306	ASN	3.8

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Mol	Chain	Res	Type	RSRZ
4	B	838	SER	3.8
6	E	185	ALA	3.8
3	A	72	GLU	3.7
4	B	325	GLN	3.7
3	A	1333	ILE	3.7
3	A	98	LYS	3.7
3	A	1284	MET	3.7
4	B	1164	GLY	3.7
6	E	16	PHE	3.6
3	A	1205	LYS	3.6
3	A	1328	TYR	3.6
3	A	59	GLY	3.6
8	H	120	GLY	3.6
6	E	110	PHE	3.6
4	B	284	ILE	3.6
3	A	764	CYS	3.6
3	A	1422	ARG	3.6
3	A	872	GLY	3.6
4	B	1101	ASP	3.5
3	A	975	HIS	3.5
3	A	293	GLU	3.5
3	A	1327	ILE	3.5
8	H	51	ALA	3.5
8	H	117	SER	3.5
3	A	49	LYS	3.5
6	E	20	LYS	3.5
3	A	1174	PHE	3.5
6	E	95	THR	3.5
3	A	445	ASN	3.5
6	E	152	LYS	3.4
3	A	1377	THR	3.4
4	B	387	LEU	3.4
3	A	1001	ARG	3.4
3	A	135	PHE	3.4
11	K	50	LEU	3.4
4	B	665	GLU	3.4
3	A	324	SER	3.4
4	B	708	GLU	3.3
4	B	535	LEU	3.3
3	A	831	THR	3.3
5	C	103	ALA	3.3
4	B	274	PRO	3.3

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Mol	Chain	Res	Type	RSRZ
3	A	503	GLN	3.3
4	B	531	GLN	3.3
9	I	6	PHE	3.3
4	B	836	GLU	3.3
10	J	1	MET	3.3
3	A	240	PRO	3.3
4	B	711	GLU	3.3
3	A	331	GLY	3.2
3	A	883	LEU	3.2
9	I	64	SER	3.2
3	A	575	LYS	3.2
3	A	1336	MET	3.2
4	B	1201	LYS	3.2
3	A	1431	GLY	3.2
4	B	998	ASP	3.2
5	C	26	ASP	3.2
5	C	115	SER	3.2
4	B	465	ASN	3.2
4	B	345	LYS	3.2
8	H	16	ASP	3.2
3	A	474	VAL	3.2
7	F	155	LEU	3.2
3	A	1433	MET	3.2
3	A	596	THR	3.1
3	A	1097	GLY	3.1
9	I	30	ARG	3.1
10	J	11	GLY	3.1
3	A	1135	ARG	3.1
4	B	428	ILE	3.1
3	A	2	VAL	3.1
3	A	495	GLU	3.1
4	B	848	ARG	3.1
3	A	996	ASN	3.1
4	B	1130	PHE	3.1
3	A	1168	GLU	3.1
4	B	296	GLU	3.1
4	B	164	LYS	3.1
4	B	841	MET	3.1
9	I	41	PRO	3.1
9	I	42	LEU	3.1
3	A	1173	HIS	3.1
3	A	172	PRO	3.0

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Mol	Chain	Res	Type	RSRZ
4	B	319	GLU	3.1
5	C	171	GLY	3.0
4	B	1074	ASN	3.0
3	A	1176	LEU	3.0
4	B	50	SER	3.0
4	B	1145	SER	3.0
9	I	4	PHE	3.0
3	A	332	LYS	3.0
4	B	39	ARG	3.0
5	C	185	LYS	3.0
3	A	308	ILE	3.0
3	A	1313	LEU	3.0
4	B	356	LEU	3.0
4	B	629	ASP	3.0
3	A	368	LYS	3.0
5	C	57	VAL	3.0
3	A	852	TYR	3.0
3	A	71	GLN	3.0
2	T	9	DC	3.0
3	A	1401	SER	3.0
3	A	1424	VAL	3.0
3	A	908	LEU	3.0
3	A	1166	ASP	3.0
9	I	57	GLY	3.0
3	A	830	LYS	3.0
6	E	122	LYS	3.0
3	A	806	ARG	3.0
4	B	1096	ARG	3.0
6	E	212	ARG	3.0
4	B	1169	MET	3.0
5	C	55	THR	3.0
4	B	1161	HIS	3.0
3	A	968	GLN	3.0
3	A	312	PRO	2.9
4	B	134	LYS	2.9
3	A	665	GLY	2.9
12	L	45	ALA	2.9
4	B	207	GLY	2.9
4	B	819	ALA	2.9
4	B	1209	ALA	2.9
8	H	29	ALA	2.9
3	A	1078	GLN	2.9

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Mol	Chain	Res	Type	RSRZ
4	B	333	PHE	2.9
3	A	1243	VAL	2.9
3	A	1303	GLU	2.9
4	B	648	HIS	2.9
3	A	822	GLU	2.9
7	F	127	GLU	2.9
3	A	505	CYS	2.9
3	A	701	LEU	2.9
8	H	131	ASN	2.9
3	A	109	HIS	2.8
4	B	768	THR	2.8
4	B	882	THR	2.8
3	A	1081	LEU	2.8
4	B	244	LEU	2.8
3	A	973	ILE	2.8
9	I	109	ILE	2.8
9	I	56	ALA	2.8
3	A	1208	THR	2.8
4	B	208	SER	2.8
4	B	782	LEU	2.8
5	C	237	SER	2.8
3	A	1256	GLU	2.8
4	B	346	GLU	2.8
5	C	235	VAL	2.8
8	H	141	TYR	2.8
3	A	955	PRO	2.8
3	A	1231	ASP	2.8
12	L	62	LYS	2.8
4	B	133	LYS	2.8
4	B	259	TYR	2.8
9	I	10	CYS	2.8
3	A	886	ILE	2.8
9	I	28	GLU	2.8
3	A	479	ASN	2.8
4	B	477	ALA	2.8
4	B	650	GLU	2.8
4	B	1221	SER	2.8
3	A	235	ILE	2.7
4	B	1216	LEU	2.7
4	B	269	ILE	2.7
4	B	323	VAL	2.7
7	F	93	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
3	A	1202	MET	2.7
6	E	93	MET	2.7
2	T	11	DC	2.7
3	A	386	ASP	2.7
6	E	19	VAL	2.7
4	B	367	LEU	2.7
6	E	211	TYR	2.7
4	B	322	PHE	2.7
4	B	489	SER	2.7
6	E	146	HIS	2.7
4	B	533	CYS	2.7
3	A	885	THR	2.7
4	B	775	LYS	2.7
3	A	340	LEU	2.7
3	A	792	TYR	2.7
3	A	862	ASN	2.7
6	E	195	VAL	2.7
9	I	8	ARG	2.7
4	B	991	GLY	2.7
8	H	8	ASP	2.7
9	I	9	ASP	2.7
4	B	986	GLN	2.7
9	I	82	GLU	2.7
4	B	490	SER	2.7
3	A	1201	ALA	2.6
3	A	214	ILE	2.6
3	A	1406	VAL	2.6
9	I	11	ASN	2.6
4	B	953	LEU	2.6
3	A	1145	SER	2.6
3	A	471	ASN	2.6
4	B	484	ASN	2.6
4	B	245	GLU	2.6
4	B	706	GLN	2.6
12	L	52	GLY	2.6
3	A	449	SER	2.6
3	A	1229	SER	2.6
3	A	545	GLN	2.6
3	A	91	PHE	2.6
3	A	452	LYS	2.6
5	C	174	ALA	2.6
9	I	107	SER	2.6

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Mol	Chain	Res	Type	RSRZ
3	A	321	PRO	2.6
9	I	120	GLN	2.6
3	A	1067	LEU	2.6
4	B	996	ARG	2.6
4	B	828	ALA	2.6
5	C	225	ALA	2.6
4	B	628	THR	2.6
3	A	80	HIS	2.6
4	B	709	ASP	2.6
9	I	20	LYS	2.6
3	A	819	GLY	2.6
3	A	1384	VAL	2.6
2	T	1	DA	2.6
3	A	514	PRO	2.6
4	B	466	TRP	2.5
8	H	135	LEU	2.5
4	B	617	ARG	2.5
3	A	287	HIS	2.5
4	B	754	SER	2.5
6	E	88	VAL	2.5
3	A	1110	ASN	2.5
5	C	221	TYR	2.5
3	A	466	SER	2.5
4	B	372	SER	2.5
8	H	18	GLY	2.5
12	L	65	VAL	2.5
7	F	145	ASP	2.5
6	E	43	LYS	2.5
3	A	916	GLY	2.5
3	A	457	ALA	2.5
3	A	749	ALA	2.5
12	L	44	ASP	2.5
3	A	1207	LEU	2.5
3	A	175	ARG	2.5
3	A	839	ARG	2.5
12	L	63	ARG	2.5
3	A	100	LYS	2.5
3	A	481	ASP	2.5
4	B	785	TYR	2.5
3	A	1371	LEU	2.5
3	A	963	ILE	2.5
4	B	281	PRO	2.5

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Mol	Chain	Res	Type	RSRZ
4	B	547	VAL	2.5
4	B	918	ILE	2.5
3	A	220	THR	2.4
3	A	96	ILE	2.4
3	A	882	SER	2.4
6	E	119	SER	2.4
4	B	917	PRO	2.4
4	B	643	ASP	2.4
8	H	23	VAL	2.4
4	B	792	MET	2.4
3	A	354	SER	2.4
8	H	7	ASP	2.4
4	B	1042	GLY	2.4
6	E	201	LYS	2.4
3	A	1172	LEU	2.4
3	A	174	ILE	2.4
4	B	890	TYR	2.4
3	A	467	THR	2.4
4	B	388	CYS	2.4
4	B	691	GLU	2.4
4	B	800	GLN	2.4
8	H	50	ALA	2.4
5	C	178	PHE	2.4
4	B	767	ASN	2.4
3	A	335	ARG	2.4
3	A	1128	GLN	2.4
4	B	951	GLN	2.4
10	J	48	ARG	2.4
3	A	131	SER	2.4
3	A	866	PHE	2.4
3	A	1098	VAL	2.4
4	B	625	LYS	2.4
3	A	624	SER	2.4
4	B	883	LEU	2.4
4	B	283	VAL	2.4
3	A	1387	HIS	2.4
4	B	393	LYS	2.4
5	C	149	LYS	2.4
3	A	76	GLU	2.4
8	H	55	LEU	2.4
4	B	253	THR	2.4
6	E	139	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
8	H	84	ALA	2.4
11	K	39	ASP	2.4
4	B	496	ARG	2.4
3	A	597	LEU	2.4
3	A	626	ASN	2.4
11	K	57	LEU	2.4
4	B	988	GLY	2.3
6	E	101	GLN	2.3
3	A	204	THR	2.3
4	B	436	VAL	2.3
3	A	676	MET	2.3
4	B	987	LYS	2.3
4	B	583	ASN	2.3
4	B	776	GLN	2.3
5	C	68	GLY	2.3
3	A	233	TRP	2.3
3	A	21	LEU	2.3
9	I	26	LEU	2.3
3	A	1332	PHE	2.3
4	B	250	PHE	2.3
11	K	62	LYS	2.3
12	L	43	THR	2.3
3	A	388	LEU	2.3
6	E	202	SER	2.3
3	A	1235	LYS	2.3
6	E	56	LYS	2.3
3	A	1101	LEU	2.3
4	B	386	LEU	2.3
5	C	202	PRO	2.3
3	A	750	GLY	2.3
3	A	1204	ASP	2.3
4	B	107	GLY	2.3
3	A	759	ALA	2.3
5	C	52	GLU	2.3
5	C	207	CYS	2.3
8	H	35	GLN	2.3
3	A	1079	MET	2.3
3	A	139	TRP	2.3
3	A	327	ALA	2.3
3	A	1367	HIS	2.3
4	B	584	GLY	2.3
3	A	528	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
3	A	788	SER	2.3
3	A	1118	VAL	2.3
4	B	1070	GLU	2.2
3	A	439	ASN	2.2
3	A	854	ASN	2.2
6	E	42	PHE	2.2
7	F	143	PHE	2.2
9	I	32	CYS	2.2
8	H	76	THR	2.2
9	I	31	THR	2.2
3	A	186	LYS	2.2
3	A	859	SER	2.2
4	B	91	SER	2.2
3	A	322	VAL	2.2
3	A	344	ARG	2.2
3	A	85	ASP	2.2
4	B	481	GLN	2.2
5	C	40	GLU	2.2
3	A	30	ILE	2.2
3	A	700	ASN	2.2
3	A	1341	ILE	2.2
4	B	459	TYR	2.2
6	E	79	TRP	2.2
4	B	939	THR	2.2
4	B	636	PRO	2.2
4	B	252	SER	2.2
5	C	208	GLU	2.2
9	I	18	GLU	2.2
3	A	1194	ARG	2.2
4	B	916	THR	2.2
4	B	1172	ILE	2.2
7	F	120	ILE	2.2
3	A	307	ASP	2.2
4	B	246	LYS	2.2
3	A	1108	ALA	2.2
5	C	173	ALA	2.2
3	A	1314	SER	2.2
4	B	824	ILE	2.2
3	A	698	GLN	2.2
3	A	1034	GLU	2.2
4	B	174	LEU	2.2
4	B	294	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
4	B	394	ASP	2.2
5	C	226	ASP	2.2
5	C	268	ASP	2.2
3	A	1374	VAL	2.2
4	B	165	VAL	2.2
4	B	601	ARG	2.2
4	B	172	ILE	2.2
4	B	289	LEU	2.2
3	A	1154	TYR	2.2
5	C	78	GLU	2.2
5	C	210	GLU	2.2
8	H	106	GLU	2.2
3	A	711	ARG	2.2
4	B	230	ALA	2.2
3	A	274	ILE	2.2
3	A	540	PHE	2.2
4	B	487	THR	2.2
4	B	1204	PHE	2.2
4	B	622	LYS	2.2
9	I	104	LEU	2.2
6	E	81	GLU	2.2
3	A	3	GLY	2.1
3	A	828	ALA	2.1
3	A	1134	ILE	2.1
4	B	1195	HIS	2.1
11	K	40	HIS	2.1
3	A	1066	VAL	2.1
3	A	5	GLN	2.1
3	A	590	ARG	2.1
4	B	46	GLN	2.1
6	E	102	GLU	2.1
3	A	342	GLY	2.1
3	A	141	LEU	2.1
3	A	1409	LEU	2.1
4	B	70	ILE	2.1
3	A	46	THR	2.1
3	A	1438	THR	2.1
9	I	2	THR	2.1
4	B	237	VAL	2.1
4	B	723	VAL	2.1
3	A	1014	ALA	2.1
4	B	816	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
8	H	60	ALA	2.1
3	A	211	PHE	2.1
3	A	1102	LYS	2.1
3	A	1105	LEU	2.1
3	A	1221	LYS	2.1
4	B	212	LEU	2.1
6	E	171	LYS	2.1
8	H	59	ILE	2.1
6	E	2	ASP	2.1
3	A	152	VAL	2.1
3	A	182	VAL	2.1
5	C	121	VAL	2.1
3	A	69	THR	2.1
4	B	692	TYR	2.1
3	A	611	GLN	2.1
4	B	1019	SER	2.1
3	A	506	ALA	2.1
6	E	66	GLU	2.1
3	A	756	ILE	2.1
4	B	365	THR	2.1
4	B	1062	HIS	2.1
5	C	128	ASN	2.1
4	B	649	LYS	2.1
3	A	333	GLU	2.1
3	A	1271	ILE	2.1
4	B	1087	PHE	2.1
4	B	901	PRO	2.1
10	J	4	PRO	2.1
4	B	318	VAL	2.1
4	B	1129	ARG	2.1
3	A	271	LYS	2.1
3	A	1418	LEU	2.1
4	B	295	GLY	2.1
3	A	232	GLU	2.1
3	A	337	ARG	2.1
8	H	136	LYS	2.1
12	L	28	LYS	2.1
4	B	947	GLY	2.1
4	B	877	PRO	2.1
3	A	663	SER	2.1
6	E	77	SER	2.1
4	B	373	ARG	2.0

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Mol	Chain	Res	Type	RSRZ
5	C	35	ARG	2.0
3	A	6	TYR	2.0
4	B	205	ILE	2.0
3	A	148	CYS	2.0
3	A	1187	GLN	2.0
4	B	224	GLN	2.0
5	C	110	THR	2.0
9	I	23	ASN	2.0
2	T	3	DG	2.0
4	B	1135	ARG	2.0
4	B	277	LYS	2.0
8	H	63	LEU	2.0
3	A	35	ILE	2.0
4	B	303	TYR	2.0
8	H	47	PHE	2.0
2	T	10	DT	2.0
3	A	151	ASP	2.0
3	A	1206	ASP	2.0
4	B	832	GLY	2.0
9	I	39	GLY	2.0
3	A	26	GLU	2.0
3	A	149	GLU	2.0
4	B	223	VAL	2.0
8	H	133	ASN	2.0
5	C	152	GLU	2.0
3	A	415	LEU	2.0
3	A	614	PHE	2.0
3	A	836	TYR	2.0
4	B	334	ILE	2.0
4	B	756	ILE	2.0
4	B	1075	GLY	2.0
3	A	512	VAL	2.0
3	A	863	VAL	2.0
3	A	1282	VAL	2.0
3	A	1330	ASN	2.0
3	A	1382	THR	2.0
4	B	425	THR	2.0
4	B	1072	MET	2.0
9	I	22	ASN	2.0
5	C	22	LEU	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](#)

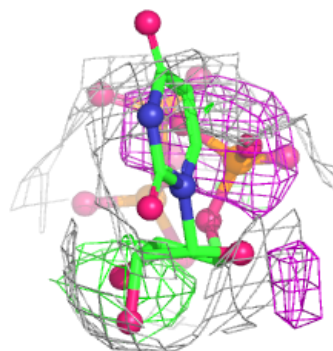
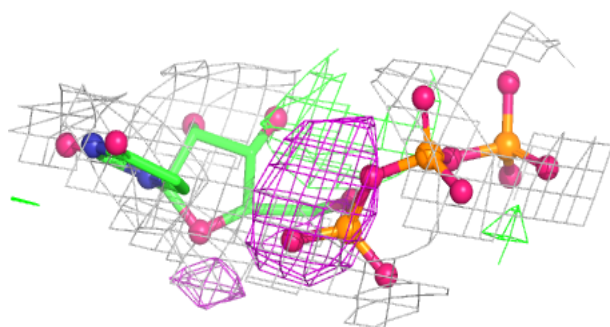
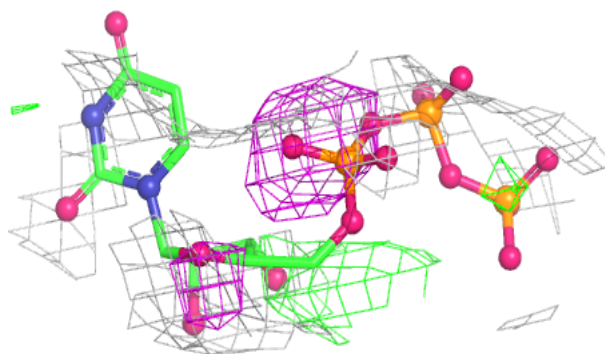
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
14	UTP	R	3000	29/29	0.75	0.18	78,78,78,78	0
15	ZN	I	203	1/1	0.84	0.14	90,90,90,90	0
13	MG	A	2002	1/1	0.86	0.13	44,44,44,44	0
15	ZN	B	1307	1/1	0.90	0.06	90,90,90,90	0
15	ZN	A	1734	1/1	0.95	0.12	90,90,90,90	0
15	ZN	A	1735	1/1	0.95	0.06	90,90,90,90	0
13	MG	R	2001	1/1	0.96	0.10	36,36,36,36	0
15	ZN	L	105	1/1	0.96	0.19	90,90,90,90	0
15	ZN	J	101	1/1	0.98	0.04	90,90,90,90	0
15	ZN	C	319	1/1	0.99	0.03	90,90,90,90	0
15	ZN	I	204	1/1	0.99	0.04	90,90,90,90	0

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

Electron density around UTP R 3000:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.