



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:22 PM UTC

PDB ID : 3GTP / pdb_00003gtp
Title : Backtracked RNA polymerase II complex with 24mer RNA
Authors : Wang, D.; Bushnell, D.A.; Huang, X.; Westover, K.D.; Levitt, M.; Kornberg, R.D.
Deposited on : 2009-03-27
Resolution : 3.90 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

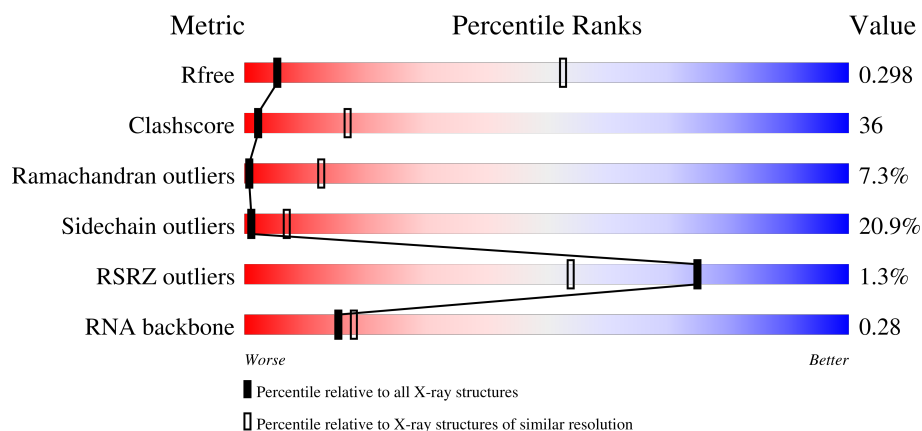
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.90 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.



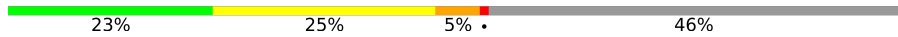
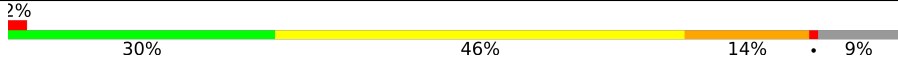
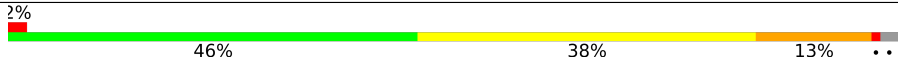
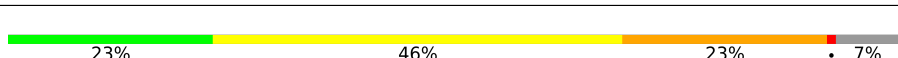
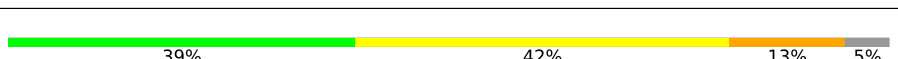
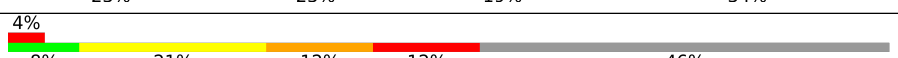
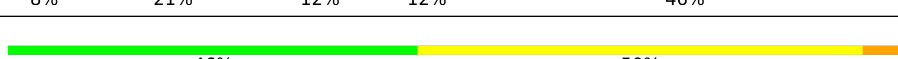
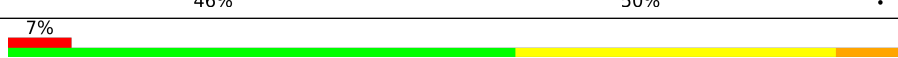
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1270 (4.10-3.70)
Clashscore	190562	1034 (4.08-3.72)
Ramachandran outliers	187476	1251 (4.10-3.70)
Sidechain outliers	187428	1243 (4.10-3.70)
RSRZ outliers	180081	1269 (4.10-3.70)
RNA backbone	3983	1014 (4.70-3.10)

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

Mol	Chain	Length	Quality of chain
1	A	1733	28% 38% 12% • 20%
2	B	1224	31% 45% 12% • 10%
3	C	318	27% 40% 15% • 16%
4	E	215	45% 42% 11% •

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Mol	Chain	Length	Quality of chain
5	F	155	
6	H	146	
7	I	122	
8	J	70	
9	K	120	
10	L	70	
11	R	24	
12	T	28	
13	N	14	

2 Entry composition [i](#)

There are 15 unique types of molecules in this entry. The entry contains 29279 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called DNA-directed RNA polymerase II subunit RPB1.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	R	13	Total	C	N	O	P	0	0	0
			280	126	55	87	12			

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

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

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

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

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

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

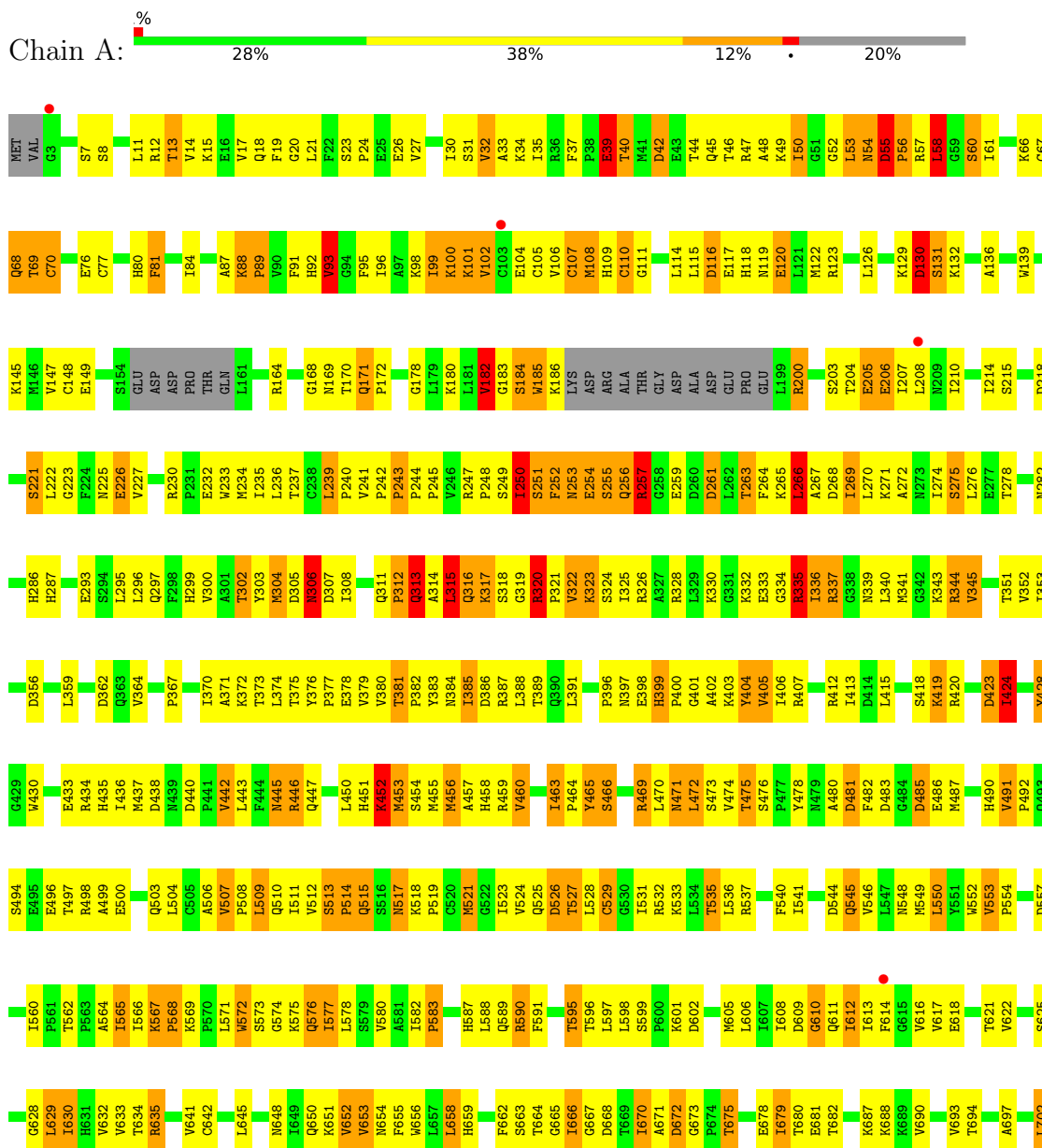
- Molecule 15 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

3 Residue-property plots

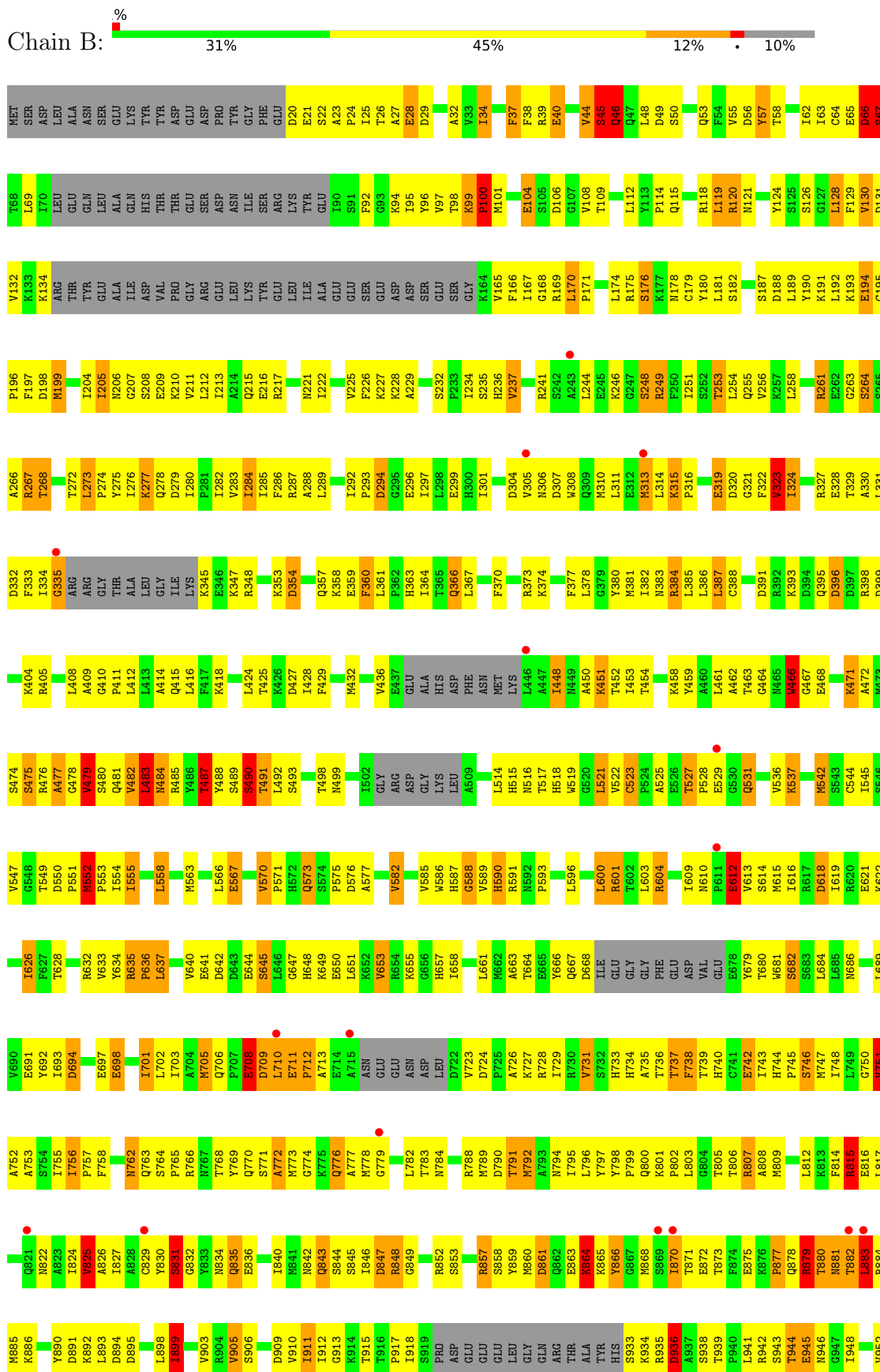
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

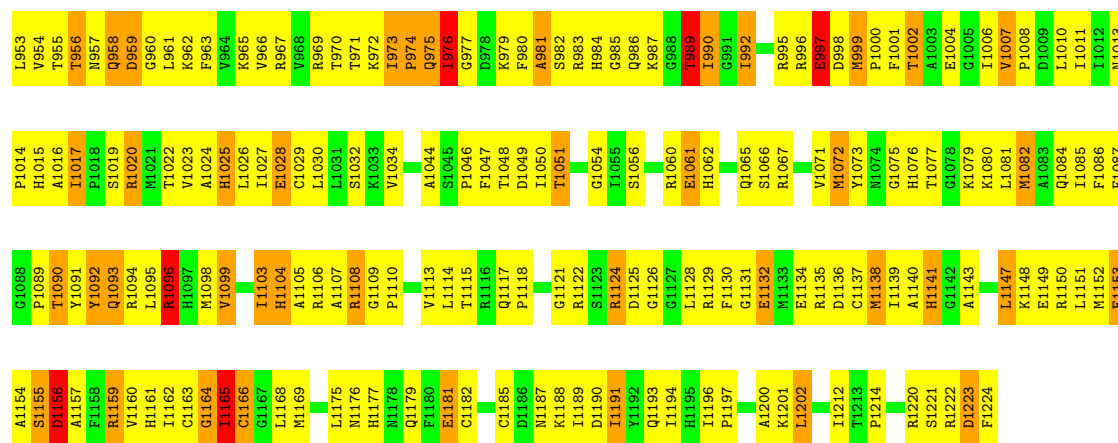
- Molecule 1: DNA-directed RNA polymerase II subunit RPB1



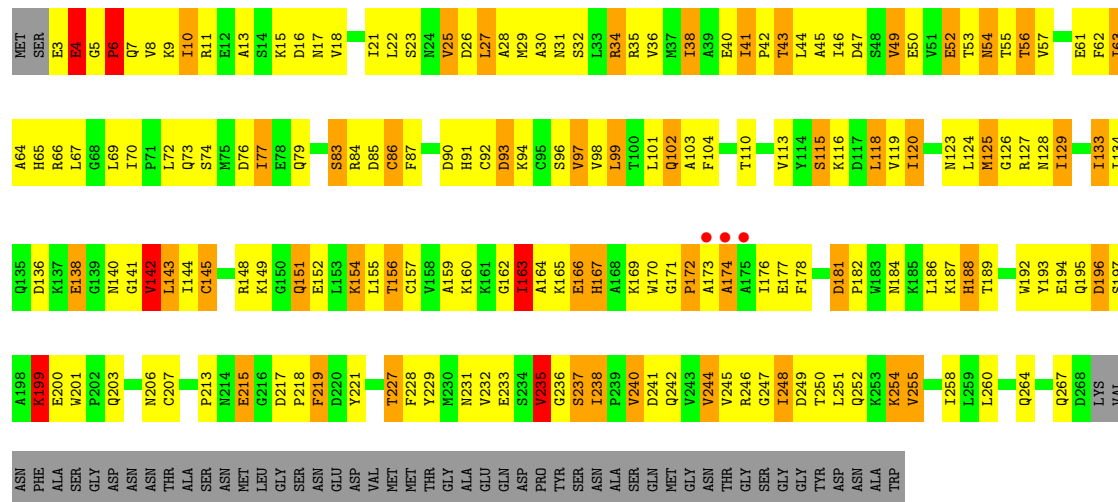


- Molecule 2: DNA-directed RNA polymerase II subunit RPB2

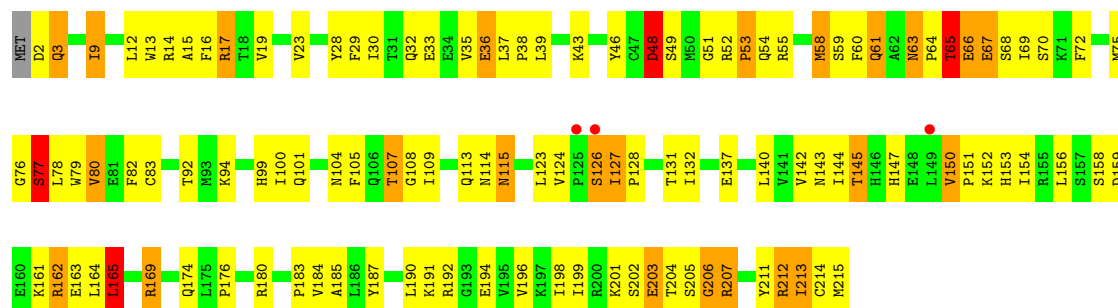
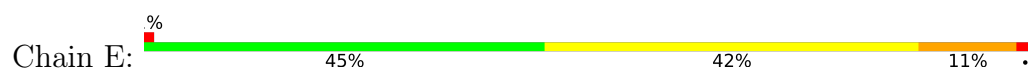




• Molecule 3: DNA-directed RNA polymerase II subunit RPB3

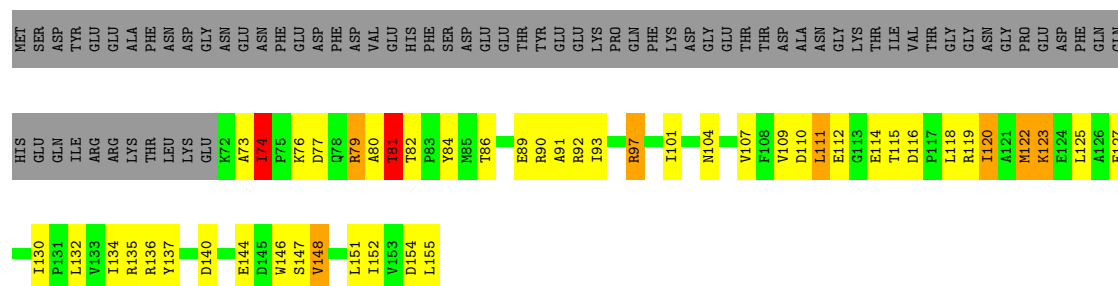


• Molecule 4: DNA-directed RNA polymerases I, II, and III subunit RPABC1

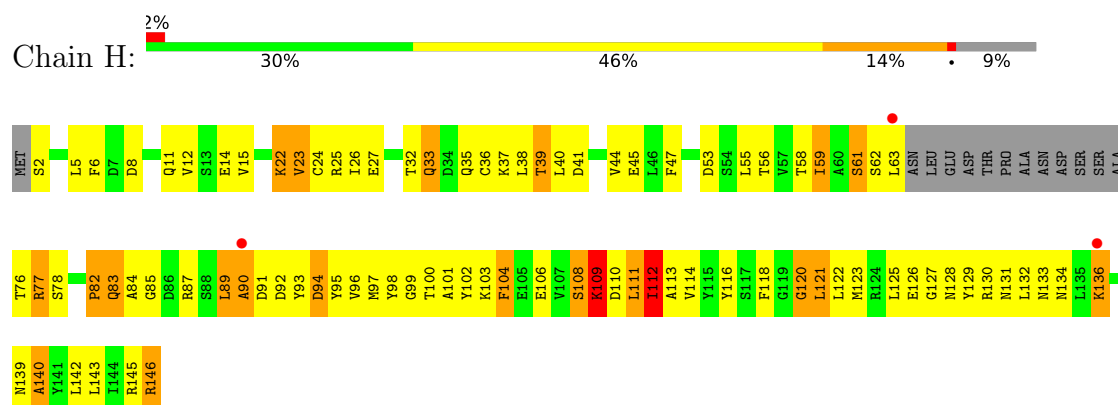


• Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC2

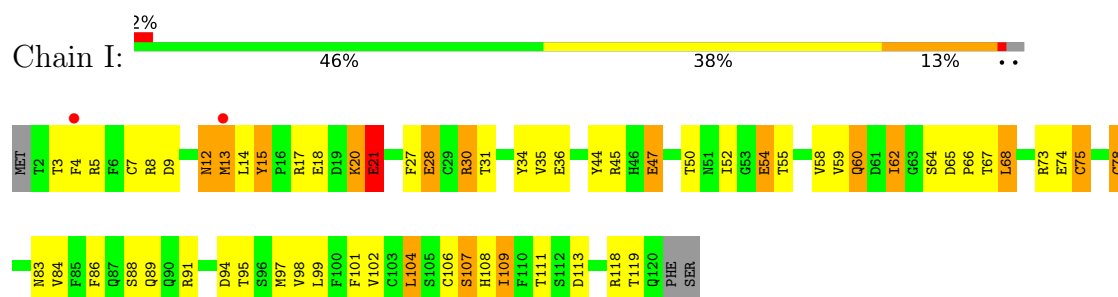




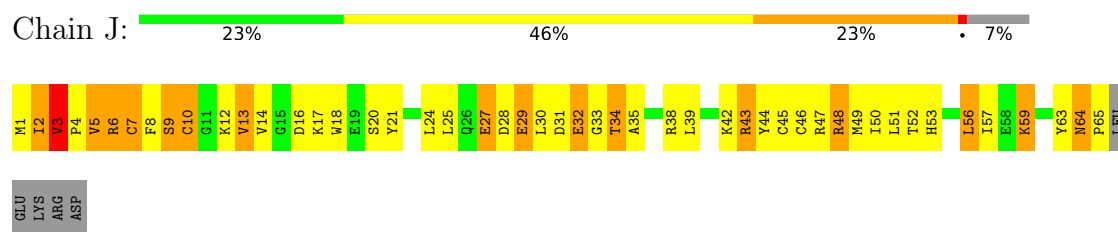
- Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC3



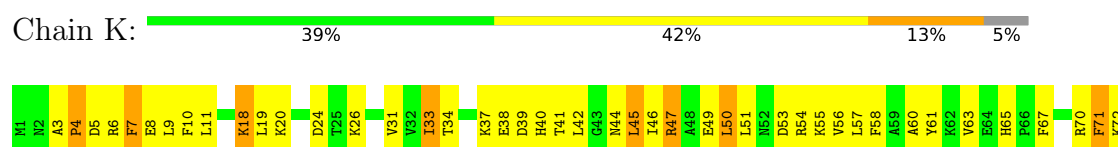
- Molecule 7: DNA-directed RNA polymerase II subunit RPB9

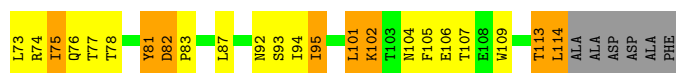


- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC5

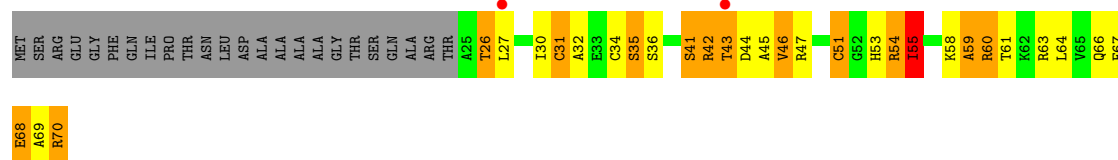


- Molecule 9: DNA-directed RNA polymerase II subunit RPB11

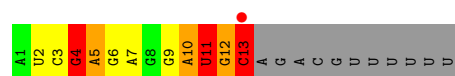




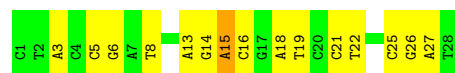
- Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC4



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



- Molecule 12: DNA (28-MER)



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



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	170.78Å 222.11Å 194.85Å 90.00° 102.06° 90.00°	Depositor
Resolution (Å)	50.00 – 3.90 50.00 – 3.90	Depositor EDS
% Data completeness (in resolution range)	91.6 (50.00-3.90) 91.6 (50.00-3.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.29 (at 3.88Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.266 , 0.299 0.269 , 0.298	Depositor DCC
R_{free} test set	3001 reflections (4.65%)	wwPDB-VP
Wilson B-factor (Å ²)	117.5	Xtriage
Anisotropy	0.095	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 75.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	29279	wwPDB-VP
Average B, all atoms (Å ²)	135.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.18% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.16	47/11163 (0.4%)	1.13	48/15091 (0.3%)
2	B	1.21	47/8963 (0.5%)	1.13	32/12086 (0.3%)
3	C	1.17	9/2133 (0.4%)	1.16	16/2891 (0.6%)
4	E	1.16	6/1788 (0.3%)	1.03	2/2406 (0.1%)
5	F	1.08	3/691 (0.4%)	0.99	0/933
6	H	1.19	8/1086 (0.7%)	1.03	3/1470 (0.2%)
7	I	1.24	3/989 (0.3%)	1.12	3/1331 (0.2%)
8	J	1.29	3/541 (0.6%)	1.28	6/727 (0.8%)
9	K	1.15	2/937 (0.2%)	1.11	4/1265 (0.3%)
10	L	1.38	3/365 (0.8%)	1.12	1/485 (0.2%)
11	R	1.00	1/314 (0.3%)	1.38	3/489 (0.6%)
12	T	0.98	3/634 (0.5%)	1.23	4/975 (0.4%)
13	N	0.90	1/317 (0.3%)	0.97	1/488 (0.2%)
All	All	1.18	136/29921 (0.5%)	1.12	123/40637 (0.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
6	H	0	1
All	All	0	2

All (136) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	T	3	DA	P-O5'	9.93	1.80	1.60
6	H	120	GLY	C-O	9.62	1.36	1.23
9	K	54	ARG	CZ-NH1	9.24	1.45	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	I	109	ILE	CG1-CD1	8.37	1.84	1.51
1	A	840	ARG	CZ-NH1	8.37	1.44	1.32
12	T	3	DA	C4'-O4'	8.33	1.62	1.45
2	B	777	ALA	C-O	8.30	1.33	1.23
3	C	219	PHE	C-O	8.11	1.33	1.23
3	C	41	ILE	CA-CB	8.04	1.61	1.53
4	E	48	ASP	CG-OD1	7.89	1.40	1.25
2	B	39	ARG	CZ-NH1	7.56	1.43	1.32
2	B	253	THR	C-O	7.54	1.33	1.24
2	B	573	GLN	CD-NE2	6.94	1.47	1.33
1	A	1382	THR	C-O	-6.93	1.15	1.23
6	H	92	ASP	CG-OD2	6.93	1.38	1.25
1	A	182	VAL	C-O	6.92	1.32	1.24
1	A	306	ASN	C-O	6.90	1.31	1.23
1	A	968	GLN	CD-NE2	6.90	1.47	1.33
1	A	833	GLU	CD-OE1	6.88	1.38	1.25
3	C	203	GLN	CD-NE2	6.78	1.47	1.33
7	I	5	ARG	CZ-NH1	6.78	1.42	1.32
2	B	772	ALA	C-O	6.77	1.32	1.24
1	A	1023	ARG	CZ-NH1	6.77	1.42	1.32
2	B	39	ARG	NE-CZ	6.77	1.40	1.33
4	E	126	SER	CB-OG	6.71	1.55	1.42
1	A	726	ARG	CZ-NH1	6.50	1.41	1.32
2	B	613	VAL	C-O	6.48	1.30	1.24
1	A	1129	GLU	CD-OE2	6.43	1.37	1.25
1	A	811	GLN	CD-NE2	6.37	1.46	1.33
6	H	22	LYS	C-O	6.36	1.33	1.24
2	B	521	LEU	CA-C	-6.34	1.47	1.52
1	A	328	ARG	CZ-NH1	6.32	1.41	1.32
2	B	936	ASP	CG-OD2	6.30	1.37	1.25
4	E	58	MET	SD-CE	6.29	1.95	1.79
2	B	1025	HIS	CE1-NE2	6.28	1.38	1.32
1	A	950	GLY	C-O	6.25	1.31	1.24
1	A	1270	ASN	C-N	6.19	1.39	1.33
1	A	1107	VAL	C-O	6.18	1.31	1.24
1	A	1215	ARG	NE-CZ	6.16	1.39	1.33
1	A	1230	GLU	CD-OE1	6.15	1.37	1.25
1	A	1423	GLY	C-O	6.15	1.32	1.23
2	B	1048	THR	CB-OG1	6.15	1.53	1.43
9	K	93	SER	CB-OG	6.13	1.54	1.42
1	A	898	ARG	CZ-NH1	6.13	1.41	1.32
2	B	588	GLY	C-O	6.11	1.28	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	776	GLN	C-O	6.10	1.31	1.24
4	E	162	ARG	CZ-NH1	6.09	1.41	1.32
13	N	12	DT	C5-C7	6.03	1.62	1.50
2	B	131	ASP	CG-OD2	6.02	1.36	1.25
2	B	698	GLU	CD-OE2	6.01	1.36	1.25
2	B	989	THR	CA-CB	6.01	1.62	1.53
2	B	1164	GLY	C-O	5.98	1.32	1.23
2	B	1224	PHE	C-O	5.98	1.35	1.23
2	B	335	GLY	C-O	5.95	1.35	1.23
1	A	994	GLN	CD-NE2	5.94	1.45	1.33
2	B	558	LEU	CG-CD2	5.94	1.72	1.52
1	A	1305	VAL	C-O	5.94	1.30	1.24
1	A	1232	ASN	CG-OD1	5.93	1.34	1.23
3	C	52	GLU	CD-OE2	5.89	1.36	1.25
1	A	1221	LYS	C-O	5.88	1.31	1.24
1	A	1215	ARG	CZ-NH1	5.87	1.41	1.32
2	B	46	GLN	CD-OE1	5.83	1.34	1.23
1	A	205	GLU	CD-OE1	5.83	1.36	1.25
1	A	447	GLN	CD-NE2	5.74	1.45	1.33
3	C	41	ILE	N-CA	5.73	1.50	1.46
2	B	1096	ARG	CZ-NH1	5.73	1.40	1.32
3	C	219	PHE	C-N	5.72	1.41	1.33
1	A	653	VAL	C-O	5.71	1.30	1.24
1	A	1275	GLY	C-O	5.70	1.31	1.23
1	A	1034	GLU	CD-OE2	5.70	1.36	1.25
6	H	146	ARG	CZ-NH1	5.69	1.40	1.32
4	E	9	ILE	CA-CB	5.68	1.60	1.54
8	J	20	SER	C-O	5.68	1.30	1.24
1	A	1023	ARG	NE-CZ	5.66	1.39	1.33
2	B	612	GLU	CD-OE1	5.66	1.36	1.25
12	T	3	DA	C3'-C2'	5.66	1.64	1.52
2	B	120	ARG	CZ-NH1	5.64	1.40	1.32
2	B	531	GLN	CD-OE1	5.64	1.34	1.23
1	A	1129	GLU	CD-OE1	5.62	1.36	1.25
2	B	487	THR	CB-OG1	5.60	1.52	1.43
10	L	41	SER	C-O	5.59	1.31	1.23
3	C	118	LEU	C-O	5.59	1.30	1.23
1	A	1444	MET	SD-CE	5.59	1.93	1.79
6	H	100	THR	CB-OG1	5.58	1.52	1.43
5	F	155	LEU	C-OXT	5.58	1.34	1.23
1	A	996	ASN	CG-ND2	5.58	1.45	1.33
1	A	39	GLU	C-N	5.58	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	990	ILE	CA-CB	5.54	1.61	1.53
2	B	573	GLN	CD-OE1	5.54	1.34	1.23
1	A	761	MET	SD-CE	5.53	1.93	1.79
2	B	708	GLU	CD-OE1	5.52	1.35	1.25
1	A	1080	THR	CA-CB	5.51	1.62	1.53
3	C	254	LYS	C-O	5.50	1.31	1.24
2	B	958	GLN	CD-NE2	5.47	1.44	1.33
11	R	4	G	P-O5'	5.47	1.68	1.59
1	A	221	SER	C-O	5.46	1.30	1.24
7	I	67	THR	C-N	5.45	1.40	1.33
1	A	820	GLY	C-O	5.43	1.31	1.23
5	F	122	MET	SD-CE	5.43	1.93	1.79
2	B	353	LYS	CG-CD	5.42	1.68	1.52
8	J	34	THR	CB-OG1	5.41	1.52	1.43
10	L	60	ARG	CZ-NH1	5.41	1.40	1.32
2	B	590	HIS	CE1-NE2	5.41	1.38	1.32
3	C	138	GLU	CD-OE1	5.40	1.35	1.25
4	E	63	ASN	CG-OD1	5.39	1.33	1.23
2	B	209	GLU	C-O	5.38	1.30	1.24
1	A	679	ILE	CG1-CD1	-5.38	1.30	1.51
1	A	1055	ARG	CZ-NH1	5.36	1.40	1.32
5	F	116	ASP	CG-OD2	5.36	1.35	1.25
2	B	1049	ASP	C-O	5.35	1.29	1.23
1	A	838	GLN	CD-NE2	5.35	1.44	1.33
1	A	335	ARG	CZ-NH1	5.33	1.40	1.32
2	B	448	ILE	C-O	5.33	1.29	1.24
2	B	772	ALA	C-N	5.31	1.41	1.33
1	A	1199	ARG	NE-CZ	5.31	1.38	1.33
1	A	945	GLU	CD-OE2	5.29	1.35	1.25
6	H	99	GLY	C-N	5.26	1.41	1.33
2	B	613	VAL	C-N	5.26	1.40	1.33
2	B	1075	GLY	C-O	5.24	1.30	1.23
1	A	372	LYS	CG-CD	5.22	1.68	1.52
2	B	1114	LEU	C-O	5.21	1.30	1.24
2	B	100	PRO	CB-CG	5.20	1.75	1.49
6	H	61	SER	C-O	5.20	1.28	1.23
2	B	713	ALA	C-O	5.19	1.29	1.23
6	H	14	GLU	CD-OE1	5.15	1.35	1.25
2	B	529	GLU	CD-OE1	5.14	1.35	1.25
2	B	466	TRP	C-O	5.13	1.30	1.24
1	A	311	GLN	CD-OE1	5.13	1.33	1.23
1	A	1368	MET	SD-CE	5.12	1.92	1.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	996	ASN	CG-OD1	5.07	1.33	1.23
2	B	106	ASP	CG-OD2	5.06	1.34	1.25
8	J	42	LYS	C-O	5.05	1.30	1.24
2	B	918	ILE	CA-CB	5.05	1.60	1.54
10	L	36	SER	CB-OG	5.03	1.52	1.42
2	B	267	ARG	CZ-NH1	5.03	1.39	1.32
2	B	1061	GLU	CD-OE1	5.00	1.34	1.25

All (123) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	R	13	C	C1'-O4'-C4'	-8.52	101.18	109.70
12	T	3	DA	C5'-C4'-C3'	8.24	127.26	114.90
6	H	85	GLY	N-CA-C	-8.23	104.54	115.32
4	E	65	THR	N-CA-C	-7.49	98.37	110.20
2	B	895	ASP	N-CA-C	7.32	120.13	111.71
1	A	275	SER	N-CA-C	-7.06	105.29	114.04
2	B	323	VAL	N-CA-C	-7.01	106.17	112.90
9	K	82	ASP	CA-C-N	6.99	128.57	119.84
9	K	82	ASP	C-N-CA	6.99	128.57	119.84
6	H	92	ASP	N-CA-C	-6.82	104.70	113.16
1	A	1323	ASP	CA-C-N	6.74	128.27	119.84
1	A	1323	ASP	C-N-CA	6.74	128.27	119.84
1	A	398	GLU	N-CA-C	-6.74	101.84	110.53
1	A	88	LYS	CA-C-N	6.66	128.17	119.84
1	A	88	LYS	C-N-CA	6.66	128.17	119.84
3	C	181	ASP	CA-C-N	6.66	126.44	119.05
3	C	181	ASP	C-N-CA	6.66	126.44	119.05
1	A	886	ILE	N-CA-C	6.56	116.71	110.74
7	I	68	LEU	CA-C-N	6.56	126.94	119.92
7	I	68	LEU	C-N-CA	6.56	126.94	119.92
1	A	239	LEU	CA-C-N	6.53	126.29	119.76
1	A	239	LEU	C-N-CA	6.53	126.29	119.76
2	B	37	PHE	N-CA-C	-6.53	101.88	110.43
1	A	513	SER	N-CA-C	6.51	118.28	110.07
2	B	825	VAL	N-CA-C	6.50	118.40	108.71
2	B	846	ILE	N-CA-C	6.47	116.63	110.42
1	A	857	ARG	N-CA-C	6.43	117.93	108.86
1	A	345	VAL	N-CA-C	6.42	118.39	108.44
1	A	964	ILE	N-CA-C	6.34	116.38	110.42
1	A	236	LEU	N-CA-C	6.33	119.03	108.20
12	T	15	DA	P-O3'-C3'	6.29	129.63	120.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1332	PHE	N-CA-C	-6.28	105.78	113.50
4	E	165	LEU	N-CA-C	6.26	120.47	112.34
8	J	5	VAL	N-CA-C	-6.25	100.92	109.55
2	B	276	ILE	N-CA-C	6.22	117.43	108.48
1	A	993	LEU	N-CA-C	-6.21	104.43	111.14
2	B	66	ASP	N-CA-C	-6.21	105.35	113.17
1	A	406	ILE	N-CA-C	6.20	117.05	108.12
1	A	582	ILE	CA-C-N	6.16	127.54	119.84
1	A	582	ILE	C-N-CA	6.16	127.54	119.84
12	T	3	DA	C5'-C4'-O4'	6.14	118.62	109.40
3	C	103	ALA	N-CA-C	-6.14	100.26	108.74
2	B	99	LYS	CA-C-N	6.07	127.42	119.84
2	B	99	LYS	C-N-CA	6.07	127.42	119.84
2	B	779	GLY	N-CA-C	6.04	120.86	111.08
2	B	479	VAL	N-CA-C	-6.03	100.25	109.78
1	A	921	GLY	N-CA-C	-5.99	106.16	111.67
3	C	188	HIS	N-CA-C	-5.97	105.48	112.89
10	L	67	PHE	N-CA-C	5.95	117.17	107.23
2	B	944	THR	CB-CA-C	-5.87	101.48	109.28
2	B	899	ILE	CB-CA-C	-5.82	105.19	111.59
11	R	5	A	N9-C1'-C2'	5.78	120.67	112.00
8	J	10	CYS	CA-CB-SG	5.78	127.69	114.40
1	A	1215	ARG	NE-CZ-NH2	-5.77	114.01	119.20
3	C	235	VAL	N-CA-C	-5.74	104.74	111.00
2	B	248	SER	CB-CA-C	-5.74	109.97	116.63
8	J	10	CYS	CB-CA-C	5.71	118.98	109.56
3	C	41	ILE	N-CA-C	5.70	112.75	107.56
9	K	75	ILE	N-CA-C	5.70	116.21	107.77
13	N	10	DG	P-O3'-C3'	5.70	128.75	120.20
2	B	774	GLY	N-CA-C	-5.65	105.84	113.24
3	C	41	ILE	N-CA-CB	5.63	117.45	111.20
2	B	273	LEU	CA-C-N	5.61	126.85	119.84
2	B	273	LEU	C-N-CA	5.61	126.85	119.84
1	A	793	SER	CA-C-N	5.60	125.27	119.05
1	A	793	SER	C-N-CA	5.60	125.27	119.05
1	A	673	GLY	CA-C-N	5.58	125.28	119.82
1	A	673	GLY	C-N-CA	5.58	125.28	119.82
2	B	751	VAL	N-CA-C	5.53	120.85	109.34
2	B	165	VAL	N-CA-C	5.53	116.08	108.12
1	A	55	ASP	N-CA-C	5.51	121.98	109.81
1	A	628	GLY	N-CA-C	5.50	120.92	112.51
1	A	58	LEU	CD1-CG-CD2	5.49	122.89	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	238	ILE	CA-C-N	-5.47	114.32	119.85
3	C	238	ILE	C-N-CA	-5.47	114.32	119.85
1	A	491	VAL	CA-C-N	5.46	125.41	119.78
1	A	491	VAL	C-N-CA	5.46	125.41	119.78
2	B	69	LEU	N-CA-C	5.43	118.70	108.65
3	C	40	GLU	N-CA-C	5.41	119.58	112.92
1	A	595	THR	N-CA-C	5.39	117.78	107.75
1	A	243	PRO	CA-C-N	5.38	125.92	120.38
1	A	243	PRO	C-N-CA	5.38	125.92	120.38
3	C	163	ILE	N-CA-C	5.38	116.41	108.45
2	B	523	CYS	CA-C-N	5.36	124.87	119.19
2	B	523	CYS	C-N-CA	5.36	124.87	119.19
1	A	929	LEU	N-CA-C	5.34	118.02	111.82
11	R	11	U	N1-C1'-C2'	5.33	120.00	112.00
8	J	3	VAL	CB-CA-C	-5.32	101.67	111.36
2	B	320	ASP	N-CA-C	-5.32	106.56	113.16
1	A	261	ASP	N-CA-C	5.30	119.00	112.54
1	A	452	LYS	N-CA-C	-5.29	105.52	111.28
2	B	756	ILE	N-CA-C	5.27	113.09	107.76
1	A	664	THR	N-CA-C	5.25	116.75	107.61
1	A	973	ILE	N-CA-C	5.25	116.28	108.46
1	A	1155	ASP	CA-C-N	5.23	126.38	119.84
1	A	1155	ASP	C-N-CA	5.23	126.38	119.84
8	J	29	GLU	N-CA-C	5.23	118.54	111.17
2	B	635	ARG	CA-C-N	5.21	126.35	119.84
2	B	635	ARG	C-N-CA	5.21	126.35	119.84
3	C	237	SER	N-CA-C	-5.19	105.54	111.14
2	B	205	ILE	CB-CA-C	-5.19	102.78	111.29
1	A	565	ILE	CB-CA-C	5.16	117.86	110.84
2	B	663	ALA	N-CA-C	-5.14	105.85	111.82
1	A	171	GLN	CA-C-N	5.12	125.40	119.92
1	A	171	GLN	C-N-CA	5.12	125.40	119.92
7	I	28	GLU	N-CA-C	5.12	116.07	108.60
3	C	199	LYS	N-CA-C	-5.11	106.36	112.59
3	C	91	HIS	N-CA-C	5.07	117.96	110.46
3	C	4	GLU	N-CA-C	5.07	119.45	113.12
8	J	5	VAL	CB-CA-C	-5.05	104.66	111.63
1	A	652	VAL	N-CA-C	5.04	115.33	110.74
1	A	776	ALA	N-CA-C	5.04	116.60	110.41
2	B	723	VAL	N-CA-C	5.04	115.70	107.24
1	A	1328	TYR	N-CA-C	5.03	117.27	108.76
6	H	36	CYS	N-CA-C	5.03	116.89	108.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	861	ASP	N-CA-C	5.03	115.94	108.60
3	C	255	VAL	N-CA-C	-5.02	105.09	110.36
12	T	22	DT	O3'-P-O5'	-5.02	96.47	104.00
2	B	616	ILE	N-CA-C	5.02	114.00	106.42
2	B	976	ILE	N-CA-C	5.02	119.77	109.34
1	A	242	PRO	CA-C-N	5.01	125.54	120.38
1	A	242	PRO	C-N-CA	5.01	125.54	120.38
9	K	95	ILE	N-CA-C	-5.00	105.11	110.36

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	523	ILE	Peptide
6	H	61	SER	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	10969	0	11070	918	0
2	B	8792	0	8825	695	0
3	C	2095	0	2051	173	0
4	E	1752	0	1776	98	0
5	F	679	0	701	41	0
6	H	1068	0	1040	100	0
7	I	971	0	928	49	0
8	J	532	0	544	77	0
9	K	919	0	929	75	0
10	L	363	0	387	27	0
11	R	280	0	143	19	0
12	T	566	0	314	20	0
13	N	284	0	161	5	0
14	A	2	0	0	1	0
14	B	1	0	0	1	0
14	C	1	0	0	0	0
14	I	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	J	1	0	0	1	0
14	L	1	0	0	1	0
15	A	1	0	0	0	0
All	All	29279	0	28869	2104	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 36.

All (2104) 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)
6:H:104:PHE:CZ	6:H:136:LYS:HB3	1.37	1.55
7:I:109:ILE:CG1	7:I:109:ILE:CD1	1.84	1.53
2:B:100:PRO:CG	2:B:100:PRO:CB	1.75	1.48
1:A:256:GLN:CA	1:A:257:ARG:HB3	1.42	1.47
6:H:109:LYS:HB3	6:H:110:ASP:C	1.43	1.40
1:A:1364:ASN:ND2	1:A:1366:ARG:HG2	1.37	1.35
1:A:253:ASN:HB2	1:A:256:GLN:C	1.56	1.29
1:A:351:THR:HG23	2:B:1103:ILE:CD1	1.64	1.25
1:A:315:LEU:CB	1:A:316:GLN:HA	1.61	1.25
6:H:109:LYS:HB3	6:H:110:ASP:CA	1.66	1.24
6:H:109:LYS:CA	6:H:110:ASP:HB2	1.66	1.23
2:B:1106:ARG:HD3	2:B:1126:GLY:O	1.36	1.23
1:A:868:TYR:CE1	1:A:1064:VAL:HG11	1.73	1.21
1:A:315:LEU:HB3	1:A:316:GLN:CA	1.68	1.21
2:B:976:ILE:O	2:B:990:ILE:HB	1.41	1.19
6:H:109:LYS:CB	6:H:110:ASP:HB2	1.74	1.18
6:H:109:LYS:CG	6:H:111:LEU:HD22	1.74	1.18
1:A:900:ASP:O	1:A:906:HIS:O	1.60	1.17
1:A:1116:LEU:HD13	1:A:1329:THR:OG1	1.43	1.17
2:B:757:PRO:HG3	2:B:983:ARG:NH2	1.58	1.16
1:A:256:GLN:CB	1:A:257:ARG:HB3	1.76	1.15
1:A:1391:ARG:O	1:A:1391:ARG:HD3	1.47	1.14
6:H:109:LYS:HA	6:H:110:ASP:HB2	1.27	1.14
1:A:256:GLN:HA	1:A:257:ARG:CB	1.68	1.14
8:J:48:ARG:HH21	8:J:49:MET:HE1	1.06	1.14
1:A:567:LYS:HB2	1:A:568:PRO:HD2	1.17	1.14
2:B:1073:TYR:CE2	2:B:1080:LYS:HG3	1.83	1.14
6:H:109:LYS:HB3	6:H:110:ASP:CB	1.77	1.13
3:C:70:ILE:HD11	3:C:144:ILE:HD11	1.26	1.13
1:A:253:ASN:HB2	1:A:256:GLN:O	1.48	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:351:THR:CG2	2:B:1103:ILE:HD12	1.78	1.11
6:H:104:PHE:CZ	6:H:136:LYS:CB	2.32	1.11
1:A:257:ARG:O	1:A:257:ARG:HG2	1.44	1.11
2:B:981:ALA:CB	2:B:987:LYS:HA	1.81	1.10
5:F:114:GLU:OE2	5:F:119:ARG:HG2	1.50	1.10
11:R:4:G:H2'	11:R:5:A:H8	1.16	1.10
6:H:109:LYS:CB	6:H:110:ASP:CB	2.30	1.09
1:A:256:GLN:CB	1:A:257:ARG:CD	2.31	1.09
1:A:351:THR:HG22	1:A:352:VAL:H	1.09	1.08
2:B:983:ARG:HG3	2:B:1093:GLN:NE2	1.66	1.08
1:A:119:ASN:O	1:A:123:ARG:HG3	1.53	1.08
2:B:635:ARG:HB2	2:B:636:PRO:HD2	1.12	1.07
1:A:256:GLN:CB	1:A:257:ARG:HD2	1.85	1.07
7:I:75:CYS:SG	7:I:78:CYS:HB3	1.94	1.07
1:A:567:LYS:HB2	1:A:568:PRO:CD	1.84	1.06
9:K:113:THR:O	9:K:114:LEU:HB2	1.49	1.06
1:A:256:GLN:HB3	1:A:257:ARG:HD2	1.37	1.05
1:A:351:THR:HG22	1:A:352:VAL:N	1.70	1.05
6:H:109:LYS:HG2	6:H:111:LEU:HD22	1.30	1.05
3:C:45:ALA:HA	3:C:72:LEU:HD12	1.38	1.05
1:A:765:VAL:CG2	1:A:800:VAL:HB	1.86	1.05
2:B:373:ARG:HA	2:B:566:LEU:HD23	1.34	1.05
1:A:256:GLN:CA	1:A:257:ARG:CB	2.30	1.04
2:B:882:THR:HG21	2:B:935:ARG:HA	1.38	1.04
1:A:351:THR:HG23	2:B:1103:ILE:HD12	1.10	1.04
1:A:382:PRO:HD3	1:A:428:TYR:HE2	1.19	1.04
1:A:1394:THR:HG22	1:A:1398:MET:HE3	1.33	1.04
1:A:256:GLN:HB2	1:A:257:ARG:HD3	1.40	1.04
1:A:507:VAL:HG13	1:A:521:MET:HE1	1.34	1.03
6:H:109:LYS:CB	6:H:110:ASP:C	2.30	1.03
8:J:1:MET:N	8:J:56:LEU:H	1.55	1.03
6:H:109:LYS:HG2	6:H:111:LEU:CD2	1.88	1.03
1:A:256:GLN:HB2	1:A:257:ARG:CD	1.88	1.02
1:A:567:LYS:CB	1:A:568:PRO:HD2	1.90	1.02
1:A:315:LEU:HD12	1:A:318:SER:O	1.58	1.01
3:C:3:GLU:HG3	3:C:4:GLU:H	1.20	1.01
2:B:213:ILE:HD11	2:B:481:GLN:OE1	1.61	1.01
2:B:634:TYR:HE1	2:B:692:TYR:CD1	1.79	1.01
2:B:706:GLN:O	2:B:710:LEU:HB2	1.61	1.01
2:B:981:ALA:HB2	2:B:987:LYS:HA	1.37	1.01
1:A:446:ARG:HD2	1:A:480:ALA:HB2	1.41	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:667:GLY:HA2	1:A:670:ILE:HG13	1.44	1.00
1:A:868:TYR:HE1	1:A:1064:VAL:CG1	1.74	1.00
11:R:4:G:H2'	11:R:5:A:C8	1.95	1.00
1:A:382:PRO:HD3	1:A:428:TYR:CE2	1.97	1.00
3:C:102:GLN:HG2	3:C:154:LYS:HD3	1.43	1.00
4:E:29:PHE:O	4:E:30:ILE:HG13	1.60	0.99
1:A:573:SER:H	1:A:576:GLN:HG3	1.27	0.99
8:J:10:CYS:SG	8:J:43:ARG:HD2	2.03	0.99
1:A:256:GLN:HB3	1:A:257:ARG:CD	1.92	0.99
1:A:855:THR:HG21	1:A:857:ARG:HE	1.26	0.98
1:A:1348:LEU:HD23	1:A:1372:VAL:HG22	1.44	0.98
1:A:1364:ASN:HD22	1:A:1366:ARG:HG2	1.29	0.98
2:B:1076:HIS:ND1	9:K:40:HIS:CD2	2.32	0.98
1:A:39:GLU:O	1:A:53:LEU:HD12	1.62	0.97
1:A:1364:ASN:HD21	1:A:1366:ARG:HG2	1.23	0.97
1:A:344:ARG:HG3	1:A:344:ARG:HH11	1.24	0.97
2:B:726:ALA:HB1	2:B:1051:THR:HG21	1.43	0.97
2:B:807:ARG:HG3	2:B:807:ARG:HH11	1.25	0.96
1:A:868:TYR:HE1	1:A:1064:VAL:HG11	0.81	0.96
1:A:860:LEU:CD1	1:A:1393:ASN:HD22	1.78	0.96
1:A:1364:ASN:ND2	1:A:1366:ARG:CG	2.27	0.96
1:A:860:LEU:HD13	1:A:1393:ASN:HD22	1.28	0.96
8:J:44:TYR:HA	8:J:47:ARG:HB2	1.47	0.96
1:A:662:PHE:HD2	2:B:829:CYS:HG	1.13	0.96
8:J:35:ALA:O	8:J:39:LEU:HD12	1.64	0.95
8:J:7:CYS:SG	8:J:10:CYS:N	2.38	0.95
1:A:249:SER:C	1:A:250:ILE:HG12	1.91	0.95
1:A:630:ILE:H	1:A:630:ILE:HD12	1.28	0.94
1:A:901:LEU:HA	1:A:907:THR:HG23	1.49	0.94
2:B:642:ASP:HB3	2:B:649:LYS:HG3	1.50	0.93
11:R:3:C:H42	12:T:26:DG:H1	1.17	0.93
1:A:1172:LEU:O	1:A:1173:HIS:HB3	1.69	0.93
1:A:256:GLN:HA	1:A:257:ARG:HB3	0.95	0.93
2:B:992:ILE:HD11	9:K:67:PHE:HE2	1.33	0.93
1:A:573:SER:O	1:A:576:GLN:HB2	1.69	0.93
1:A:253:ASN:CB	1:A:256:GLN:C	2.41	0.93
1:A:1394:THR:CG2	1:A:1398:MET:HE3	1.99	0.92
1:A:662:PHE:HD2	2:B:829:CYS:SG	1.92	0.92
6:H:104:PHE:HZ	6:H:136:LYS:HB3	1.12	0.92
1:A:765:VAL:HG23	1:A:800:VAL:HB	1.50	0.92
2:B:64:CYS:HA	2:B:67:SER:HB2	1.50	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:757:PRO:HG3	2:B:983:ARG:HH22	1.26	0.91
1:A:341:MET:HE2	1:A:1401:SER:HB2	1.51	0.90
1:A:875:ALA:HA	1:A:878:ILE:HD12	1.53	0.90
3:C:66:ARG:NH2	8:J:4:PRO:HA	1.86	0.90
1:A:257:ARG:HG3	1:A:257:ARG:HH11	1.35	0.90
2:B:634:TYR:CE1	2:B:692:TYR:CD1	2.59	0.90
2:B:635:ARG:HB2	2:B:636:PRO:CD	2.02	0.90
8:J:48:ARG:NH2	8:J:49:MET:HE1	1.87	0.89
1:A:925:LEU:O	1:A:929:LEU:HB2	1.73	0.89
1:A:239:LEU:HD12	1:A:240:PRO:HD2	1.54	0.89
1:A:590:ARG:HG3	1:A:590:ARG:HH11	1.38	0.89
6:H:109:LYS:CA	6:H:110:ASP:CB	2.48	0.88
1:A:1156:PRO:O	1:A:1158:PRO:HD3	1.74	0.88
1:A:256:GLN:HB3	1:A:257:ARG:HB3	1.56	0.88
2:B:1032:SER:HB3	2:B:1089:PRO:HG2	1.53	0.88
1:A:382:PRO:CD	1:A:428:TYR:HE2	1.85	0.88
1:A:1436:ILE:HD13	2:B:1139:ILE:HG23	1.56	0.88
7:I:75:CYS:SG	7:I:78:CYS:CB	2.63	0.87
1:A:1407:GLU:CD	1:A:1407:GLU:H	1.83	0.87
1:A:630:ILE:HD12	1:A:630:ILE:N	1.89	0.87
2:B:1117:GLN:HG2	2:B:1156:ASP:OD2	1.75	0.87
2:B:829:CYS:SG	2:B:1014:PRO:CG	2.63	0.86
2:B:100:PRO:HD3	2:B:126:SER:OG	1.75	0.86
1:A:105:CYS:O	1:A:114:LEU:HG	1.75	0.86
4:E:28:TYR:CE1	4:E:78:LEU:HD13	2.10	0.86
6:H:82:PRO:O	6:H:83:GLN:HB2	1.72	0.86
1:A:351:THR:CG2	1:A:352:VAL:H	1.89	0.86
2:B:770:GLN:NE2	2:B:1093:GLN:HE22	1.73	0.86
1:A:1118:VAL:HG23	1:A:1306:LEU:HB2	1.57	0.86
1:A:793:SER:HB2	1:A:794:PRO:HD2	1.58	0.86
1:A:751:SER:OG	2:B:1015:HIS:HE1	1.57	0.86
2:B:913:GLY:HA2	2:B:938:SER:HB3	1.56	0.85
1:A:276:LEU:HD21	1:A:293:GLU:HG2	1.57	0.85
2:B:955:THR:HG22	2:B:956:THR:H	1.39	0.85
2:B:610:ASN:OD1	2:B:612:GLU:HB2	1.76	0.85
2:B:829:CYS:SG	2:B:1014:PRO:HG3	2.16	0.85
2:B:577:ALA:HB1	2:B:589:VAL:HG11	1.56	0.85
6:H:110:ASP:O	6:H:111:LEU:HD13	1.77	0.85
1:A:343:LYS:HD2	2:B:1151:LEU:HG	1.57	0.85
1:A:814:PHE:CE1	2:B:514:LEU:HD21	2.12	0.84
6:H:104:PHE:HD2	6:H:114:VAL:HG12	1.43	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:635:ARG:HE	1:A:877:HIS:HA	1.41	0.84
2:B:778:MET:HE3	2:B:853:SER:HB3	1.59	0.84
1:A:512:VAL:HA	1:A:519:PRO:HA	1.59	0.84
1:A:751:SER:OG	2:B:1015:HIS:CE1	2.31	0.84
6:H:47:PHE:HB3	6:H:95:TYR:CD1	2.12	0.84
1:A:253:ASN:CB	1:A:257:ARG:N	2.40	0.84
1:A:264:PHE:CZ	1:A:317:LYS:HB2	2.12	0.84
1:A:840:ARG:HE	1:A:1385:THR:HG23	1.42	0.84
9:K:65:HIS:HD2	9:K:67:PHE:H	1.26	0.84
1:A:855:THR:CG2	1:A:857:ARG:HE	1.89	0.84
8:J:3:VAL:HG21	8:J:18:TRP:CG	2.12	0.83
2:B:1096:ARG:HG2	2:B:1096:ARG:HH11	1.42	0.83
1:A:1118:VAL:HA	1:A:1327:ILE:HG13	1.57	0.83
1:A:903:ASN:O	1:A:907:THR:OG1	1.95	0.83
2:B:892:LYS:HG2	2:B:903:VAL:HG11	1.61	0.83
2:B:1099:VAL:HG12	2:B:1103:ILE:HD11	1.58	0.83
2:B:1136:ASP:HA	2:B:1139:ILE:HD12	1.61	0.83
2:B:37:PHE:O	2:B:38:PHE:HB2	1.77	0.83
2:B:955:THR:HG22	2:B:956:THR:N	1.93	0.83
4:E:61:GLN:HB3	4:E:79:TRP:HE3	1.43	0.83
3:C:260:LEU:O	3:C:264:GLN:HG3	1.79	0.82
1:A:251:SER:O	1:A:252:PHE:CD2	2.32	0.82
2:B:1032:SER:CB	2:B:1089:PRO:HG2	2.09	0.82
1:A:106:VAL:HG11	1:A:214:ILE:HD11	1.61	0.82
2:B:174:LEU:HD22	2:B:204:ILE:HD11	1.60	0.82
3:C:46:ILE:HD13	3:C:159:ALA:HB2	1.59	0.82
1:A:909:ASP:OD1	1:A:911:SER:HB3	1.79	0.82
2:B:870:ILE:O	2:B:871:THR:OG1	1.97	0.82
6:H:38:LEU:HD13	6:H:125:LEU:HD13	1.60	0.82
1:A:672:ASP:N	1:A:736:ASN:HD21	1.78	0.82
6:H:47:PHE:CB	6:H:95:TYR:HD1	1.93	0.82
1:A:567:LYS:HB3	6:H:96:VAL:H	1.43	0.81
2:B:329:THR:HA	2:B:332:ASP:HB2	1.61	0.81
1:A:401:GLY:C	1:A:435:HIS:CD2	2.58	0.81
1:A:889:SER:HB2	1:A:892:ALA:H	1.44	0.81
2:B:986:GLN:NE2	2:B:1016:ALA:HB1	1.95	0.81
1:A:115:LEU:HD22	1:A:119:ASN:HD22	1.45	0.81
1:A:528:LEU:HD23	1:A:751:SER:HA	1.63	0.81
2:B:803:LEU:N	2:B:822:ASN:HD21	1.79	0.81
3:C:70:ILE:HD11	3:C:144:ILE:CD1	2.09	0.81
2:B:577:ALA:HB1	2:B:589:VAL:CG1	2.09	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:600:LEU:HD12	2:B:615:MET:SD	2.20	0.81
1:A:120:GLU:OE2	1:A:123:ARG:HD3	1.80	0.81
1:A:675:THR:O	1:A:679:ILE:HD12	1.81	0.80
1:A:110:CYS:SG	1:A:111:GLY:N	2.53	0.80
1:A:630:ILE:H	1:A:630:ILE:CD1	1.93	0.80
2:B:634:TYR:CE1	2:B:692:TYR:HD1	2.00	0.80
2:B:1073:TYR:CE2	2:B:1080:LYS:CG	2.64	0.80
3:C:74:SER:O	3:C:77:ILE:HB	1.81	0.80
1:A:101:LYS:HG2	1:A:139:TRP:NE1	1.96	0.80
2:B:1076:HIS:ND1	9:K:40:HIS:HD2	1.79	0.80
3:C:56:THR:HG21	3:C:145:CYS:SG	2.22	0.80
4:E:63:ASN:HB3	4:E:64:PRO:CD	2.12	0.80
4:E:114:ASN:O	4:E:115:ASN:HB3	1.80	0.80
1:A:182:VAL:HG12	1:A:183:GLY:H	1.46	0.80
5:F:81:THR:HB	5:F:136:ARG:HH11	1.46	0.80
2:B:636:PRO:HB3	2:B:743:ILE:CG1	2.11	0.80
1:A:98:LYS:O	1:A:102:VAL:HG23	1.82	0.79
1:A:337:ARG:HD3	2:B:1132:GLU:OE1	1.82	0.79
1:A:256:GLN:CB	1:A:257:ARG:CB	2.60	0.79
1:A:909:ASP:O	1:A:911:SER:N	2.15	0.79
2:B:870:ILE:CG2	2:B:871:THR:N	2.45	0.79
2:B:982:SER:O	2:B:1093:GLN:HG3	1.81	0.79
3:C:167:HIS:CE1	10:L:70:ARG:HB3	2.17	0.79
1:A:722:LEU:HD11	1:A:794:PRO:HB3	1.64	0.79
1:A:890:ASP:H	1:A:1296:GLY:HA3	1.48	0.79
1:A:253:ASN:ND2	1:A:257:ARG:HA	1.96	0.79
1:A:1155:ASP:OD1	1:A:1162:VAL:HG23	1.82	0.79
3:C:166:GLU:HG3	9:K:10:PHE:HZ	1.48	0.79
8:J:1:MET:H1	8:J:56:LEU:H	1.31	0.79
3:C:3:GLU:HG3	3:C:4:GLU:N	1.97	0.79
5:F:109:VAL:HG12	5:F:110:ASP:N	1.98	0.79
2:B:636:PRO:HB3	2:B:743:ILE:HG13	1.63	0.78
3:C:70:ILE:CD1	3:C:144:ILE:HD11	2.11	0.78
3:C:102:GLN:HG2	3:C:154:LYS:CD	2.13	0.78
1:A:672:ASP:H	1:A:736:ASN:HD21	1.31	0.78
7:I:35:VAL:HG12	7:I:36:GLU:H	1.47	0.78
1:A:345:VAL:HG12	2:B:1155:SER:HB2	1.64	0.78
5:F:114:GLU:OE2	5:F:119:ARG:CG	2.31	0.78
1:A:1105:LEU:HD23	1:A:1384:VAL:HG21	1.66	0.78
1:A:264:PHE:CZ	1:A:317:LYS:CB	2.67	0.78
1:A:315:LEU:HB3	1:A:316:GLN:HA	0.82	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1063:MET:CG	1:A:1436:ILE:HG23	2.13	0.78
2:B:762:ASN:OD1	2:B:984:HIS:HD2	1.67	0.78
2:B:653:VAL:HG22	2:B:689:LEU:HB3	1.66	0.78
5:F:109:VAL:HG12	5:F:110:ASP:H	1.49	0.78
2:B:757:PRO:CG	2:B:983:ARG:NH2	2.45	0.77
2:B:770:GLN:HE22	2:B:1093:GLN:HE22	1.31	0.77
3:C:166:GLU:HG3	9:K:10:PHE:CZ	2.18	0.77
8:J:35:ALA:O	8:J:39:LEU:CD1	2.31	0.77
1:A:344:ARG:HG3	1:A:344:ARG:NH1	1.96	0.77
1:A:860:LEU:CD1	1:A:1393:ASN:ND2	2.46	0.77
4:E:61:GLN:HB3	4:E:79:TRP:CE3	2.19	0.77
2:B:635:ARG:CB	2:B:636:PRO:HD2	2.01	0.77
6:H:104:PHE:HZ	6:H:136:LYS:CB	1.84	0.77
6:H:109:LYS:HB2	6:H:111:LEU:HB2	1.66	0.77
1:A:253:ASN:CB	1:A:256:GLN:O	2.30	0.77
2:B:363:HIS:O	2:B:364:ILE:HB	1.83	0.77
2:B:911:ILE:HG22	2:B:912:ILE:HG13	1.65	0.77
5:F:76:LYS:O	5:F:79:ARG:HD2	1.85	0.77
1:A:552:TRP:NE1	1:A:655:PHE:CD1	2.53	0.77
2:B:807:ARG:HH11	2:B:807:ARG:CG	1.97	0.77
3:C:167:HIS:HD2	3:C:169:LYS:H	1.33	0.77
9:K:58:PHE:HB3	9:K:76:GLN:HB3	1.65	0.77
1:A:452:LYS:HB2	2:B:1141:HIS:CE1	2.20	0.77
1:A:1172:LEU:O	1:A:1173:HIS:CB	2.31	0.77
1:A:250:ILE:O	1:A:251:SER:CB	2.33	0.77
1:A:351:THR:CG2	2:B:1103:ILE:CD1	2.49	0.76
1:A:666:ILE:HD11	2:B:1030:LEU:HD13	1.64	0.76
8:J:1:MET:N	8:J:56:LEU:N	2.33	0.76
2:B:522:VAL:HG11	2:B:537:LYS:HB3	1.67	0.76
1:A:1025:ARG:HG2	1:A:1025:ARG:HH11	1.50	0.76
2:B:796:LEU:HB3	2:B:799:PRO:HD3	1.66	0.76
3:C:142:VAL:HG13	3:C:143:LEU:N	1.98	0.76
2:B:996:ARG:NH2	3:C:38:ILE:HD13	2.00	0.76
2:B:1073:TYR:CD2	2:B:1080:LYS:HG3	2.21	0.76
2:B:1084:GLN:HG2	3:C:201:TRP:CZ2	2.20	0.76
4:E:28:TYR:HE1	4:E:78:LEU:HD13	1.51	0.76
8:J:5:VAL:HG12	8:J:6:ARG:HG3	1.67	0.76
2:B:293:PRO:O	2:B:297:ILE:HG12	1.86	0.76
2:B:842:ASN:HD22	2:B:845:SER:HB3	1.49	0.76
2:B:981:ALA:HB2	2:B:987:LYS:CA	2.14	0.75
3:C:258:ILE:HD11	9:K:42:LEU:HD21	1.66	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1222:ASN:O	1:A:1223:ASP:HB3	1.86	0.75
6:H:47:PHE:HB3	6:H:95:TYR:HD1	1.50	0.75
9:K:57:LEU:HD12	9:K:76:GLN:HG2	1.68	0.75
1:A:19:PHE:HE1	1:A:1396:ALA:HB3	1.50	0.75
1:A:257:ARG:HH11	1:A:257:ARG:CG	2.00	0.75
1:A:364:VAL:HG12	1:A:459:ARG:O	1.87	0.75
2:B:976:ILE:HD11	2:B:992:ILE:HD12	1.68	0.75
2:B:825:VAL:HG23	2:B:1010:LEU:HG	1.69	0.75
5:F:111:LEU:HD13	5:F:111:LEU:H	1.51	0.75
7:I:7:CYS:SG	7:I:8:ARG:O	2.44	0.75
1:A:253:ASN:HB2	1:A:257:ARG:N	1.98	0.75
2:B:899:ILE:HD11	2:B:911:ILE:HG23	1.68	0.75
2:B:1154:ALA:O	2:B:1155:SER:CB	2.35	0.75
2:B:25:ILE:HD11	2:B:653:VAL:HB	1.67	0.75
1:A:15:LYS:HE2	2:B:1220:ARG:HG2	1.69	0.75
1:A:252:PHE:CG	1:A:252:PHE:O	2.39	0.75
1:A:423:ASP:C	1:A:424:ILE:HG13	2.11	0.74
2:B:824:ILE:HG12	8:J:48:ARG:HH12	1.51	0.74
1:A:482:PHE:O	2:B:989:THR:HG23	1.88	0.74
1:A:671:ALA:HB1	1:A:736:ASN:ND2	2.02	0.74
1:A:853:ASP:OD1	1:A:855:THR:HG22	1.86	0.74
3:C:252:GLN:HG3	9:K:95:ILE:HG23	1.69	0.74
7:I:35:VAL:HG12	7:I:36:GLU:N	2.02	0.74
2:B:64:CYS:HA	2:B:67:SER:CB	2.16	0.74
1:A:1391:ARG:HD3	1:A:1391:ARG:C	2.12	0.74
1:A:1441:PHE:CZ	5:F:89:GLU:HA	2.22	0.74
2:B:475:SER:C	2:B:477:ALA:H	1.95	0.74
1:A:535:THR:HG21	1:A:617:VAL:H	1.50	0.74
2:B:628:THR:O	2:B:628:THR:HG22	1.87	0.74
12:T:15:DA:H2''	12:T:16:DC:O5'	1.87	0.74
2:B:549:THR:HG22	2:B:550:ASP:H	1.53	0.74
1:A:567:LYS:NZ	6:H:97:MET:HG2	2.03	0.74
2:B:364:ILE:HD13	2:B:585:VAL:HG13	1.68	0.74
2:B:789:MET:CE	2:B:965:LYS:HB3	2.18	0.74
6:H:111:LEU:HD12	6:H:127:GLY:O	1.87	0.73
5:F:101:ILE:HD13	5:F:120:ILE:HG22	1.69	0.73
2:B:373:ARG:HA	2:B:566:LEU:CD2	2.15	0.73
2:B:475:SER:C	2:B:477:ALA:N	2.45	0.73
2:B:1065:GLN:NE2	2:B:1067:ARG:H	1.86	0.73
1:A:667:GLY:HA2	1:A:670:ILE:CG1	2.19	0.73
1:A:250:ILE:O	1:A:251:SER:HB3	1.89	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1173:HIS:ND1	1:A:1174:PHE:N	2.36	0.73
1:A:116:ASP:C	1:A:118:HIS:H	1.97	0.73
12:T:26:DG:N3	12:T:27:DA:H1'	2.03	0.73
1:A:7:SER:HB3	2:B:1193:GLN:OE1	1.89	0.73
1:A:1175:SER:OG	1:A:1176:LEU:N	2.21	0.73
2:B:992:ILE:HD11	9:K:67:PHE:CE2	2.22	0.73
10:L:42:ARG:O	10:L:44:ASP:N	2.22	0.73
2:B:701:ILE:HD11	2:B:703:ILE:HD11	1.71	0.72
2:B:983:ARG:CG	2:B:1093:GLN:NE2	2.51	0.72
1:A:265:LYS:C	1:A:267:ALA:H	1.96	0.72
1:A:871:ASP:OD1	1:A:1366:ARG:NH2	2.23	0.72
1:A:940:ARG:CZ	1:A:944:ARG:HH21	2.02	0.72
2:B:287:ARG:NH1	2:B:324:ILE:O	2.22	0.72
1:A:67:CYS:HB3	1:A:70:CYS:SG	2.29	0.72
2:B:1164:GLY:HA3	2:B:1190:ASP:HB3	1.70	0.72
1:A:100:LYS:HD3	1:A:104:GLU:OE1	1.90	0.72
1:A:269:ILE:HG13	1:A:299:HIS:HB3	1.70	0.72
1:A:457:ALA:HB3	1:A:506:ALA:HA	1.70	0.72
1:A:148:CYS:HB3	1:A:168:GLY:HA2	1.71	0.72
2:B:980:PHE:O	2:B:981:ALA:HB3	1.90	0.72
1:A:1063:MET:HG3	1:A:1436:ILE:HG23	1.71	0.72
2:B:1166:CYS:O	2:B:1166:CYS:SG	2.47	0.72
1:A:107:CYS:SG	1:A:108:MET:N	2.62	0.71
1:A:312:PRO:O	1:A:313:GLN:HB2	1.90	0.71
1:A:332:LYS:C	1:A:334:GLY:H	1.98	0.71
1:A:261:ASP:HB3	1:A:323:LYS:HD2	1.73	0.71
1:A:351:THR:HG23	2:B:1103:ILE:HD13	1.71	0.71
2:B:636:PRO:HB2	2:B:637:LEU:HB3	1.70	0.71
1:A:629:LEU:HD23	1:A:633:VAL:HG23	1.70	0.71
6:H:109:LYS:HG3	6:H:111:LEU:HD22	1.70	0.71
1:A:256:GLN:HB3	1:A:257:ARG:CB	2.20	0.71
1:A:402:ALA:HB2	1:A:434:ARG:HA	1.70	0.71
1:A:1424:VAL:HG13	1:A:1436:ILE:HD11	1.71	0.71
3:C:166:GLU:O	3:C:167:HIS:HB2	1.90	0.71
2:B:762:ASN:OD1	2:B:984:HIS:CD2	2.43	0.71
2:B:778:MET:CE	2:B:853:SER:HB3	2.21	0.71
1:A:252:PHE:O	1:A:252:PHE:CD1	2.43	0.71
2:B:770:GLN:OE1	2:B:983:ARG:HA	1.90	0.71
2:B:880:THR:O	2:B:881:ASN:HB2	1.89	0.71
9:K:102:LYS:O	9:K:106:GLU:HG2	1.91	0.71
1:A:129:LYS:O	1:A:130:ASP:HB2	1.91	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1025:ARG:HG2	1:A:1025:ARG:NH1	2.02	0.71
2:B:292:ILE:HD11	2:B:327:ARG:HG2	1.71	0.71
3:C:77:ILE:HA	3:C:129:ILE:HD11	1.73	0.71
6:H:58:THR:HG22	6:H:59:ILE:N	2.06	0.71
1:A:68:GLN:O	1:A:70:CYS:N	2.24	0.70
2:B:23:ALA:HB1	2:B:24:PRO:HD2	1.72	0.70
10:L:42:ARG:C	10:L:44:ASP:H	1.99	0.70
2:B:1077:THR:HG23	2:B:1079:LYS:H	1.57	0.70
10:L:46:VAL:HG12	10:L:47:ARG:H	1.56	0.70
1:A:901:LEU:H	1:A:926:GLN:NE2	1.89	0.70
2:B:589:VAL:HG12	2:B:590:HIS:N	2.05	0.70
2:B:744:HIS:HD2	2:B:746:SER:OG	1.73	0.70
2:B:1163:CYS:HB3	2:B:1166:CYS:O	1.90	0.70
1:A:326:ARG:HG2	1:A:1406:VAL:HG21	1.71	0.70
2:B:567:GLU:H	2:B:567:GLU:CD	1.99	0.70
2:B:870:ILE:HG23	2:B:871:THR:H	1.56	0.70
2:B:830:TYR:O	2:B:831:SER:C	2.33	0.70
8:J:45:CYS:SG	8:J:46:CYS:N	2.64	0.70
1:A:1273:LEU:O	1:A:1274:ARG:HB3	1.91	0.70
2:B:1096:ARG:HG2	2:B:1096:ARG:NH1	2.05	0.70
6:H:104:PHE:CE1	6:H:136:LYS:HB3	2.22	0.70
1:A:1342:GLU:HG3	4:E:198:ILE:HD13	1.73	0.70
3:C:148:ARG:NH1	8:J:64:ASN:HA	2.07	0.70
2:B:34:ILE:HD13	2:B:542:MET:HE1	1.73	0.69
1:A:445:ASN:HB2	1:A:454:SER:O	1.92	0.69
2:B:975:GLN:HG2	2:B:976:ILE:H	1.56	0.69
3:C:22:LEU:CD2	3:C:25:VAL:HG21	2.23	0.69
5:F:135:ARG:HG2	5:F:137:TYR:CE1	2.27	0.69
1:A:629:LEU:HD23	1:A:633:VAL:CG2	2.21	0.69
1:A:1404:GLU:O	1:A:1408:ILE:HG12	1.92	0.69
2:B:211:VAL:O	2:B:480:SER:HA	1.92	0.69
1:A:842:VAL:HG11	2:B:1136:ASP:OD2	1.92	0.69
1:A:1116:LEU:H	1:A:1308:THR:HB	1.57	0.69
2:B:682:SER:O	2:B:686:ASN:ND2	2.25	0.69
3:C:66:ARG:HH22	8:J:4:PRO:HA	1.56	0.69
1:A:367:PRO:HB3	1:A:466:SER:HA	1.74	0.69
1:A:765:VAL:CG2	1:A:800:VAL:CB	2.68	0.69
2:B:1051:THR:HB	2:B:1054:GLY:H	1.58	0.69
1:A:1025:ARG:HH11	1:A:1025:ARG:CG	2.06	0.69
1:A:1111:MET:HG2	1:A:1114:PRO:HG3	1.73	0.69
2:B:589:VAL:HG12	2:B:590:HIS:H	1.56	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:636:PRO:CB	2:B:637:LEU:HA	2.22	0.69
2:B:852:ARG:NH2	10:L:70:ARG:O	2.26	0.69
2:B:976:ILE:O	2:B:990:ILE:CB	2.34	0.69
1:A:525:GLN:O	1:A:526:ASP:C	2.36	0.69
2:B:702:LEU:HD21	2:B:735:ALA:HB1	1.74	0.69
1:A:264:PHE:HZ	1:A:317:LYS:CB	2.05	0.69
2:B:373:ARG:HD3	2:B:566:LEU:CD2	2.22	0.69
1:A:14:VAL:H	1:A:1432:GLN:NE2	1.91	0.68
1:A:37:PHE:HB2	1:A:52:GLY:CA	2.23	0.68
1:A:1222:ASN:O	1:A:1223:ASP:CB	2.41	0.68
2:B:986:GLN:HE22	2:B:1016:ALA:HB1	1.56	0.68
2:B:273:LEU:HD11	2:B:285:ILE:HD11	1.75	0.68
1:A:873:MET:HG2	1:A:957:PRO:HG3	1.75	0.68
9:K:65:HIS:CD2	9:K:67:PHE:HB2	2.28	0.68
2:B:637:LEU:HD11	2:B:693:ILE:HG13	1.76	0.68
1:A:845:LEU:O	1:A:848:ILE:HG12	1.94	0.68
1:A:1021:LEU:O	1:A:1024:SER:N	2.27	0.68
1:A:731:ARG:HG3	1:A:755:PHE:CZ	2.28	0.68
1:A:1015:VAL:HG12	1:A:1019:CYS:SG	2.34	0.68
6:H:109:LYS:CG	6:H:110:ASP:HB2	2.24	0.68
1:A:37:PHE:HB2	1:A:52:GLY:HA3	1.76	0.67
2:B:983:ARG:HH11	2:B:1091:TYR:HB3	1.58	0.67
2:B:784:ASN:CG	2:B:788:ARG:HD2	2.20	0.67
5:F:111:LEU:H	5:F:111:LEU:CD1	2.06	0.67
2:B:32:ALA:HB3	2:B:658:ILE:HD11	1.76	0.67
4:E:19:VAL:O	4:E:23:VAL:HG23	1.94	0.67
1:A:855:THR:HG21	1:A:857:ARG:NE	2.04	0.67
2:B:724:ASP:HB3	2:B:727:LYS:HG3	1.76	0.67
1:A:504:LEU:HD11	5:F:91:ALA:CB	2.24	0.67
2:B:487:THR:O	2:B:490:SER:HB3	1.93	0.67
3:C:35:ARG:NH1	9:K:41:THR:OG1	2.27	0.67
1:A:814:PHE:HE1	2:B:514:LEU:HD21	1.60	0.67
1:A:1101:LEU:O	1:A:1105:LEU:HD12	1.95	0.67
2:B:1159:ARG:HD3	2:B:1193:GLN:HG3	1.75	0.67
1:A:19:PHE:CE1	1:A:1396:ALA:HB3	2.30	0.67
1:A:264:PHE:HZ	1:A:317:LYS:HB3	1.59	0.67
1:A:883:LEU:HD11	1:A:1017:LEU:HD21	1.77	0.67
2:B:955:THR:CG2	2:B:956:THR:H	2.07	0.67
2:B:221:ASN:N	2:B:241:ARG:O	2.21	0.67
6:H:89:LEU:O	6:H:91:ASP:N	2.27	0.67
8:J:6:ARG:H	8:J:14:VAL:H	1.43	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:474:SER:C	2:B:476:ARG:H	2.03	0.66
2:B:603:LEU:HB3	2:B:609:ILE:HG12	1.76	0.66
3:C:52:GLU:HA	10:L:64:LEU:HD22	1.77	0.66
1:A:1392:SER:O	1:A:1393:ASN:C	2.38	0.66
2:B:213:ILE:CD1	2:B:481:GLN:OE1	2.40	0.66
1:A:527:THR:HG22	1:A:653:VAL:HB	1.78	0.66
1:A:1410:PHE:HD2	2:B:1212:ILE:HD11	1.59	0.66
2:B:615:MET:HG2	2:B:626:ILE:HG23	1.77	0.66
2:B:956:THR:HA	2:B:961:LEU:O	1.96	0.66
1:A:344:ARG:HH11	1:A:344:ARG:CG	2.05	0.66
2:B:547:VAL:HG12	2:B:612:GLU:OE2	1.95	0.66
2:B:847:ASP:N	2:B:847:ASP:OD1	2.28	0.66
1:A:507:VAL:HG13	1:A:521:MET:CE	2.18	0.66
1:A:1434:ALA:O	1:A:1436:ILE:N	2.29	0.66
1:A:577:ILE:O	1:A:580:VAL:HG23	1.95	0.66
2:B:1181:GLU:HG2	2:B:1188:LYS:HG2	1.77	0.66
3:C:165:LYS:O	9:K:6:ARG:NH1	2.29	0.66
2:B:471:LYS:HG3	2:B:472:ALA:N	2.09	0.66
1:A:119:ASN:O	1:A:123:ARG:CG	2.40	0.66
1:A:567:LYS:HZ1	6:H:97:MET:HG2	1.60	0.66
3:C:124:LEU:O	3:C:127:ARG:HG2	1.96	0.66
1:A:256:GLN:HB3	1:A:257:ARG:CG	2.26	0.66
1:A:399:HIS:HB3	1:A:400:PRO:HD3	1.76	0.66
1:A:751:SER:HG	2:B:1015:HIS:HE1	1.43	0.66
2:B:199:MET:HE2	2:B:492:LEU:HD23	1.75	0.66
2:B:635:ARG:O	2:B:636:PRO:O	2.14	0.66
2:B:1166:CYS:SG	14:B:1307:ZN:ZN	1.84	0.66
1:A:252:PHE:HE2	12:T:27:DA:H61	1.43	0.65
2:B:980:PHE:CE1	2:B:990:ILE:HG13	2.31	0.65
3:C:143:LEU:C	3:C:143:LEU:HD12	2.20	0.65
1:A:185:TRP:O	1:A:186:LYS:HB2	1.96	0.65
1:A:445:ASN:HB2	1:A:455:MET:HG2	1.78	0.65
1:A:892:ALA:HA	1:A:895:LYS:HE3	1.78	0.65
2:B:384:ARG:HH22	2:B:621:GLU:CG	2.08	0.65
1:A:1116:LEU:HD13	1:A:1329:THR:HG1	1.62	0.65
1:A:1349:TYR:CE1	1:A:1368:MET:HE3	2.32	0.65
1:A:1144:LYS:HA	1:A:1268:LEU:HD22	1.77	0.65
1:A:907:THR:HG21	1:A:920:LEU:HG	1.78	0.65
2:B:129:PHE:CE2	2:B:166:PHE:HB2	2.31	0.65
2:B:999:MET:HG2	2:B:1008:PRO:HD2	1.78	0.65
5:F:84:TYR:CE1	5:F:152:ILE:HD12	2.32	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:104:PHE:CE2	6:H:136:LYS:HB3	2.24	0.65
1:A:77:CYS:SG	14:A:1735:ZN:ZN	1.85	0.65
2:B:345:LYS:O	2:B:348:ARG:HG2	1.96	0.65
2:B:980:PHE:CE1	2:B:990:ILE:HD11	2.31	0.65
1:A:115:LEU:HD11	1:A:145:LYS:HE3	1.79	0.65
1:A:575:LYS:HB3	1:A:612:ILE:HG12	1.78	0.65
2:B:549:THR:HG22	2:B:550:ASP:N	2.11	0.65
2:B:834:ASN:HB3	2:B:840:ILE:HG13	1.77	0.65
3:C:3:GLU:HB3	9:K:104:ASN:OD1	1.96	0.65
1:A:1130:GLN:HG3	1:A:1134:ILE:HD11	1.78	0.65
2:B:976:ILE:HD11	2:B:992:ILE:HA	1.78	0.65
1:A:503:GLN:HB2	1:A:504:LEU:HD12	1.78	0.65
8:J:45:CYS:SG	14:J:101:ZN:ZN	1.85	0.65
2:B:1094:ARG:HH22	2:B:1098:MET:HG2	1.62	0.64
3:C:186:LEU:HB3	3:C:188:HIS:CD2	2.32	0.64
6:H:109:LYS:CB	6:H:111:LEU:N	2.60	0.64
2:B:370:PHE:HD2	2:B:373:ARG:HG3	1.62	0.64
2:B:864:LYS:HB3	2:B:872:GLU:H	1.60	0.64
1:A:1134:ILE:O	1:A:1138:ILE:HG12	1.97	0.64
6:H:93:TYR:HA	6:H:145:ARG:HB3	1.79	0.64
1:A:401:GLY:O	1:A:435:HIS:CD2	2.50	0.64
1:A:1319:VAL:HG13	1:A:1320:PRO:HD2	1.77	0.64
6:H:130:ARG:HB3	6:H:134:ASN:HD22	1.63	0.64
1:A:567:LYS:O	1:A:569:LYS:N	2.30	0.64
1:A:900:ASP:HB3	1:A:906:HIS:O	1.98	0.64
2:B:62:ILE:HD12	2:B:418:LYS:HG3	1.80	0.64
1:A:68:GLN:C	1:A:70:CYS:H	2.06	0.64
1:A:809:THR:HB	1:A:810:PRO:HD2	1.79	0.64
2:B:803:LEU:H	2:B:822:ASN:HD21	1.45	0.64
4:E:63:ASN:HB3	4:E:64:PRO:HD3	1.79	0.64
4:E:66:GLU:O	4:E:68:SER:N	2.31	0.64
1:A:380:VAL:HG21	1:A:430:TRP:HB2	1.78	0.64
1:A:1291:VAL:HG22	1:A:1292:PRO:HD2	1.80	0.64
4:E:185:ALA:HA	4:E:190:LEU:HD23	1.80	0.64
9:K:57:LEU:HD12	9:K:76:GLN:CG	2.27	0.64
1:A:343:LYS:NZ	2:B:1197:PRO:HB3	2.12	0.64
3:C:47:ASP:HA	10:L:69:ALA:HB3	1.78	0.64
11:R:4:G:C2'	11:R:5:A:H8	2.04	0.64
2:B:378:LEU:O	2:B:382:ILE:HG12	1.99	0.63
3:C:247:GLY:O	3:C:248:ILE:C	2.39	0.63
6:H:97:MET:HB2	6:H:118:PHE:CD2	2.32	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:J:48:ARG:HH21	8:J:49:MET:CE	1.97	0.63
1:A:532:ARG:HH22	1:A:745:GLN:HE21	1.46	0.63
1:A:535:THR:CG2	1:A:616:VAL:HA	2.28	0.63
2:B:955:THR:HG23	10:L:54:ARG:O	1.98	0.63
3:C:123:ASN:HD22	3:C:125:MET:HG2	1.62	0.63
1:A:269:ILE:HD11	1:A:300:VAL:HA	1.81	0.63
1:A:1312:ASN:O	1:A:1316:VAL:HG23	1.99	0.63
2:B:636:PRO:HB2	2:B:637:LEU:CA	2.28	0.63
5:F:135:ARG:HG2	5:F:137:TYR:HE1	1.63	0.63
1:A:401:GLY:H	1:A:435:HIS:HD2	1.44	0.63
2:B:45:SER:OG	2:B:46:GLN:N	2.29	0.63
6:H:23:VAL:HG21	6:H:121:LEU:HD21	1.81	0.63
1:A:500:GLU:HG2	2:B:1143:ALA:HB1	1.81	0.63
1:A:810:PRO:HD3	2:B:1047:PHE:CD2	2.33	0.63
6:H:104:PHE:CD2	6:H:114:VAL:HG12	2.31	0.63
1:A:206:GLU:O	1:A:210:ILE:HG12	1.99	0.63
1:A:315:LEU:CB	1:A:316:GLN:CA	2.46	0.63
1:A:401:GLY:N	1:A:435:HIS:HD2	1.97	0.63
1:A:1342:GLU:HG2	4:E:212:ARG:HH11	1.64	0.63
2:B:763:GLN:O	2:B:766:ARG:HB2	1.97	0.63
12:T:13:DA:H61	13:N:2:DT:C7	2.12	0.63
1:A:455:MET:HE1	2:B:1130:PHE:HE1	1.63	0.63
1:A:768:GLN:HG2	1:A:816:HIS:HA	1.79	0.63
2:B:824:ILE:HG12	8:J:48:ARG:NH1	2.14	0.63
1:A:261:ASP:HB3	1:A:323:LYS:CD	2.29	0.62
1:A:451:HIS:HB3	1:A:453:MET:H	1.64	0.62
1:A:596:THR:C	1:A:598:LEU:H	2.06	0.62
1:A:1189:SER:OG	1:A:1190:PRO:HD2	1.99	0.62
1:A:767:GLN:OE1	1:A:767:GLN:HA	1.99	0.62
2:B:783:THR:HG21	8:J:59:LYS:HB3	1.81	0.62
2:B:999:MET:HG3	2:B:1000:PRO:HD2	1.81	0.62
1:A:14:VAL:H	1:A:1432:GLN:HE22	1.46	0.62
1:A:352:VAL:HG12	1:A:353:ILE:N	2.13	0.62
1:A:1393:ASN:N	1:A:1393:ASN:OD1	2.32	0.62
8:J:45:CYS:O	8:J:48:ARG:HG3	1.99	0.62
1:A:1342:GLU:HG2	4:E:212:ARG:NH1	2.15	0.62
2:B:711:GLU:H	2:B:712:PRO:HD3	1.63	0.62
2:B:980:PHE:CE1	2:B:990:ILE:CD1	2.83	0.62
6:H:109:LYS:HG2	6:H:111:LEU:HD23	1.81	0.62
8:J:3:VAL:HG21	8:J:18:TRP:CB	2.29	0.62
10:L:51:CYS:SG	14:L:105:ZN:ZN	1.89	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:315:LEU:CD1	1:A:318:SER:O	2.40	0.62
1:A:545:GLN:HB3	1:A:549:MET:HE3	1.81	0.62
2:B:622:LYS:HE3	7:I:59:VAL:HG22	1.82	0.62
2:B:1130:PHE:HZ	2:B:1138:MET:HG2	1.64	0.62
5:F:74:ILE:HG21	5:F:144:GLU:HG2	1.80	0.62
6:H:47:PHE:CB	6:H:95:TYR:CD1	2.75	0.62
3:C:144:ILE:HG22	3:C:145:CYS:HB3	1.80	0.62
2:B:273:LEU:HD11	2:B:285:ILE:CD1	2.30	0.62
2:B:636:PRO:HB3	2:B:743:ILE:HG12	1.81	0.62
2:B:807:ARG:HG3	2:B:807:ARG:NH1	2.00	0.62
2:B:955:THR:CG2	2:B:956:THR:N	2.63	0.62
8:J:6:ARG:HG2	8:J:13:VAL:HA	1.81	0.62
7:I:111:THR:HG22	7:I:113:ASP:H	1.63	0.62
3:C:102:GLN:CG	3:C:154:LYS:HD3	2.26	0.62
4:E:58:MET:HE3	4:E:82:PHE:CD2	2.35	0.62
9:K:92:ASN:HA	9:K:95:ILE:HD12	1.81	0.62
1:A:675:THR:C	1:A:679:ILE:HD12	2.25	0.62
2:B:865:LYS:O	2:B:866:TYR:C	2.43	0.62
3:C:45:ALA:HA	3:C:72:LEU:CD1	2.23	0.62
1:A:590:ARG:HH11	1:A:590:ARG:CG	2.12	0.61
3:C:92:CYS:SG	3:C:94:LYS:HB3	2.40	0.61
1:A:869:GLY:O	4:E:204:THR:HG21	2.00	0.61
1:A:709:THR:HB	1:A:712:GLU:H	1.65	0.61
1:A:826:ASP:O	1:A:830:LYS:N	2.27	0.61
1:A:909:ASP:C	1:A:911:SER:N	2.56	0.61
1:A:1173:HIS:ND1	1:A:1173:HIS:C	2.58	0.61
1:A:900:ASP:O	1:A:907:THR:HA	2.00	0.61
2:B:636:PRO:HB2	2:B:637:LEU:CB	2.29	0.61
2:B:982:SER:OG	2:B:983:ARG:N	2.30	0.61
6:H:108:SER:OG	6:H:109:LYS:N	2.33	0.61
9:K:47:ARG:HD2	9:K:60:ALA:HA	1.81	0.61
2:B:490:SER:O	2:B:493:SER:N	2.33	0.61
3:C:248:ILE:HG12	9:K:101:LEU:HD13	1.83	0.61
4:E:61:GLN:CB	4:E:79:TRP:HE3	2.11	0.61
1:A:302:THR:HG21	1:A:313:GLN:NE2	2.16	0.61
1:A:567:LYS:CG	1:A:568:PRO:HD2	2.30	0.61
2:B:830:TYR:O	2:B:832:GLY:N	2.34	0.61
7:I:55:THR:HG23	7:I:58:VAL:HG21	1.81	0.61
1:A:116:ASP:O	1:A:118:HIS:N	2.34	0.61
1:A:860:LEU:HD11	1:A:1393:ASN:ND2	2.15	0.61
2:B:849:GLY:HA2	2:B:852:ARG:HD2	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:969:ARG:NH1	3:C:61:GLU:OE1	2.32	0.61
3:C:49:VAL:HG12	3:C:155:LEU:HD22	1.83	0.61
8:J:1:MET:H2	8:J:56:LEU:H	1.48	0.61
1:A:335:ARG:NH1	2:B:1202:LEU:HD12	2.16	0.61
1:A:336:ILE:HA	1:A:340:LEU:HD12	1.83	0.61
1:A:446:ARG:CD	1:A:480:ALA:HB2	2.23	0.61
1:A:901:LEU:HD22	1:A:919:ILE:HG22	1.82	0.61
2:B:981:ALA:HB1	2:B:987:LYS:HA	1.80	0.61
1:A:203:SER:O	1:A:207:ILE:HD12	2.01	0.61
1:A:315:LEU:HD13	1:A:319:GLY:O	2.01	0.61
3:C:182:PRO:HB2	3:C:207:CYS:SG	2.41	0.61
5:F:81:THR:HB	5:F:136:ARG:NH1	2.14	0.61
1:A:809:THR:H	1:A:812:GLU:HB2	1.64	0.60
1:A:899:VAL:HB	1:A:929:LEU:HD11	1.83	0.60
2:B:999:MET:HE2	2:B:1011:ILE:HD11	1.83	0.60
1:A:253:ASN:HD22	1:A:257:ARG:HA	1.66	0.60
1:A:351:THR:HG21	1:A:466:SER:O	2.01	0.60
1:A:553:VAL:HG23	1:A:652:VAL:CG2	2.30	0.60
1:A:1134:ILE:O	1:A:1138:ILE:CG1	2.49	0.60
2:B:980:PHE:CD1	2:B:990:ILE:HG13	2.36	0.60
3:C:98:VAL:C	3:C:99:LEU:HD23	2.25	0.60
6:H:96:VAL:HG13	6:H:143:LEU:HG	1.82	0.60
1:A:913:LEU:HG	1:A:915:SER:H	1.67	0.60
1:A:648:ASN:O	1:A:652:VAL:HG23	2.01	0.60
1:A:1227:ILE:HG22	1:A:1228:TRP:N	2.15	0.60
2:B:957:ASN:HB3	2:B:961:LEU:HB2	1.83	0.60
4:E:29:PHE:O	4:E:30:ILE:CG1	2.45	0.60
6:H:109:LYS:HA	6:H:110:ASP:CB	2.16	0.60
10:L:41:SER:O	10:L:42:ARG:O	2.18	0.60
1:A:899:VAL:HG23	1:A:1029:ARG:HG3	1.84	0.60
3:C:93:ASP:O	3:C:127:ARG:NH2	2.35	0.60
1:A:553:VAL:HG23	1:A:652:VAL:HG22	1.83	0.60
2:B:745:PRO:C	2:B:747:MET:H	2.09	0.60
2:B:770:GLN:HG2	2:B:983:ARG:O	2.01	0.60
2:B:1104:HIS:HB2	2:B:1122:ARG:HD2	1.84	0.60
3:C:173:ALA:O	3:C:174:ALA:HB2	2.02	0.60
1:A:535:THR:HG22	1:A:616:VAL:HA	1.84	0.60
1:A:490:HIS:HB3	2:B:1150:ARG:CZ	2.32	0.60
1:A:1333:ILE:O	1:A:1333:ILE:HD13	2.02	0.60
2:B:870:ILE:HG22	2:B:871:THR:N	2.16	0.60
8:J:7:CYS:HB2	8:J:49:MET:CE	2.31	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:93:VAL:HG21	1:A:304:MET:HB3	1.82	0.60
3:C:76:ASP:OD2	3:C:128:ASN:HB3	2.01	0.60
1:A:380:VAL:HG23	1:A:430:TRP:O	2.02	0.59
1:A:775:ILE:HG13	1:A:798:GLY:HA3	1.84	0.59
1:A:956:LEU:HD11	1:A:1017:LEU:HD22	1.84	0.59
1:A:463:ILE:HB	1:A:464:PRO:HD2	1.83	0.59
1:A:902:LEU:HG	1:A:926:GLN:HG3	1.83	0.59
2:B:322:PHE:HZ	7:I:30:ARG:HH11	1.47	0.59
2:B:383:ASN:O	2:B:387:LEU:HB2	2.01	0.59
8:J:3:VAL:HG22	8:J:53:HIS:CE1	2.38	0.59
1:A:105:CYS:O	1:A:114:LEU:CG	2.48	0.59
1:A:909:ASP:C	1:A:911:SER:H	2.10	0.59
2:B:373:ARG:HD3	2:B:566:LEU:HD23	1.82	0.59
8:J:2:ILE:HG23	8:J:2:ILE:O	2.02	0.59
1:A:253:ASN:ND2	1:A:257:ARG:CA	2.66	0.59
1:A:257:ARG:O	1:A:257:ARG:CG	2.30	0.59
1:A:741:ASN:HD22	1:A:744:LYS:H	1.49	0.59
3:C:184:ASN:ND2	3:C:187:LYS:HA	2.17	0.59
6:H:108:SER:OG	6:H:109:LYS:HE2	2.02	0.59
8:J:7:CYS:HB2	8:J:49:MET:HE2	1.84	0.59
9:K:70:ARG:O	9:K:71:PHE:HB3	2.01	0.59
1:A:100:LYS:O	1:A:104:GLU:HG3	2.03	0.59
1:A:264:PHE:CZ	1:A:317:LYS:HB3	2.35	0.59
1:A:741:ASN:ND2	1:A:744:LYS:H	2.00	0.59
2:B:515:HIS:H	2:B:518:HIS:CD2	2.20	0.59
3:C:115:SER:HB3	3:C:142:VAL:HG12	1.83	0.59
1:A:95:PHE:O	1:A:99:ILE:HG13	2.01	0.59
1:A:583:PRO:O	1:A:610:GLY:HA2	2.02	0.59
1:A:840:ARG:HG3	1:A:1402:PHE:HZ	1.67	0.59
1:A:419:LYS:HG3	1:A:420:ARG:HG3	1.84	0.59
1:A:922:ASP:OD1	1:A:923:LEU:N	2.34	0.59
2:B:190:TYR:CZ	2:B:196:PRO:HG2	2.37	0.59
2:B:308:TRP:HA	2:B:311:LEU:HD12	1.84	0.59
9:K:24:ASP:OD2	9:K:74:ARG:HD2	2.02	0.59
2:B:210:LYS:NZ	2:B:482:VAL:HG13	2.17	0.59
2:B:800:GLN:HB3	8:J:52:THR:CG2	2.32	0.59
3:C:167:HIS:ND1	10:L:70:ARG:HB3	2.18	0.59
4:E:176:PRO:O	4:E:212:ARG:HA	2.02	0.59
6:H:109:LYS:CG	6:H:110:ASP:CB	2.81	0.59
6:H:139:ASN:O	6:H:140:ALA:HB2	2.02	0.59
12:T:27:DA:H2'	12:T:27:DA:N3	2.17	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:107:CYS:SG	1:A:108:MET:O	2.60	0.59
1:A:249:SER:C	1:A:250:ILE:CG1	2.72	0.59
1:A:565:ILE:HG12	1:A:567:LYS:NZ	2.18	0.59
2:B:515:HIS:CD2	2:B:517:THR:H	2.20	0.59
2:B:636:PRO:CB	2:B:637:LEU:CA	2.80	0.59
2:B:814:PHE:C	2:B:816:GLU:H	2.09	0.59
2:B:870:ILE:HG23	2:B:871:THR:N	2.14	0.59
2:B:980:PHE:HE1	2:B:990:ILE:CD1	2.16	0.59
2:B:1138:MET:HA	2:B:1138:MET:HE3	1.85	0.59
1:A:517:ASN:HD22	1:A:1364:ASN:HB2	1.66	0.59
1:A:1168:GLU:HG2	1:A:1168:GLU:O	2.03	0.59
2:B:179:CYS:SG	2:B:180:TYR:N	2.75	0.59
6:H:89:LEU:HB2	6:H:91:ASP:OD1	2.03	0.59
1:A:1324:PRO:HB2	4:E:142:VAL:HG11	1.84	0.58
2:B:708:GLU:O	2:B:710:LEU:N	2.35	0.58
1:A:1276:VAL:HB	1:A:1279:ILE:HD13	1.86	0.58
1:A:1319:VAL:HG12	1:A:1320:PRO:O	2.02	0.58
3:C:73:GLN:NE2	3:C:237:SER:O	2.36	0.58
5:F:111:LEU:CD1	5:F:111:LEU:N	2.67	0.58
6:H:58:THR:HG22	6:H:59:ILE:H	1.68	0.58
1:A:1400:CYS:O	1:A:1405:THR:HG23	2.04	0.58
2:B:745:PRO:O	2:B:747:MET:N	2.36	0.58
1:A:116:ASP:C	1:A:118:HIS:N	2.61	0.58
1:A:1116:LEU:HD22	1:A:1311:VAL:HG22	1.85	0.58
2:B:23:ALA:HB1	2:B:24:PRO:CD	2.33	0.58
3:C:97:VAL:HG21	3:C:129:ILE:HG23	1.85	0.58
3:C:177:GLU:HB2	3:C:231:ASN:HB3	1.86	0.58
1:A:256:GLN:CB	1:A:257:ARG:HD3	2.10	0.58
1:A:1152:ILE:HD12	7:I:44:TYR:HD2	1.68	0.58
1:A:1220:PHE:CD1	1:A:1224:LEU:CD2	2.86	0.58
2:B:770:GLN:HB2	2:B:983:ARG:O	2.04	0.58
2:B:1154:ALA:O	2:B:1155:SER:HB2	2.03	0.58
3:C:134:ILE:HD12	3:C:141:GLY:H	1.68	0.58
3:C:238:ILE:HG23	3:C:242:GLN:HB2	1.86	0.58
1:A:1019:CYS:O	1:A:1022:LEU:HB3	2.03	0.58
3:C:124:LEU:C	3:C:126:GLY:N	2.61	0.58
1:A:58:LEU:HD22	1:A:244:PRO:HD2	1.85	0.58
1:A:251:SER:O	1:A:252:PHE:HD2	1.86	0.58
1:A:1025:ARG:HG3	1:A:1030:ARG:NH1	2.18	0.58
2:B:293:PRO:HG2	2:B:296:GLU:HB2	1.86	0.58
4:E:77:SER:HB3	4:E:105:PHE:HD2	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:55:ASP:H	1:A:56:PRO:HD2	1.69	0.58
1:A:58:LEU:HD21	1:A:243:PRO:HB3	1.86	0.58
1:A:253:ASN:HD22	1:A:257:ARG:CA	2.17	0.58
1:A:265:LYS:C	1:A:267:ALA:N	2.60	0.58
2:B:976:ILE:HG23	2:B:977:GLY:N	2.18	0.58
4:E:66:GLU:C	4:E:68:SER:N	2.61	0.58
1:A:265:LYS:HD3	1:A:302:THR:HG22	1.86	0.57
1:A:335:ARG:O	1:A:339:ASN:HB2	2.04	0.57
1:A:527:THR:HG21	1:A:650:GLN:HA	1.86	0.57
6:H:5:LEU:HD22	6:H:133:ASN:O	2.04	0.57
1:A:567:LYS:CB	1:A:568:PRO:CD	2.57	0.57
1:A:1127:ASP:HB3	1:A:1130:GLN:HB3	1.86	0.57
1:A:899:VAL:HB	1:A:929:LEU:CD1	2.34	0.57
1:A:1433:MET:HE1	5:F:92:ARG:NH1	2.19	0.57
2:B:451:LYS:O	2:B:452:THR:C	2.48	0.57
2:B:913:GLY:HA2	2:B:938:SER:CB	2.31	0.57
4:E:100:ILE:HG23	4:E:105:PHE:HB2	1.85	0.57
5:F:109:VAL:CG1	5:F:110:ASP:H	2.16	0.57
1:A:55:ASP:O	1:A:58:LEU:N	2.37	0.57
1:A:446:ARG:HD3	1:A:478:TYR:O	2.05	0.57
1:A:55:ASP:O	1:A:57:ARG:N	2.37	0.57
1:A:381:THR:HG22	1:A:384:ASN:ND2	2.19	0.57
1:A:690:VAL:HG13	1:A:718:VAL:HG22	1.86	0.57
1:A:840:ARG:HG3	1:A:1402:PHE:CZ	2.39	0.57
2:B:120:ARG:HE	2:B:955:THR:CG2	2.17	0.57
2:B:361:LEU:HD11	2:B:381:MET:HE1	1.86	0.57
2:B:522:VAL:CG1	2:B:537:LYS:HB3	2.34	0.57
2:B:635:ARG:O	2:B:636:PRO:C	2.46	0.57
4:E:190:LEU:HD12	4:E:194:GLU:O	2.03	0.57
6:H:47:PHE:HB2	6:H:95:TYR:HD1	1.68	0.57
12:T:26:DG:C2	12:T:27:DA:H1'	2.39	0.57
1:A:54:ASN:O	1:A:55:ASP:HB2	2.04	0.57
1:A:709:THR:HG23	7:I:94:ASP:HA	1.86	0.57
2:B:957:ASN:HD22	2:B:959:ASP:H	1.52	0.57
9:K:46:ILE:O	9:K:50:LEU:HB2	2.04	0.57
1:A:535:THR:HG21	1:A:617:VAL:N	2.19	0.57
1:A:635:ARG:NE	1:A:877:HIS:HA	2.16	0.57
1:A:1195:LEU:HD11	1:A:1267:MET:HE1	1.87	0.57
2:B:357:GLN:HA	2:B:374:LYS:NZ	2.19	0.57
4:E:66:GLU:C	4:E:68:SER:H	2.13	0.57
7:I:84:VAL:HG13	7:I:84:VAL:O	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:T:18:DA:C2	12:T:19:DT:N3	2.72	0.57
1:A:498:ARG:O	1:A:499:ALA:C	2.48	0.57
1:A:659:HIS:O	2:B:1081:LEU:HD23	2.03	0.57
1:A:679:ILE:HG23	1:A:729:ALA:HB1	1.87	0.57
1:A:1073:GLY:O	1:A:1076:ALA:HB3	2.05	0.57
2:B:384:ARG:HH22	2:B:621:GLU:HG3	1.68	0.57
6:H:38:LEU:CD1	6:H:125:LEU:HD13	2.33	0.57
1:A:1151:GLU:OE2	7:I:45:ARG:NH1	2.38	0.57
1:A:1170:ILE:O	1:A:1171:GLN:C	2.47	0.57
1:A:1261:LYS:C	1:A:1263:ILE:H	2.12	0.57
2:B:115:GLN:O	2:B:119:LEU:HD12	2.05	0.57
2:B:235:SER:OG	2:B:236:HIS:HD2	1.88	0.57
5:F:109:VAL:CG1	5:F:110:ASP:N	2.67	0.57
2:B:211:VAL:HG23	2:B:483:LEU:HA	1.87	0.56
1:A:99:ILE:HG12	1:A:234:MET:SD	2.45	0.56
1:A:378:GLU:OE1	1:A:434:ARG:HD3	2.05	0.56
2:B:120:ARG:HE	2:B:955:THR:HG21	1.69	0.56
2:B:1106:ARG:CD	2:B:1126:GLY:O	2.30	0.56
4:E:213:ILE:HG12	4:E:214:CYS:H	1.69	0.56
2:B:322:PHE:CD1	2:B:322:PHE:O	2.58	0.56
2:B:552:MET:HA	2:B:555:ILE:HB	1.86	0.56
2:B:733:HIS:O	2:B:735:ALA:N	2.30	0.56
2:B:801:LYS:O	8:J:52:THR:CG2	2.52	0.56
2:B:983:ARG:NH1	2:B:1091:TYR:HB3	2.19	0.56
2:B:1149:GLU:HG3	2:B:1153:GLU:HB2	1.86	0.56
2:B:1187:ASN:ND2	2:B:1190:ASP:HB2	2.21	0.56
6:H:41:ASP:O	6:H:121:LEU:HD13	2.06	0.56
9:K:63:VAL:HG23	9:K:63:VAL:O	2.04	0.56
1:A:356:ASP:OD2	9:K:65:HIS:HE1	1.88	0.56
2:B:474:SER:C	2:B:476:ARG:N	2.63	0.56
2:B:750:GLY:O	2:B:752:ALA:N	2.39	0.56
2:B:806:THR:H	2:B:809:MET:HG3	1.71	0.56
2:B:815:ARG:HB2	2:B:816:GLU:OE1	2.05	0.56
2:B:980:PHE:O	2:B:981:ALA:CB	2.53	0.56
4:E:29:PHE:HD1	4:E:65:THR:HB	1.69	0.56
1:A:404:TYR:HA	1:A:413:ILE:O	2.06	0.56
2:B:277:LYS:NZ	2:B:335:GLY:HA2	2.20	0.56
9:K:47:ARG:HB3	9:K:47:ARG:HH11	1.71	0.56
1:A:13:THR:HG22	1:A:1432:GLN:NE2	2.20	0.56
1:A:722:LEU:HD13	1:A:799:PHE:CD1	2.41	0.56
1:A:1017:LEU:HB2	4:E:205:SER:HA	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1025:ARG:NH1	1:A:1025:ARG:CG	2.68	0.56
1:A:1319:VAL:CG1	1:A:1320:PRO:HD2	2.35	0.56
2:B:100:PRO:HD3	2:B:126:SER:HG	1.70	0.56
3:C:173:ALA:O	3:C:235:VAL:HG22	2.05	0.56
1:A:451:HIS:HB3	1:A:453:MET:N	2.19	0.56
1:A:678:GLU:HA	1:A:681:GLU:HG2	1.87	0.56
1:A:751:SER:HG	2:B:1015:HIS:CE1	2.20	0.56
1:A:1336:MET:HE2	1:A:1341:ILE:HD13	1.88	0.56
5:F:76:LYS:O	5:F:79:ARG:CD	2.54	0.56
1:A:1364:ASN:ND2	1:A:1364:ASN:C	2.63	0.56
3:C:148:ARG:HG2	3:C:149:LYS:H	1.70	0.56
6:H:82:PRO:O	6:H:83:GLN:CB	2.48	0.56
1:A:694:THR:HA	1:A:714:PHE:CE1	2.40	0.56
2:B:801:LYS:O	8:J:52:THR:HG23	2.05	0.56
8:J:1:MET:H1	8:J:56:LEU:N	2.00	0.56
1:A:451:HIS:CE1	1:A:1074:GLU:HG3	2.41	0.56
2:B:288:ALA:N	2:B:330:ALA:HB1	2.21	0.56
3:C:52:GLU:HB3	3:C:154:LYS:HB3	1.88	0.56
11:R:3:C:N4	12:T:26:DG:H1	1.95	0.56
1:A:253:ASN:HB3	1:A:257:ARG:N	2.21	0.55
1:A:1021:LEU:O	1:A:1022:LEU:C	2.48	0.55
2:B:115:GLN:OE1	2:B:115:GLN:HA	2.06	0.55
4:E:29:PHE:C	4:E:30:ILE:HG13	2.30	0.55
1:A:775:ILE:HG23	1:A:818:MET:HE1	1.88	0.55
2:B:1166:CYS:HB3	2:B:1185:CYS:SG	2.46	0.55
4:E:28:TYR:CZ	4:E:75:MET:HE2	2.41	0.55
1:A:598:LEU:HB3	6:H:25:ARG:HH12	1.72	0.55
1:A:1072:ILE:HD11	1:A:1368:MET:HA	1.88	0.55
2:B:169:ARG:HB2	2:B:454:THR:HG23	1.88	0.55
2:B:881:ASN:HB2	2:B:933:SER:N	2.21	0.55
3:C:46:ILE:HG23	3:C:157:CYS:HB3	1.88	0.55
1:A:483:ASP:OD1	11:R:11:U:OP1	2.25	0.55
1:A:876:ALA:HB3	1:A:877:HIS:CD2	2.40	0.55
1:A:1017:LEU:HB2	4:E:206:GLY:H	1.71	0.55
1:A:1173:HIS:C	1:A:1175:SER:H	2.13	0.55
1:A:1254:ALA:O	1:A:1255:GLU:HB2	2.07	0.55
2:B:294:ASP:HB2	7:I:12:ASN:HA	1.88	0.55
2:B:842:ASN:O	2:B:843:GLN:C	2.47	0.55
2:B:983:ARG:HG3	2:B:1093:GLN:HE21	1.64	0.55
3:C:42:PRO:HA	3:C:163:ILE:HG23	1.87	0.55
3:C:178:PHE:C	3:C:178:PHE:CD2	2.83	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:J:3:VAL:HG21	8:J:18:TRP:HB2	1.89	0.55
9:K:37:LYS:O	9:K:38:GLU:HG2	2.06	0.55
1:A:500:GLU:HG2	2:B:1143:ALA:CB	2.37	0.55
1:A:911:SER:O	1:A:978:PRO:HB3	2.06	0.55
2:B:744:HIS:CD2	2:B:746:SER:OG	2.57	0.55
2:B:753:ALA:HA	2:B:756:ILE:HD12	1.88	0.55
2:B:274:PRO:HB2	2:B:359:GLU:HB3	1.87	0.55
2:B:490:SER:O	2:B:491:THR:C	2.49	0.55
1:A:1239:ARG:C	1:A:1240:CYS:SG	2.89	0.55
1:A:1242:VAL:HG12	1:A:1243:VAL:H	1.72	0.55
2:B:45:SER:O	2:B:46:GLN:C	2.50	0.55
2:B:34:ILE:HD13	2:B:542:MET:CE	2.37	0.55
4:E:77:SER:CB	4:E:105:PHE:HA	2.37	0.55
8:J:44:TYR:CA	8:J:47:ARG:HB2	2.29	0.55
1:A:119:ASN:HB3	1:A:122:MET:HB3	1.88	0.55
1:A:464:PRO:HG2	9:K:67:PHE:CD1	2.42	0.55
1:A:485:ASP:OD1	1:A:485:ASP:N	2.33	0.55
1:A:525:GLN:O	1:A:528:LEU:N	2.38	0.55
1:A:765:VAL:HG23	1:A:766:GLY:H	1.71	0.55
1:A:1436:ILE:O	1:A:1437:GLY:C	2.49	0.55
2:B:644:GLU:HB3	2:B:647:GLY:O	2.06	0.55
3:C:66:ARG:HH21	8:J:4:PRO:HA	1.68	0.55
6:H:109:LYS:N	6:H:109:LYS:HD3	2.20	0.55
2:B:637:LEU:H	2:B:637:LEU:HD12	1.72	0.55
2:B:745:PRO:C	2:B:747:MET:N	2.62	0.55
1:A:104:GLU:O	1:A:171:GLN:OE1	2.26	0.54
1:A:344:ARG:HB3	2:B:1118:PRO:HD2	1.89	0.54
1:A:851:HIS:HD2	1:A:857:ARG:HG3	1.70	0.54
1:A:896:ARG:HH11	1:A:897:TYR:HE1	1.54	0.54
2:B:980:PHE:CE1	2:B:990:ILE:CG1	2.90	0.54
6:H:84:ALA:HA	6:H:87:ARG:HB2	1.88	0.54
1:A:272:ALA:HA	1:A:275:SER:HB3	1.89	0.54
1:A:751:SER:CB	2:B:1015:HIS:HE1	2.19	0.54
1:A:1173:HIS:C	1:A:1175:SER:N	2.65	0.54
2:B:62:ILE:HD12	2:B:418:LYS:CG	2.37	0.54
2:B:101:MET:HE3	2:B:169:ARG:HH22	1.73	0.54
3:C:9:LYS:HG3	3:C:21:ILE:HB	1.89	0.54
4:E:191:LYS:H	4:E:194:GLU:HB2	1.72	0.54
1:A:1384:VAL:HA	1:A:1389:PHE:HD2	1.73	0.54
1:A:120:GLU:OE2	1:A:120:GLU:HA	2.07	0.54
1:A:843:LYS:HD3	1:A:846:GLU:OE2	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:913:LEU:HD23	1:A:915:SER:HB2	1.88	0.54
2:B:835:GLN:HA	2:B:1013:ASN:HD22	1.72	0.54
1:A:253:ASN:HB3	1:A:257:ARG:H	1.73	0.54
1:A:947:PHE:CD2	1:A:954:TRP:CE2	2.96	0.54
2:B:983:ARG:HG3	2:B:1093:GLN:CD	2.32	0.54
9:K:6:ARG:O	9:K:8:GLU:N	2.41	0.54
1:A:471:ASN:O	1:A:472:LEU:C	2.50	0.54
1:A:919:ILE:HG23	1:A:925:LEU:HD12	1.90	0.54
2:B:708:GLU:HG3	2:B:709:ASP:H	1.73	0.54
2:B:917:PRO:HA	2:B:934:LYS:HA	1.90	0.54
3:C:148:ARG:HH12	8:J:64:ASN:HA	1.72	0.54
7:I:109:ILE:CD1	7:I:109:ILE:CB	2.80	0.54
1:A:67:CYS:CB	1:A:70:CYS:SG	2.96	0.54
1:A:98:LYS:O	1:A:102:VAL:CG2	2.54	0.54
1:A:101:LYS:HG2	1:A:139:TRP:HE1	1.72	0.54
1:A:535:THR:O	1:A:575:LYS:HE2	2.08	0.54
1:A:1015:VAL:CG1	1:A:1019:CYS:SG	2.96	0.54
1:A:1220:PHE:CD1	1:A:1224:LEU:HD22	2.42	0.54
1:A:1313:LEU:C	1:A:1315:GLU:H	2.16	0.54
2:B:1128:LEU:HD23	12:T:21:DC:OP1	2.08	0.54
1:A:391:LEU:HB3	1:A:401:GLY:HA2	1.90	0.54
1:A:996:ASN:HA	1:A:998:LEU:HD23	1.88	0.54
2:B:980:PHE:O	2:B:1095:LEU:CD1	2.56	0.54
3:C:22:LEU:HD23	3:C:25:VAL:CG2	2.38	0.54
3:C:123:ASN:ND2	3:C:125:MET:HG2	2.22	0.54
1:A:265:LYS:NZ	1:A:323:LYS:HE2	2.23	0.54
1:A:928:LEU:O	1:A:931:GLU:HB3	2.07	0.54
1:A:1170:ILE:O	1:A:1171:GLN:O	2.26	0.54
2:B:176:SER:O	2:B:182:SER:HB2	2.08	0.54
2:B:1072:MET:HE2	2:B:1085:ILE:HG21	1.90	0.54
3:C:8:VAL:HG11	9:K:105:PHE:HD1	1.73	0.54
7:I:106:CYS:O	7:I:107:SER:C	2.51	0.54
1:A:541:ILE:HG21	1:A:549:MET:HE3	1.89	0.54
1:A:605:MET:HE1	1:A:612:ILE:HD12	1.88	0.54
1:A:1224:LEU:O	1:A:1226:VAL:HG23	2.08	0.54
1:A:1349:TYR:HB2	1:A:1372:VAL:HG21	1.90	0.54
2:B:361:LEU:HD21	2:B:377:PHE:CD2	2.43	0.54
3:C:22:LEU:HD23	3:C:25:VAL:HG21	1.90	0.54
9:K:61:TYR:HA	9:K:72:LYS:O	2.08	0.54
1:A:257:ARG:CG	1:A:257:ARG:NH1	2.62	0.53
1:A:507:VAL:CG1	1:A:521:MET:HE1	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:947:PHE:HE2	1:A:954:TRP:CD2	2.26	0.53
2:B:464:GLY:HA2	2:B:479:VAL:O	2.08	0.53
4:E:61:GLN:HG2	4:E:79:TRP:HE3	1.73	0.53
5:F:81:THR:O	5:F:82:THR:C	2.51	0.53
6:H:109:LYS:CB	6:H:111:LEU:HD22	2.37	0.53
8:J:12:LYS:NZ	8:J:17:LYS:NZ	2.56	0.53
1:A:786:HIS:ND1	2:B:703:ILE:HB	2.23	0.53
2:B:705:MET:HA	2:B:705:MET:HE3	1.90	0.53
2:B:1175:LEU:O	2:B:1176:ASN:HB3	2.09	0.53
1:A:532:ARG:O	1:A:535:THR:N	2.40	0.53
1:A:889:SER:HB2	1:A:892:ALA:N	2.19	0.53
1:A:896:ARG:HB3	1:A:897:TYR:CD1	2.43	0.53
1:A:108:MET:C	1:A:110:CYS:H	2.16	0.53
1:A:249:SER:O	1:A:250:ILE:HG12	2.06	0.53
1:A:871:ASP:HB3	4:E:204:THR:HG22	1.89	0.53
1:A:1173:HIS:O	1:A:1175:SER:N	2.41	0.53
1:A:1191:TRP:HB3	1:A:1260:LEU:HD22	1.90	0.53
1:A:37:PHE:HB2	1:A:52:GLY:HA2	1.91	0.53
1:A:511:ILE:HG12	1:A:521:MET:HE2	1.89	0.53
1:A:786:HIS:CE1	2:B:705:MET:HE1	2.43	0.53
2:B:25:ILE:CD1	2:B:653:VAL:HB	2.38	0.53
2:B:204:ILE:O	2:B:205:ILE:HD13	2.08	0.53
4:E:52:ARG:HB3	4:E:53:PRO:CD	2.38	0.53
8:J:12:LYS:HZ2	8:J:17:LYS:HZ3	1.56	0.53
1:A:1116:LEU:CD2	1:A:1311:VAL:HA	2.39	0.53
1:A:1364:ASN:ND2	1:A:1366:ARG:H	2.06	0.53
2:B:614:SER:H	2:B:632:ARG:HH12	1.57	0.53
2:B:800:GLN:HB3	8:J:52:THR:HG22	1.91	0.53
2:B:1187:ASN:HD21	2:B:1190:ASP:HB2	1.73	0.53
3:C:178:PHE:C	3:C:178:PHE:HD2	2.16	0.53
6:H:127:GLY:HA3	6:H:130:ARG:CZ	2.39	0.53
1:A:940:ARG:CZ	1:A:944:ARG:NH2	2.69	0.53
2:B:653:VAL:HG13	2:B:689:LEU:HD13	1.89	0.53
2:B:702:LEU:HD23	2:B:738:PHE:N	2.22	0.53
1:A:388:LEU:O	1:A:389:THR:C	2.52	0.53
1:A:445:ASN:CB	1:A:455:MET:HG2	2.38	0.53
1:A:1420:ASP:O	1:A:1421:CYS:HB2	2.09	0.53
2:B:736:THR:O	2:B:736:THR:HG22	2.09	0.53
3:C:124:LEU:C	3:C:126:GLY:H	2.16	0.53
4:E:14:ARG:HH12	4:E:142:VAL:HG22	1.74	0.53
6:H:23:VAL:CG2	6:H:121:LEU:HD21	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:L:32:ALA:HB3	10:L:55:ILE:HD12	1.91	0.53
1:A:399:HIS:CB	1:A:400:PRO:HD3	2.39	0.53
1:A:540:PHE:HB3	1:A:571:LEU:HD23	1.91	0.53
4:E:2:ASP:O	4:E:3:GLN:HB3	2.09	0.53
9:K:45:LEU:HG	9:K:94:ILE:HD13	1.90	0.53
1:A:119:ASN:HB3	1:A:122:MET:CB	2.39	0.53
1:A:605:MET:HE3	1:A:614:PHE:O	2.10	0.53
1:A:809:THR:CB	1:A:810:PRO:HD2	2.38	0.53
1:A:863:VAL:HG11	1:A:866:PHE:CE2	2.43	0.53
2:B:314:LEU:O	2:B:315:LYS:C	2.52	0.53
2:B:498:THR:O	2:B:536:VAL:HA	2.09	0.53
2:B:797:TYR:HB3	2:B:798:TYR:CD1	2.44	0.53
7:I:75:CYS:SG	7:I:78:CYS:HB2	2.48	0.53
8:J:43:ARG:HB3	8:J:43:ARG:HH11	1.74	0.53
9:K:53:ASP:OD1	9:K:56:VAL:HG23	2.08	0.53
1:A:754:SER:H	1:A:757:ASN:ND2	2.07	0.52
1:A:1030:ARG:O	1:A:1031:VAL:C	2.52	0.52
1:A:1161:THR:HG22	1:A:1162:VAL:H	1.74	0.52
2:B:44:VAL:O	2:B:45:SER:C	2.52	0.52
2:B:770:GLN:CG	2:B:983:ARG:O	2.57	0.52
2:B:1072:MET:O	2:B:1081:LEU:HB2	2.08	0.52
2:B:1162:ILE:HD13	2:B:1168:LEU:O	2.08	0.52
6:H:63:LEU:C	6:H:90:ALA:HB3	2.34	0.52
1:A:755:PHE:O	1:A:758:ILE:N	2.42	0.52
1:A:868:TYR:CE1	1:A:1064:VAL:CG1	2.63	0.52
1:A:913:LEU:HD11	1:A:981:LEU:O	2.09	0.52
2:B:516:ASN:HD22	2:B:516:ASN:H	1.57	0.52
3:C:16:ASP:O	3:C:233:GLU:HA	2.10	0.52
4:E:69:ILE:O	4:E:69:ILE:HG22	2.09	0.52
1:A:27:VAL:O	1:A:30:ILE:HG22	2.10	0.52
1:A:863:VAL:HG11	1:A:866:PHE:CD2	2.43	0.52
2:B:459:TYR:C	2:B:459:TYR:CD2	2.87	0.52
2:B:1148:LYS:O	2:B:1152:MET:HB2	2.09	0.52
7:I:35:VAL:CG1	7:I:36:GLU:N	2.72	0.52
1:A:130:ASP:C	1:A:132:LYS:H	2.17	0.52
1:A:518:LYS:HB2	1:A:519:PRO:HD2	1.92	0.52
1:A:642:CYS:O	1:A:645:LEU:HB3	2.08	0.52
1:A:982:THR:C	1:A:984:LYS:H	2.17	0.52
2:B:476:ARG:O	2:B:478:GLY:N	2.43	0.52
1:A:856:THR:O	1:A:864:ILE:HG12	2.10	0.52
1:A:901:LEU:HG	1:A:926:GLN:HE21	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1362:TYR:CD1	1:A:1362:TYR:C	2.86	0.52
2:B:263:GLY:O	2:B:264:SER:C	2.52	0.52
2:B:482:VAL:HG11	12:T:25:DC:H5"	1.91	0.52
1:A:332:LYS:O	1:A:334:GLY:N	2.40	0.52
1:A:1109:LYS:HE2	13:N:3:DG:OP2	2.09	0.52
1:A:1424:VAL:HG13	1:A:1436:ILE:CD1	2.39	0.52
2:B:358:LYS:HA	2:B:366:GLN:HG2	1.91	0.52
2:B:981:ALA:O	2:B:1092:TYR:CD2	2.63	0.52
2:B:1084:GLN:NE2	3:C:192:TRP:HB2	2.25	0.52
3:C:49:VAL:CG1	3:C:155:LEU:HD22	2.39	0.52
3:C:167:HIS:CD2	3:C:169:LYS:HG2	2.45	0.52
5:F:90:ARG:O	5:F:91:ALA:C	2.52	0.52
6:H:109:LYS:CB	6:H:110:ASP:CA	2.49	0.52
7:I:55:THR:HG23	7:I:58:VAL:CG2	2.40	0.52
8:J:7:CYS:HA	8:J:49:MET:HG2	1.92	0.52
1:A:320:ARG:HD3	2:B:471:LYS:HG2	1.91	0.52
2:B:208:SER:OG	2:B:210:LYS:HE2	2.10	0.52
2:B:483:LEU:HD22	2:B:484:ASN:H	1.75	0.52
2:B:542:MET:HE3	2:B:747:MET:HE2	1.92	0.52
2:B:825:VAL:HG12	2:B:1090:THR:OG1	2.09	0.52
7:I:35:VAL:CG1	7:I:36:GLU:H	2.19	0.52
8:J:44:TYR:HA	8:J:47:ARG:CB	2.31	0.52
9:K:5:ASP:O	9:K:6:ARG:C	2.52	0.52
2:B:65:GLU:OE1	2:B:65:GLU:N	2.43	0.52
2:B:521:LEU:HD22	2:B:633:VAL:HG12	1.91	0.52
3:C:57:VAL:CG2	8:J:57:ILE:HD11	2.40	0.52
8:J:56:LEU:O	8:J:57:ILE:C	2.53	0.52
1:A:401:GLY:C	1:A:435:HIS:HD2	2.11	0.52
1:A:541:ILE:HD11	1:A:574:GLY:HA2	1.91	0.52
1:A:575:LYS:HG2	1:A:612:ILE:HD11	1.90	0.52
1:A:731:ARG:HG3	1:A:755:PHE:CE1	2.44	0.52
1:A:901:LEU:CG	1:A:926:GLN:HE21	2.23	0.52
2:B:249:ARG:HA	2:B:249:ARG:HE	1.75	0.52
2:B:549:THR:CG2	2:B:550:ASP:H	2.22	0.52
2:B:879:ARG:H	2:B:879:ARG:CZ	2.23	0.52
2:B:915:THR:HB	2:B:934:LYS:HB3	1.92	0.52
2:B:1002:THR:HG22	2:B:1006:ILE:H	1.75	0.52
1:A:19:PHE:HB3	1:A:1413:GLY:HA2	1.91	0.52
1:A:352:VAL:CG1	1:A:353:ILE:N	2.72	0.52
1:A:504:LEU:HD11	5:F:91:ALA:HB1	1.91	0.52
1:A:573:SER:N	1:A:576:GLN:HG3	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:754:SER:H	1:A:757:ASN:HD22	1.58	0.52
1:A:830:LYS:HD3	1:A:1079:MET:O	2.10	0.52
1:A:894:GLU:C	1:A:896:ARG:H	2.17	0.52
1:A:1267:MET:O	1:A:1271:ILE:HB	2.09	0.52
1:A:1420:ASP:O	1:A:1421:CYS:CB	2.57	0.52
2:B:770:GLN:HE22	2:B:1093:GLN:NE2	2.03	0.52
2:B:784:ASN:OD1	2:B:788:ARG:HD2	2.09	0.52
2:B:859:TYR:OH	2:B:941:LEU:HD22	2.09	0.52
4:E:61:GLN:HG2	4:E:79:TRP:CE3	2.45	0.52
11:R:12:G:O2'	11:R:13:C:O5'	2.23	0.52
1:A:268:ASP:O	1:A:299:HIS:ND1	2.43	0.51
2:B:791:THR:HA	2:B:858:SER:HB2	1.91	0.51
2:B:905:VAL:HG12	2:B:909:ASP:HB2	1.92	0.51
3:C:241:ASP:O	3:C:245:VAL:HG23	2.10	0.51
5:F:132:LEU:O	5:F:148:VAL:HG23	2.10	0.51
6:H:58:THR:CG2	6:H:59:ILE:N	2.73	0.51
2:B:53:GLN:HG2	2:B:547:VAL:HG22	1.92	0.51
2:B:384:ARG:O	2:B:385:LEU:C	2.52	0.51
3:C:31:ASN:O	3:C:34:ARG:N	2.42	0.51
10:L:42:ARG:C	10:L:44:ASP:N	2.61	0.51
1:A:120:GLU:OE2	1:A:123:ARG:CD	2.55	0.51
1:A:252:PHE:CD1	1:A:252:PHE:C	2.87	0.51
1:A:474:VAL:O	1:A:478:TYR:HD1	1.94	0.51
1:A:815:PHE:O	1:A:818:MET:N	2.43	0.51
1:A:226:GLU:O	1:A:230:ARG:HD2	2.10	0.51
2:B:373:ARG:HD3	2:B:566:LEU:HD22	1.92	0.51
2:B:515:HIS:HD2	2:B:517:THR:OG1	1.92	0.51
1:A:765:VAL:HG21	1:A:800:VAL:CG1	2.41	0.51
1:A:1166:ASP:OD1	1:A:1237:ILE:HD13	2.10	0.51
2:B:329:THR:HA	2:B:332:ASP:CB	2.35	0.51
3:C:193:TYR:HA	3:C:200:GLU:OE1	2.11	0.51
1:A:755:PHE:O	1:A:757:ASN:N	2.44	0.51
1:A:903:ASN:ND2	1:A:906:HIS:HB2	2.26	0.51
1:A:1116:LEU:CD1	1:A:1329:THR:OG1	2.36	0.51
2:B:92:PHE:HD2	2:B:132:VAL:HG22	1.76	0.51
10:L:34:CYS:O	10:L:35:SER:HB2	2.11	0.51
1:A:568:PRO:HD3	6:H:94:ASP:O	2.09	0.51
1:A:765:VAL:HG21	1:A:800:VAL:HG11	1.92	0.51
1:A:893:PHE:C	1:A:893:PHE:CD2	2.89	0.51
1:A:919:ILE:HD12	1:A:925:LEU:CD1	2.41	0.51
2:B:299:GLU:OE2	2:B:571:PRO:HG2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:525:ALA:O	2:B:527:THR:HG22	2.09	0.51
1:A:343:LYS:HZ1	2:B:1197:PRO:HB3	1.74	0.51
2:B:114:PRO:HG3	2:B:181:LEU:HD21	1.93	0.51
2:B:589:VAL:CG1	2:B:590:HIS:N	2.74	0.51
2:B:893:LEU:HD11	2:B:910:VAL:HG12	1.92	0.51
1:A:587:HIS:HE2	1:A:969:GLN:HG2	1.76	0.51
1:A:653:VAL:O	1:A:654:ASN:C	2.53	0.51
2:B:1137:CYS:HA	2:B:1140:ALA:HB3	1.93	0.51
4:E:94:LYS:HE3	4:E:123:LEU:HD11	1.92	0.51
8:J:1:MET:H2	8:J:56:LEU:N	2.05	0.51
1:A:343:LYS:NZ	2:B:1156:ASP:HB2	2.25	0.51
1:A:1189:SER:O	1:A:1241:ARG:HD3	2.11	0.51
2:B:1154:ALA:O	2:B:1155:SER:HB3	2.09	0.51
6:H:109:LYS:HB2	6:H:111:LEU:N	2.26	0.51
1:A:567:LYS:HZ1	6:H:97:MET:CG	2.24	0.50
1:A:860:LEU:HD21	1:A:1394:THR:H	1.75	0.50
1:A:1192:LEU:HD11	1:A:1239:ARG:HB3	1.93	0.50
2:B:840:ILE:HG23	2:B:992:ILE:HG22	1.93	0.50
2:B:1023:VAL:O	2:B:1026:LEU:HB2	2.12	0.50
2:B:1056:SER:HB3	2:B:1066:SER:HB2	1.93	0.50
1:A:243:PRO:HB2	1:A:245:PRO:HD2	1.93	0.50
2:B:212:LEU:HD12	2:B:409:ALA:HB1	1.92	0.50
2:B:286:PHE:HB3	2:B:297:ILE:HD12	1.93	0.50
2:B:770:GLN:NE2	2:B:1093:GLN:NE2	2.53	0.50
2:B:879:ARG:H	2:B:879:ARG:NE	2.09	0.50
2:B:1032:SER:HB3	2:B:1089:PRO:CG	2.35	0.50
2:B:198:ASP:OD1	2:B:485:ARG:NH2	2.44	0.50
11:R:13:C:O4'	11:R:13:C:OP2	2.30	0.50
1:A:296:LEU:O	1:A:300:VAL:HG23	2.11	0.50
1:A:567:LYS:HG3	1:A:568:PRO:HD2	1.93	0.50
1:A:650:GLN:HB3	1:A:654:ASN:HD21	1.77	0.50
2:B:168:GLY:HA2	2:B:454:THR:OG1	2.12	0.50
2:B:215:GLN:OE1	2:B:479:VAL:HG13	2.11	0.50
3:C:46:ILE:HD12	3:C:157:CYS:HB3	1.93	0.50
4:E:213:ILE:HG12	4:E:214:CYS:N	2.25	0.50
1:A:532:ARG:HG3	1:A:616:VAL:HG11	1.94	0.50
2:B:999:MET:HA	2:B:999:MET:HE3	1.93	0.50
2:B:1071:VAL:HG11	2:B:1080:LYS:HE2	1.94	0.50
3:C:35:ARG:NH1	9:K:41:THR:H	2.09	0.50
7:I:58:VAL:O	7:I:58:VAL:HG12	2.11	0.50
1:A:982:THR:C	1:A:984:LYS:N	2.67	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:212:LEU:HD21	2:B:461:LEU:CD1	2.41	0.50
2:B:604:ARG:HA	2:B:609:ILE:O	2.11	0.50
3:C:241:ASP:HB3	9:K:109:TRP:CZ2	2.46	0.50
1:A:265:LYS:O	1:A:267:ALA:N	2.44	0.50
1:A:332:LYS:C	1:A:334:GLY:N	2.67	0.50
1:A:383:TYR:HB3	5:F:115:THR:HB	1.94	0.50
1:A:537:ARG:HG3	1:A:602:ASP:OD2	2.11	0.50
1:A:629:LEU:O	1:A:633:VAL:HG23	2.12	0.50
1:A:1063:MET:SD	1:A:1436:ILE:HG23	2.52	0.50
1:A:1299:VAL:HG12	1:A:1300:LYS:H	1.77	0.50
2:B:205:ILE:C	2:B:207:GLY:H	2.20	0.50
2:B:1106:ARG:HG3	2:B:1107:ALA:N	2.27	0.50
1:A:1140:HIS:HB3	1:A:1279:ILE:O	2.12	0.50
1:A:1393:ASN:O	1:A:1394:THR:O	2.30	0.50
1:A:1410:PHE:CD2	2:B:1212:ILE:HD11	2.45	0.50
2:B:128:LEU:HB2	2:B:167:ILE:O	2.11	0.50
1:A:514:PRO:O	1:A:515:GLN:C	2.55	0.50
1:A:596:THR:O	1:A:598:LEU:N	2.45	0.50
2:B:65:GLU:CD	2:B:66:ASP:H	2.20	0.50
2:B:942:ARG:HB2	2:B:945:GLU:HB2	1.94	0.50
2:B:954:VAL:O	10:L:55:ILE:O	2.29	0.50
2:B:1107:ALA:O	2:B:1108:ARG:HB3	2.11	0.50
4:E:144:ILE:HG13	4:E:145:THR:N	2.27	0.50
10:L:41:SER:C	10:L:42:ARG:O	2.55	0.50
1:A:402:ALA:CB	1:A:434:ARG:HA	2.42	0.49
1:A:860:LEU:HD13	1:A:1393:ASN:ND2	2.10	0.49
2:B:1124:ARG:O	2:B:1125:ASP:C	2.53	0.49
2:B:315:LYS:N	2:B:316:PRO:HD2	2.27	0.49
2:B:884:ARG:O	2:B:936:ASP:HB3	2.11	0.49
2:B:1004:GLU:O	3:C:177:GLU:HG2	2.13	0.49
2:B:1084:GLN:H	2:B:1084:GLN:CD	2.20	0.49
3:C:167:HIS:CD2	3:C:169:LYS:H	2.20	0.49
1:A:313:GLN:HB3	1:A:322:VAL:CG1	2.41	0.49
1:A:1006:ILE:HD11	4:E:163:GLU:HG3	1.93	0.49
1:A:1174:PHE:O	1:A:1175:SER:O	2.30	0.49
2:B:34:ILE:HD11	2:B:743:ILE:HG22	1.94	0.49
2:B:235:SER:CB	2:B:236:HIS:HD2	2.25	0.49
3:C:22:LEU:HD21	3:C:25:VAL:HG21	1.93	0.49
3:C:62:PHE:O	3:C:65:HIS:HB3	2.12	0.49
1:A:407:ARG:HD3	1:A:413:ILE:CD1	2.43	0.49
1:A:836:TYR:CZ	1:A:840:ARG:HD2	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1237:ILE:HG22	1:A:1238:ILE:N	2.27	0.49
2:B:636:PRO:HB3	2:B:637:LEU:HA	1.91	0.49
2:B:1077:THR:HG23	2:B:1079:LYS:N	2.27	0.49
4:E:46:TYR:CE2	4:E:58:MET:HA	2.47	0.49
6:H:109:LYS:CD	6:H:110:ASP:HB2	2.42	0.49
9:K:10:PHE:CD1	9:K:11:LEU:HD13	2.47	0.49
1:A:757:ASN:O	1:A:761:MET:HG3	2.12	0.49
1:A:1222:ASN:O	1:A:1223:ASP:OD1	2.30	0.49
1:A:1261:LYS:C	1:A:1263:ILE:N	2.70	0.49
1:A:1424:VAL:HG11	2:B:1139:ILE:HD13	1.95	0.49
2:B:210:LYS:HZ3	2:B:482:VAL:HG13	1.75	0.49
3:C:181:ASP:CG	3:C:186:LEU:HD13	2.38	0.49
4:E:48:ASP:OD2	4:E:49:SER:N	2.45	0.49
5:F:80:ALA:O	5:F:81:THR:C	2.55	0.49
6:H:89:LEU:C	6:H:91:ASP:H	2.18	0.49
7:I:7:CYS:HB2	7:I:14:LEU:HD21	1.94	0.49
1:A:108:MET:O	1:A:110:CYS:N	2.41	0.49
1:A:1152:ILE:HD12	7:I:44:TYR:CD2	2.47	0.49
1:A:1191:TRP:CE3	1:A:1191:TRP:HA	2.46	0.49
1:A:1392:SER:O	1:A:1393:ASN:O	2.30	0.49
2:B:701:ILE:HG12	2:B:702:LEU:N	2.26	0.49
2:B:890:TYR:CD2	2:B:910:VAL:HG11	2.48	0.49
5:F:97:ARG:HD2	5:F:101:ILE:HG13	1.93	0.49
6:H:98:TYR:CE1	6:H:139:ASN:OD1	2.65	0.49
10:L:68:GLU:OE1	10:L:68:GLU:O	2.30	0.49
1:A:66:LYS:C	1:A:68:GLN:H	2.20	0.49
1:A:738:LYS:NZ	3:C:194:GLU:HA	2.28	0.49
1:A:1242:VAL:HG12	1:A:1243:VAL:N	2.28	0.49
2:B:57:TYR:CD1	2:B:57:TYR:N	2.81	0.49
2:B:783:THR:CG2	8:J:59:LYS:HB3	2.41	0.49
2:B:1002:THR:HG23	2:B:1004:GLU:H	1.77	0.49
3:C:186:LEU:HB3	3:C:188:HIS:HD2	1.77	0.49
1:A:265:LYS:HZ1	1:A:323:LYS:HE2	1.77	0.49
1:A:1364:ASN:HD22	1:A:1366:ARG:CG	2.10	0.49
2:B:25:ILE:HG23	2:B:29:ASP:HB2	1.94	0.49
2:B:666:TYR:CD1	2:B:666:TYR:O	2.66	0.49
2:B:953:LEU:HB3	2:B:965:LYS:HB2	1.94	0.49
3:C:57:VAL:HG23	8:J:57:ILE:HD11	1.95	0.49
4:E:61:GLN:CG	4:E:79:TRP:HE3	2.25	0.49
8:J:3:VAL:CG2	8:J:18:TRP:CG	2.90	0.49
8:J:12:LYS:NZ	8:J:17:LYS:HZ3	2.09	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:930:ASP:O	1:A:931:GLU:C	2.56	0.49
1:A:979:SER:OG	1:A:980:ASP:N	2.44	0.49
1:A:1132:LYS:O	1:A:1135:ARG:HB3	2.13	0.49
1:A:1400:CYS:SG	1:A:1409:LEU:HG	2.53	0.49
1:A:1402:PHE:CD2	1:A:1403:GLU:HB2	2.48	0.49
2:B:789:MET:HE3	2:B:965:LYS:HB3	1.94	0.49
4:E:94:LYS:HE3	4:E:123:LEU:CD1	2.43	0.49
1:A:483:ASP:OD1	11:R:11:U:P	2.71	0.49
2:B:644:GLU:CB	2:B:647:GLY:O	2.60	0.49
2:B:848:ARG:HH22	2:B:996:ARG:NH1	2.11	0.49
2:B:1152:MET:O	2:B:1153:GLU:C	2.55	0.49
4:E:77:SER:HB3	4:E:105:PHE:HA	1.94	0.49
6:H:101:ALA:HB2	6:H:116:TYR:CE2	2.48	0.49
12:T:13:DA:C2	12:T:14:DG:N3	2.81	0.49
1:A:106:VAL:HG12	1:A:107:CYS:N	2.28	0.48
1:A:380:VAL:HG23	1:A:430:TRP:C	2.38	0.48
1:A:650:GLN:O	1:A:651:LYS:C	2.56	0.48
1:A:777:PHE:HD2	1:A:782:ARG:C	2.20	0.48
1:A:782:ARG:NH1	1:A:785:PRO:HA	2.28	0.48
1:A:840:ARG:CG	1:A:1402:PHE:HZ	2.26	0.48
1:A:1006:ILE:HD11	4:E:163:GLU:CG	2.42	0.48
1:A:1167:GLU:O	1:A:1167:GLU:HG2	2.12	0.48
1:A:1227:ILE:CG2	1:A:1228:TRP:N	2.76	0.48
2:B:48:LEU:O	2:B:49:ASP:C	2.56	0.48
2:B:844:SER:OG	2:B:996:ARG:N	2.39	0.48
2:B:1082:MET:HA	3:C:189:THR:HA	1.94	0.48
5:F:136:ARG:HD2	5:F:146:TRP:CD1	2.48	0.48
1:A:20:GLY:O	1:A:21:LEU:HD23	2.13	0.48
1:A:101:LYS:HD3	1:A:139:TRP:CE2	2.48	0.48
1:A:591:PHE:HA	1:A:595:THR:HG21	1.94	0.48
1:A:599:SER:C	1:A:601:LYS:H	2.21	0.48
1:A:693:VAL:HG21	1:A:721:PHE:HE1	1.79	0.48
1:A:815:PHE:O	1:A:818:MET:HB2	2.12	0.48
1:A:962:ARG:HA	1:A:965:GLN:HE21	1.77	0.48
1:A:1406:VAL:HG13	1:A:1410:PHE:CE1	2.49	0.48
2:B:197:PHE:HE1	8:J:59:LYS:HD3	1.78	0.48
2:B:976:ILE:HG23	2:B:977:GLY:H	1.78	0.48
3:C:251:LEU:O	3:C:255:VAL:HG23	2.13	0.48
4:E:35:VAL:C	4:E:37:LEU:H	2.21	0.48
12:T:13:DA:H61	13:N:2:DT:H73	1.76	0.48
1:A:335:ARG:HH11	2:B:1202:LEU:HD12	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:913:LEU:CD2	1:A:915:SER:HB2	2.43	0.48
1:A:1053:PHE:O	1:A:1055:ARG:N	2.47	0.48
2:B:120:ARG:HH21	2:B:956:THR:HG23	1.77	0.48
2:B:234:ILE:HG21	2:B:237:VAL:HG22	1.93	0.48
2:B:310:MET:O	2:B:313:MET:HB2	2.13	0.48
2:B:316:PRO:HA	2:B:319:GLU:HG3	1.95	0.48
2:B:661:LEU:HD23	2:B:679:TYR:O	2.13	0.48
2:B:772:ALA:O	2:B:776:GLN:NE2	2.46	0.48
9:K:49:GLU:HG3	9:K:94:ILE:HD11	1.94	0.48
1:A:380:VAL:HG11	1:A:428:TYR:H	1.78	0.48
1:A:491:VAL:H	2:B:1150:ARG:NH2	2.11	0.48
1:A:545:GLN:O	1:A:546:VAL:C	2.56	0.48
1:A:765:VAL:HG23	1:A:766:GLY:N	2.27	0.48
1:A:1348:LEU:O	1:A:1352:VAL:HG23	2.13	0.48
4:E:48:ASP:HB3	4:E:54:GLN:HB2	1.94	0.48
1:A:388:LEU:O	1:A:391:LEU:N	2.46	0.48
1:A:544:ASP:HB2	9:K:47:ARG:HH21	1.77	0.48
1:A:569:LYS:HE3	3:C:221:TYR:O	2.14	0.48
1:A:1146:VAL:HG12	1:A:1201:ALA:HB1	1.94	0.48
1:A:1311:VAL:HG11	1:A:1329:THR:HG21	1.94	0.48
2:B:800:GLN:HB3	8:J:52:THR:HG21	1.95	0.48
2:B:898:LEU:HD13	2:B:952:VAL:HG11	1.94	0.48
4:E:16:PHE:O	4:E:19:VAL:N	2.42	0.48
1:A:56:PRO:O	1:A:57:ARG:HB2	2.13	0.48
1:A:313:GLN:HB3	1:A:322:VAL:HG11	1.96	0.48
1:A:319:GLY:CA	1:A:320:ARG:HH11	2.27	0.48
1:A:860:LEU:HD11	1:A:1393:ASN:HB2	1.94	0.48
2:B:814:PHE:C	2:B:816:GLU:N	2.72	0.48
2:B:980:PHE:O	2:B:1095:LEU:HG	2.13	0.48
4:E:201:LYS:HE2	4:E:207:ARG:HD3	1.96	0.48
10:L:34:CYS:O	10:L:35:SER:CB	2.62	0.48
2:B:118:ARG:NH2	2:B:194:GLU:OE1	2.46	0.48
2:B:266:ALA:O	2:B:268:THR:HG22	2.13	0.48
2:B:515:HIS:HD2	2:B:517:THR:H	1.62	0.48
1:A:91:PHE:HB3	1:A:96:ILE:HD11	1.96	0.48
1:A:535:THR:O	1:A:536:LEU:C	2.57	0.48
1:A:568:PRO:HB3	3:C:221:TYR:CZ	2.49	0.48
1:A:760:GLN:HE21	1:A:765:VAL:HA	1.78	0.48
2:B:593:PRO:HA	2:B:596:LEU:HB3	1.94	0.48
2:B:1084:GLN:HE21	3:C:192:TRP:HB2	1.79	0.48
3:C:43:THR:HG23	3:C:44:LEU:N	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:I:8:ARG:O	7:I:9:ASP:HB2	2.13	0.48
8:J:48:ARG:NH2	8:J:49:MET:CE	2.68	0.48
9:K:94:ILE:O	9:K:95:ILE:C	2.54	0.48
1:A:115:LEU:HD13	1:A:119:ASN:ND2	2.28	0.48
1:A:351:THR:HG21	2:B:1103:ILE:HD12	1.82	0.48
1:A:452:LYS:HB2	2:B:1141:HIS:HE1	1.74	0.48
1:A:473:SER:O	1:A:521:MET:HB3	2.14	0.48
1:A:575:LYS:HB3	1:A:612:ILE:CG1	2.43	0.48
1:A:1097:GLY:C	1:A:1099:PRO:HD2	2.39	0.48
1:A:1101:LEU:HD13	1:A:1355:VAL:HG11	1.96	0.48
1:A:1397:LEU:O	1:A:1400:CYS:HB2	2.14	0.48
2:B:635:ARG:HH12	2:B:742:GLU:CD	2.22	0.48
2:B:640:VAL:O	2:B:640:VAL:HG12	2.13	0.48
2:B:827:ILE:CD1	2:B:1086:PHE:HD2	2.27	0.48
6:H:120:GLY:O	6:H:122:LEU:HG	2.14	0.48
9:K:18:LYS:O	9:K:19:LEU:HD23	2.14	0.48
1:A:919:ILE:HD12	1:A:925:LEU:HD11	1.94	0.48
1:A:996:ASN:C	1:A:998:LEU:N	2.72	0.48
1:A:1337:GLU:O	4:E:183:PRO:HG3	2.14	0.48
1:A:1377:THR:C	1:A:1379:GLY:H	2.22	0.48
12:T:26:DG:N2	12:T:27:DA:H1'	2.29	0.48
1:A:249:SER:O	1:A:250:ILE:CG1	2.62	0.47
1:A:609:ASP:CG	1:A:610:GLY:H	2.22	0.47
1:A:1376:THR:HG23	1:A:1376:THR:O	2.14	0.47
2:B:121:ASN:HA	2:B:207:GLY:HA3	1.96	0.47
2:B:589:VAL:CG1	2:B:590:HIS:H	2.25	0.47
2:B:857:ARG:O	2:B:967:ARG:HG3	2.14	0.47
2:B:870:ILE:C	2:B:871:THR:OG1	2.56	0.47
2:B:995:ARG:HB3	2:B:997:GLU:OE2	2.14	0.47
3:C:241:ASP:HB3	9:K:109:TRP:CE2	2.49	0.47
7:I:17:ARG:HG2	7:I:18:GLU:H	1.78	0.47
1:A:384:ASN:O	1:A:385:ILE:C	2.57	0.47
2:B:55:VAL:HG12	2:B:56:ASP:N	2.29	0.47
2:B:256:VAL:HG11	2:B:382:ILE:HD13	1.95	0.47
2:B:773:MET:HE1	2:B:985:GLY:HA2	1.94	0.47
3:C:29:MET:O	3:C:32:SER:N	2.47	0.47
4:E:29:PHE:C	4:E:30:ILE:CG1	2.87	0.47
1:A:440:ASP:H	1:A:460:VAL:HG23	1.79	0.47
2:B:29:ASP:HB3	2:B:658:ILE:HG12	1.96	0.47
2:B:1153:GLU:OE2	2:B:1153:GLU:N	2.47	0.47
4:E:15:ALA:HA	4:E:140:LEU:O	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:199:ILE:O	4:E:199:ILE:HG22	2.14	0.47
12:T:5:DC:H2''	12:T:6:DG:O5'	2.14	0.47
1:A:15:LYS:HD2	2:B:1220:ARG:NH1	2.29	0.47
1:A:438:ASP:HA	1:A:460:VAL:O	2.13	0.47
2:B:254:LEU:HD22	2:B:361:LEU:HD11	1.96	0.47
2:B:395:GLN:HG2	2:B:396:ASP:H	1.78	0.47
4:E:205:SER:O	4:E:207:ARG:N	2.47	0.47
5:F:93:ILE:HG23	5:F:132:LEU:HD12	1.95	0.47
1:A:253:ASN:ND2	1:A:257:ARG:N	2.63	0.47
1:A:378:GLU:HG2	1:A:388:LEU:HD11	1.95	0.47
1:A:767:GLN:NE2	1:A:774:ARG:HE	2.12	0.47
1:A:855:THR:HG23	1:A:857:ARG:HG2	1.97	0.47
1:A:1369:ALA:O	1:A:1370:LEU:C	2.54	0.47
2:B:254:LEU:CD2	2:B:381:MET:HE1	2.44	0.47
2:B:681:TRP:O	2:B:684:LEU:HB2	2.14	0.47
2:B:875:GLU:O	2:B:877:PRO:HD3	2.14	0.47
8:J:16:ASP:OD1	8:J:17:LYS:HG3	2.14	0.47
1:A:848:ILE:HD13	1:A:858:ASN:HB3	1.97	0.47
2:B:573:GLN:O	2:B:575:PRO:HD3	2.13	0.47
2:B:757:PRO:HG3	2:B:983:ARG:CZ	2.36	0.47
2:B:972:LYS:HD3	2:B:1098:MET:SD	2.54	0.47
3:C:43:THR:CG2	3:C:44:LEU:N	2.77	0.47
3:C:54:ASN:O	3:C:54:ASN:CG	2.57	0.47
9:K:60:ALA:O	9:K:73:LEU:HA	2.14	0.47
11:R:5:A:C2	11:R:6:G:C5	3.03	0.47
1:A:256:GLN:CB	1:A:257:ARG:CG	2.90	0.47
1:A:464:PRO:CG	9:K:67:PHE:CD1	2.98	0.47
1:A:557:ASP:HA	9:K:26:LYS:HE3	1.96	0.47
1:A:949:ASP:OD1	1:A:949:ASP:N	2.38	0.47
1:A:1325:THR:HG22	1:A:1326:ARG:HG3	1.97	0.47
1:A:1370:LEU:O	1:A:1374:VAL:HG23	2.15	0.47
2:B:386:LEU:C	2:B:388:CYS:H	2.23	0.47
2:B:479:VAL:O	2:B:480:SER:HB3	2.15	0.47
2:B:765:PRO:O	2:B:769:TYR:CD1	2.68	0.47
2:B:1013:ASN:C	2:B:1015:HIS:H	2.21	0.47
2:B:1175:LEU:O	2:B:1176:ASN:CB	2.63	0.47
3:C:142:VAL:HG13	3:C:143:LEU:H	1.78	0.47
3:C:186:LEU:CB	3:C:188:HIS:HD2	2.28	0.47
8:J:25:LEU:HD21	8:J:32:GLU:HG3	1.96	0.47
1:A:182:VAL:HG12	1:A:183:GLY:N	2.23	0.47
1:A:375:THR:OG1	1:A:433:GLU:HB3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:382:PRO:N	1:A:428:TYR:HE2	2.12	0.47
1:A:463:ILE:CB	1:A:464:PRO:HD2	2.44	0.47
1:A:567:LYS:C	1:A:569:LYS:H	2.22	0.47
1:A:567:LYS:HD3	6:H:95:TYR:CD1	2.50	0.47
1:A:608:ILE:HG12	1:A:613:ILE:HG13	1.97	0.47
1:A:853:ASP:OD1	1:A:855:THR:CG2	2.58	0.47
2:B:701:ILE:HD11	2:B:703:ILE:CD1	2.43	0.47
3:C:69:LEU:H	3:C:69:LEU:CD2	2.27	0.47
4:E:127:ILE:HD13	4:E:127:ILE:H	1.80	0.47
4:E:180:ARG:HB2	4:E:215:MET:OXT	2.15	0.47
6:H:15:VAL:HA	6:H:26:ILE:HD12	1.96	0.47
12:T:8:DT:H3	13:N:7:DA:H61	1.63	0.47
1:A:49:LYS:HZ2	1:A:60:SER:HA	1.80	0.47
1:A:321:PRO:O	1:A:322:VAL:HG22	2.14	0.47
1:A:1004:ASN:OD1	1:A:1006:ILE:HG12	2.15	0.47
1:A:1173:HIS:CD2	1:A:1227:ILE:HG12	2.49	0.47
2:B:299:GLU:CD	2:B:571:PRO:HG2	2.39	0.47
2:B:519:TRP:C	2:B:519:TRP:CD1	2.93	0.47
2:B:766:ARG:HD3	2:B:766:ARG:HA	1.62	0.47
3:C:56:THR:CG2	3:C:145:CYS:SG	3.00	0.47
3:C:124:LEU:O	3:C:126:GLY:N	2.48	0.47
6:H:145:ARG:HG3	6:H:146:ARG:HG3	1.96	0.47
1:A:35:ILE:HG13	1:A:241:VAL:HG21	1.96	0.47
1:A:239:LEU:HD12	1:A:240:PRO:CD	2.37	0.47
1:A:1165:GLU:O	1:A:1166:ASP:OD1	2.33	0.47
1:A:1395:GLY:O	1:A:1398:MET:HB3	2.15	0.47
2:B:241:ARG:HA	2:B:253:THR:HG22	1.96	0.47
2:B:1006:ILE:HD11	8:J:43:ARG:HB2	1.97	0.47
2:B:1106:ARG:NH1	2:B:1110:PRO:HD2	2.29	0.47
1:A:434:ARG:NH2	1:A:440:ASP:OD2	2.48	0.46
1:A:475:THR:HG22	1:A:476:SER:N	2.29	0.46
1:A:849:MET:HG3	1:A:849:MET:O	2.13	0.46
1:A:919:ILE:O	1:A:920:LEU:C	2.58	0.46
1:A:998:LEU:HG	1:A:1001:ARG:NH1	2.30	0.46
1:A:1236:LEU:C	1:A:1237:ILE:HG13	2.40	0.46
2:B:981:ALA:CB	2:B:987:LYS:CA	2.72	0.46
2:B:1155:SER:O	2:B:1156:ASP:OD2	2.33	0.46
3:C:7:GLN:HB2	3:C:23:SER:HB2	1.97	0.46
3:C:133:ILE:HD13	3:C:236:GLY:O	2.15	0.46
1:A:571:LEU:C	1:A:572:TRP:CE3	2.93	0.46
1:A:694:THR:HA	1:A:714:PHE:HE1	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:947:PHE:HD2	1:A:954:TRP:CE2	2.31	0.46
1:A:1406:VAL:HG12	1:A:1407:GLU:N	2.30	0.46
3:C:69:LEU:H	3:C:69:LEU:HD22	1.80	0.46
7:I:109:ILE:H	7:I:109:ILE:HD12	1.79	0.46
1:A:317:LYS:HD2	1:A:317:LYS:HA	1.43	0.46
1:A:341:MET:CE	1:A:1401:SER:HB2	2.34	0.46
1:A:465:TYR:HD2	2:B:976:ILE:HB	1.81	0.46
2:B:278:GLN:HG2	2:B:279:ASP:H	1.79	0.46
3:C:50:GLU:HB2	3:C:156:THR:HB	1.97	0.46
3:C:63:ILE:HA	3:C:66:ARG:HG3	1.97	0.46
3:C:206:ASN:ND2	3:C:229:TYR:CB	2.79	0.46
10:L:59:ALA:O	10:L:60:ARG:HB2	2.14	0.46
1:A:845:LEU:HD12	1:A:1069:ALA:HB2	1.98	0.46
1:A:1373:ASP:HA	1:A:1376:THR:HG22	1.96	0.46
2:B:523:CYS:SG	2:B:750:GLY:N	2.88	0.46
2:B:655:LYS:O	2:B:658:ILE:HG22	2.16	0.46
2:B:999:MET:CG	2:B:1008:PRO:HD2	2.43	0.46
3:C:10:ILE:HG21	3:C:13:ALA:HB2	1.96	0.46
3:C:142:VAL:H	8:J:16:ASP:HB3	1.81	0.46
8:J:24:LEU:O	8:J:30:LEU:HB2	2.16	0.46
1:A:387:ARG:HD2	1:A:437:MET:HE1	1.98	0.46
1:A:1161:THR:HG22	1:A:1162:VAL:N	2.30	0.46
2:B:174:LEU:HD12	2:B:174:LEU:HA	1.59	0.46
1:A:66:LYS:C	1:A:68:GLN:N	2.74	0.46
1:A:266:LEU:HD23	1:A:303:TYR:CE1	2.50	0.46
1:A:399:HIS:O	1:A:400:PRO:C	2.56	0.46
1:A:666:ILE:CD1	2:B:1030:LEU:HD13	2.39	0.46
1:A:711:ARG:NH2	7:I:91:ARG:HH12	2.14	0.46
1:A:765:VAL:CG2	1:A:800:VAL:CG1	2.94	0.46
1:A:840:ARG:NE	1:A:1385:THR:HG23	2.22	0.46
1:A:989:GLY:O	1:A:990:VAL:C	2.59	0.46
1:A:1396:ALA:O	1:A:1397:LEU:C	2.58	0.46
2:B:411:PRO:HA	2:B:414:ALA:HB3	1.96	0.46
2:B:1094:ARG:HH22	2:B:1098:MET:CG	2.28	0.46
2:B:1121:GLY:O	2:B:1126:GLY:HA3	2.16	0.46
3:C:134:ILE:HG22	3:C:136:ASP:HB3	1.98	0.46
6:H:40:LEU:HD13	6:H:123:MET:HB2	1.98	0.46
1:A:185:TRP:HZ3	1:A:200:ARG:HB3	1.80	0.46
1:A:315:LEU:HB2	1:A:316:GLN:HA	1.79	0.46
1:A:401:GLY:CA	1:A:435:HIS:HD2	2.29	0.46
1:A:508:PRO:C	1:A:510:GLN:H	2.23	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:821:ARG:O	1:A:825:ILE:HG12	2.16	0.46
1:A:893:PHE:O	1:A:896:ARG:HB2	2.16	0.46
2:B:697:GLU:O	2:B:698:GLU:C	2.59	0.46
2:B:882:THR:HG22	2:B:884:ARG:H	1.80	0.46
2:B:952:VAL:HG13	2:B:966:VAL:HG22	1.98	0.46
1:A:92:HIS:C	1:A:92:HIS:CD2	2.94	0.46
1:A:374:LEU:C	1:A:436:ILE:HD13	2.41	0.46
1:A:658:LEU:HD13	2:B:831:SER:N	2.30	0.46
1:A:1220:PHE:CD1	1:A:1224:LEU:HD23	2.51	0.46
2:B:248:SER:HB3	2:B:249:ARG:H	1.49	0.46
2:B:377:PHE:O	2:B:380:TYR:N	2.48	0.46
2:B:1007:VAL:HG13	2:B:1008:PRO:N	2.30	0.46
2:B:1084:GLN:HE21	3:C:192:TRP:CB	2.29	0.46
3:C:64:ALA:HA	3:C:67:LEU:HD12	1.98	0.46
4:E:147:HIS:HB3	4:E:150:VAL:HG23	1.98	0.46
6:H:104:PHE:HD2	6:H:114:VAL:CG1	2.22	0.46
7:I:15:TYR:N	7:I:15:TYR:CD1	2.83	0.46
9:K:4:PRO:O	9:K:5:ASP:C	2.59	0.46
10:L:30:ILE:HG22	10:L:31:CYS:O	2.16	0.46
1:A:359:LEU:HD23	1:A:359:LEU:HA	1.81	0.46
1:A:481:ASP:OD1	1:A:483:ASP:OD2	2.34	0.46
1:A:809:THR:OG1	1:A:812:GLU:HG3	2.16	0.46
1:A:837:ILE:HD13	1:A:840:ARG:HH12	1.81	0.46
2:B:228:LYS:HE2	2:B:228:LYS:HB3	1.79	0.46
3:C:66:ARG:HH22	8:J:4:PRO:CA	2.27	0.46
3:C:67:LEU:HD11	3:C:155:LEU:HD13	1.98	0.46
4:E:165:LEU:HD22	4:E:165:LEU:HA	1.82	0.46
9:K:56:VAL:HG13	9:K:77:THR:HG22	1.98	0.46
1:A:391:LEU:HD22	1:A:400:PRO:C	2.41	0.46
1:A:848:ILE:O	1:A:1065:GLY:N	2.46	0.46
1:A:901:LEU:O	1:A:907:THR:OG1	2.34	0.46
1:A:1313:LEU:C	1:A:1315:GLU:N	2.74	0.46
2:B:550:ASP:OD1	2:B:551:PRO:CD	2.64	0.46
2:B:834:ASN:CG	2:B:1013:ASN:HB2	2.41	0.46
8:J:21:TYR:CZ	8:J:25:LEU:HD11	2.50	0.46
8:J:30:LEU:HD11	8:J:38:ARG:HH12	1.81	0.46
9:K:105:PHE:O	9:K:106:GLU:C	2.59	0.46
1:A:15:LYS:O	1:A:1420:ASP:O	2.32	0.45
1:A:19:PHE:O	1:A:1416:ALA:HA	2.16	0.45
1:A:971:PHE:O	1:A:972:HIS:O	2.34	0.45
1:A:1104:ILE:HG21	1:A:1352:VAL:HG22	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1434:ALA:HB3	1:A:1436:ILE:HD12	1.98	0.45
2:B:56:ASP:C	2:B:57:TYR:CD1	2.94	0.45
1:A:553:VAL:HG13	1:A:554:PRO:HD2	1.97	0.45
1:A:609:ASP:C	1:A:611:GLN:H	2.24	0.45
1:A:1284:MET:HE3	1:A:1304:TRP:CZ3	2.51	0.45
2:B:363:HIS:O	2:B:364:ILE:CB	2.59	0.45
2:B:737:THR:O	2:B:738:PHE:C	2.58	0.45
3:C:3:GLU:HB3	9:K:104:ASN:CG	2.41	0.45
3:C:246:ARG:HA	3:C:249:ASP:HB2	1.98	0.45
4:E:108:GLY:HA3	4:E:132:ILE:HG12	1.99	0.45
9:K:7:PHE:CD1	9:K:7:PHE:C	2.94	0.45
1:A:356:ASP:HB2	1:A:469:ARG:HH11	1.81	0.45
1:A:961:ARG:HB2	1:A:1025:ARG:HH12	1.81	0.45
1:A:1290:LYS:HA	1:A:1299:VAL:O	2.17	0.45
2:B:27:ALA:O	2:B:28:GLU:C	2.60	0.45
2:B:48:LEU:HD22	2:B:176:SER:HA	1.99	0.45
2:B:289:LEU:HD23	2:B:289:LEU:HA	1.85	0.45
2:B:458:LYS:O	2:B:462:ALA:CB	2.65	0.45
4:E:202:SER:OG	4:E:204:THR:HB	2.16	0.45
11:R:13:C:O2	11:R:13:C:O2'	2.30	0.45
1:A:512:VAL:HG23	1:A:519:PRO:N	2.31	0.45
1:A:665:GLY:O	1:A:668:ASP:HB2	2.16	0.45
2:B:1002:THR:HG22	2:B:1006:ILE:HB	1.99	0.45
2:B:1200:ALA:O	2:B:1201:LYS:C	2.59	0.45
4:E:16:PHE:O	4:E:17:ARG:C	2.59	0.45
4:E:63:ASN:CB	4:E:64:PRO:HD3	2.44	0.45
5:F:130:ILE:HG22	5:F:132:LEU:HG	1.98	0.45
13:N:11:DG:H2''	13:N:12:DT:O4'	2.16	0.45
1:A:172:PRO:HB3	1:A:183:GLY:HA3	1.98	0.45
1:A:456:MET:HE3	1:A:507:VAL:HG22	1.99	0.45
1:A:1396:ALA:HB2	1:A:1417:GLU:OE1	2.16	0.45
2:B:26:THR:O	2:B:27:ALA:C	2.59	0.45
2:B:370:PHE:CD2	2:B:373:ARG:HG3	2.46	0.45
3:C:21:ILE:HD12	3:C:229:TYR:CE2	2.52	0.45
6:H:22:LYS:O	6:H:23:VAL:HG23	2.15	0.45
6:H:111:LEU:O	6:H:112:ILE:HB	2.15	0.45
11:R:6:G:H2'	11:R:7:A:H8	1.80	0.45
1:A:53:LEU:O	1:A:56:PRO:HD2	2.15	0.45
2:B:99:LYS:O	2:B:100:PRO:O	2.34	0.45
2:B:542:MET:HB3	2:B:636:PRO:HD3	1.98	0.45
2:B:981:ALA:CA	2:B:987:LYS:HA	2.41	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:80:VAL:HG13	4:E:109:ILE:HG21	1.97	0.45
5:F:147:SER:O	5:F:151:LEU:HD12	2.16	0.45
1:A:253:ASN:HD22	1:A:257:ARG:N	2.14	0.45
1:A:1283:VAL:HG12	1:A:1284:MET:N	2.31	0.45
2:B:40:GLU:HG3	2:B:681:TRP:HB3	1.99	0.45
2:B:450:ALA:O	2:B:451:LYS:C	2.60	0.45
2:B:515:HIS:H	2:B:518:HIS:HD2	1.63	0.45
2:B:770:GLN:CB	2:B:983:ARG:O	2.64	0.45
2:B:879:ARG:HB2	2:B:880:THR:H	1.48	0.45
2:B:1073:TYR:OH	2:B:1080:LYS:HE3	2.17	0.45
3:C:35:ARG:HH11	9:K:41:THR:N	2.15	0.45
4:E:13:TRP:CZ3	4:E:39:LEU:HB2	2.51	0.45
5:F:86:THR:OG1	5:F:89:GLU:HG3	2.16	0.45
11:R:13:C:O2	11:R:13:C:C2'	2.61	0.45
1:A:302:THR:HA	1:A:305:ASP:O	2.17	0.45
1:A:323:LYS:HD3	1:A:323:LYS:N	2.32	0.45
1:A:492:PRO:HB3	1:A:497:THR:HG22	1.98	0.45
1:A:658:LEU:HD22	2:B:831:SER:HA	1.99	0.45
1:A:807:GLY:HA3	2:B:728:ARG:NH1	2.31	0.45
1:A:1109:LYS:HB2	1:A:1109:LYS:HE3	1.56	0.45
2:B:522:VAL:HG12	2:B:523:CYS:N	2.32	0.45
2:B:768:THR:O	2:B:771:SER:HB2	2.17	0.45
2:B:1027:ILE:O	2:B:1028:GLU:C	2.59	0.45
6:H:93:TYR:HA	6:H:145:ARG:CB	2.47	0.45
6:H:113:ALA:HA	6:H:125:LEU:O	2.17	0.45
2:B:248:SER:H	2:B:418:LYS:NZ	2.15	0.45
2:B:1131:GLY:O	2:B:1132:GLU:C	2.60	0.45
2:B:1175:LEU:HD23	2:B:1176:ASN:N	2.32	0.45
3:C:31:ASN:O	3:C:32:SER:C	2.57	0.45
3:C:134:ILE:CG2	3:C:136:ASP:HB3	2.46	0.45
12:T:14:DG:H2'	12:T:15:DA:C8	2.52	0.45
1:A:68:GLN:C	1:A:70:CYS:N	2.73	0.45
1:A:765:VAL:HG21	1:A:800:VAL:CB	2.44	0.45
1:A:866:PHE:CZ	4:E:211:TYR:HB2	2.52	0.45
2:B:128:LEU:HD21	2:B:170:LEU:HB3	1.98	0.45
2:B:321:GLY:C	2:B:323:VAL:H	2.25	0.45
2:B:1104:HIS:ND1	2:B:1105:ALA:N	2.65	0.45
3:C:162:GLY:HA3	3:C:170:TRP:CE2	2.51	0.45
1:A:88:LYS:HA	1:A:89:PRO:HD2	1.60	0.44
1:A:172:PRO:HA	1:A:184:SER:O	2.15	0.44
1:A:531:ILE:HG21	1:A:622:VAL:HG11	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:606:LEU:HB2	1:A:614:PHE:CE2	2.52	0.44
1:A:899:VAL:O	1:A:929:LEU:HD12	2.17	0.44
1:A:1345:ARG:HG2	1:A:1372:VAL:CG1	2.47	0.44
2:B:205:ILE:C	2:B:207:GLY:N	2.74	0.44
4:E:100:ILE:HG12	4:E:105:PHE:HD1	1.82	0.44
4:E:143:ASN:OD1	4:E:187:TYR:HE1	2.00	0.44
6:H:63:LEU:C	6:H:90:ALA:CB	2.91	0.44
7:I:45:ARG:HE	7:I:47:GLU:HG3	1.82	0.44
7:I:106:CYS:O	7:I:108:HIS:N	2.50	0.44
8:J:6:ARG:CG	8:J:13:VAL:HA	2.46	0.44
1:A:17:VAL:HB	1:A:1419:ASP:HB3	1.98	0.44
1:A:147:VAL:HG23	1:A:149:GLU:HG3	1.99	0.44
1:A:251:SER:O	1:A:252:PHE:CG	2.70	0.44
1:A:302:THR:HG21	1:A:313:GLN:HE22	1.83	0.44
1:A:565:ILE:HG12	1:A:567:LYS:HZ2	1.80	0.44
1:A:786:HIS:HD1	2:B:703:ILE:HB	1.81	0.44
1:A:966:ASN:O	1:A:1044:TRP:CH2	2.70	0.44
1:A:1117:THR:O	1:A:1117:THR:HG22	2.17	0.44
1:A:1209:MET:O	1:A:1212:VAL:HB	2.17	0.44
2:B:205:ILE:O	2:B:206:ASN:HB2	2.16	0.44
2:B:216:GLU:HB3	2:B:499:ASN:O	2.18	0.44
2:B:360:PHE:O	2:B:361:LEU:C	2.59	0.44
3:C:92:CYS:O	3:C:96:SER:N	2.45	0.44
4:E:12:LEU:HD13	4:E:55:ARG:HH21	1.81	0.44
1:A:482:PHE:HD1	2:B:835:GLN:O	2.00	0.44
1:A:1044:TRP:O	1:A:1045:VAL:C	2.60	0.44
1:A:1295:THR:OG1	1:A:1297:GLU:OE1	2.33	0.44
1:A:1351:GLU:O	1:A:1352:VAL:C	2.60	0.44
2:B:255:GLN:HB2	2:B:272:THR:HB	2.00	0.44
2:B:412:LEU:HB3	2:B:466:TRP:CZ2	2.53	0.44
3:C:120:ILE:H	3:C:120:ILE:HG12	1.62	0.44
4:E:108:GLY:O	4:E:132:ILE:HG23	2.17	0.44
4:E:113:GLN:HB3	4:E:137:GLU:OE1	2.17	0.44
9:K:55:LYS:HB2	9:K:81:TYR:CE1	2.52	0.44
1:A:11:LEU:HA	2:B:1193:GLN:O	2.18	0.44
1:A:88:LYS:HE2	1:A:205:GLU:OE2	2.18	0.44
1:A:344:ARG:CZ	2:B:1129:ARG:HB2	2.47	0.44
1:A:662:PHE:CD2	2:B:829:CYS:SG	2.83	0.44
1:A:909:ASP:O	1:A:910:PRO:C	2.60	0.44
1:A:1100:ARG:HH21	1:A:1351:GLU:HG2	1.82	0.44
2:B:551:PRO:C	2:B:553:PRO:HD2	2.43	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:711:GLU:H	2:B:712:PRO:CD	2.30	0.44
2:B:852:ARG:HG2	2:B:973:ILE:HG23	1.98	0.44
2:B:864:LYS:HD2	2:B:865:LYS:O	2.18	0.44
8:J:30:LEU:HD11	8:J:38:ARG:NH1	2.32	0.44
1:A:23:SER:O	1:A:27:VAL:HG23	2.18	0.44
1:A:996:ASN:C	1:A:998:LEU:H	2.25	0.44
1:A:1098:VAL:N	1:A:1099:PRO:HD2	2.32	0.44
1:A:1100:ARG:HH21	1:A:1351:GLU:CG	2.30	0.44
1:A:1152:ILE:HG12	1:A:1260:LEU:HD23	1.99	0.44
1:A:1313:LEU:O	1:A:1315:GLU:N	2.51	0.44
2:B:808:ALA:O	2:B:812:LEU:HG	2.18	0.44
2:B:864:LYS:N	2:B:872:GLU:OE1	2.44	0.44
5:F:134:ILE:HG22	5:F:136:ARG:HG3	1.98	0.44
1:A:532:ARG:O	1:A:533:LYS:C	2.61	0.44
1:A:1364:ASN:HD22	1:A:1364:ASN:C	2.26	0.44
2:B:258:LEU:HB2	2:B:385:LEU:HD21	1.98	0.44
2:B:905:VAL:HG12	2:B:909:ASP:CB	2.48	0.44
3:C:84:ARG:HD3	9:K:11:LEU:HD21	1.99	0.44
1:A:14:VAL:HB	1:A:1432:GLN:HE22	1.82	0.44
1:A:540:PHE:CB	1:A:571:LEU:HD23	2.48	0.44
2:B:354:ASP:O	2:B:357:GLN:N	2.48	0.44
2:B:650:GLU:HG3	2:B:651:LEU:N	2.33	0.44
2:B:766:ARG:HA	2:B:769:TYR:HD1	1.82	0.44
2:B:806:THR:HG22	2:B:808:ALA:H	1.82	0.44
2:B:829:CYS:SG	2:B:1014:PRO:HG2	2.52	0.44
6:H:26:ILE:N	6:H:40:LEU:O	2.49	0.44
7:I:21:GLU:H	7:I:21:GLU:HG3	1.45	0.44
9:K:55:LYS:HB2	9:K:81:TYR:HE1	1.82	0.44
10:L:27:LEU:HD23	10:L:27:LEU:H	1.83	0.44
1:A:756:ILE:O	1:A:760:GLN:HG2	2.18	0.44
1:A:793:SER:HB2	1:A:794:PRO:CD	2.39	0.44
1:A:947:PHE:CE2	1:A:954:TRP:CD2	3.06	0.44
2:B:175:ARG:O	2:B:175:ARG:HG2	2.18	0.44
2:B:332:ASP:C	2:B:334:ILE:H	2.26	0.44
2:B:739:THR:OG1	2:B:740:HIS:N	2.50	0.44
2:B:783:THR:HG22	8:J:63:TYR:HE1	1.82	0.44
2:B:1177:HIS:C	2:B:1179:GLN:H	2.26	0.44
3:C:148:ARG:O	3:C:151:GLN:HG3	2.18	0.44
6:H:109:LYS:HD3	6:H:109:LYS:H	1.82	0.44
9:K:101:LEU:O	9:K:102:LYS:C	2.61	0.44
1:A:405:VAL:HG23	1:A:415:LEU:HD11	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:412:ARG:NH2	1:A:433:GLU:OE2	2.51	0.44
1:A:755:PHE:O	1:A:756:ILE:C	2.61	0.44
1:A:1222:ASN:HD22	1:A:1222:ASN:HA	1.63	0.44
2:B:56:ASP:C	2:B:57:TYR:HD1	2.26	0.44
2:B:120:ARG:NE	2:B:955:THR:HG21	2.33	0.44
2:B:586:TRP:NE1	2:B:588:GLY:O	2.51	0.44
2:B:980:PHE:O	2:B:1095:LEU:HD12	2.17	0.44
2:B:1131:GLY:O	2:B:1134:GLU:N	2.50	0.44
12:T:26:DG:C2	12:T:27:DA:C8	3.06	0.44
1:A:343:LYS:HZ3	2:B:1197:PRO:HB3	1.82	0.43
1:A:353:ILE:HD12	1:A:482:PHE:HD2	1.83	0.43
1:A:853:ASP:OD1	1:A:853:ASP:C	2.61	0.43
1:A:865:GLN:NE2	1:A:1370:LEU:HA	2.33	0.43
1:A:1063:MET:SD	1:A:1436:ILE:HG12	2.58	0.43
1:A:1066:VAL:HG11	2:B:1136:ASP:O	2.18	0.43
1:A:1209:MET:SD	1:A:1236:LEU:HB3	2.58	0.43
1:A:1365:TYR:O	1:A:1366:ARG:C	2.61	0.43
1:A:1393:ASN:HB2	1:A:1394:THR:H	1.52	0.43
1:A:1406:VAL:CG1	1:A:1410:PHE:CE1	3.01	0.43
1:A:1420:ASP:HB3	1:A:1422:ARG:HG2	1.99	0.43
2:B:235:SER:OG	2:B:236:HIS:N	2.51	0.43
2:B:322:PHE:CZ	7:I:30:ARG:HD2	2.52	0.43
2:B:384:ARG:HA	2:B:384:ARG:HD2	1.59	0.43
2:B:490:SER:OG	2:B:491:THR:N	2.47	0.43
2:B:842:ASN:O	2:B:845:SER:N	2.51	0.43
2:B:890:TYR:O	2:B:892:LYS:N	2.51	0.43
3:C:184:ASN:CG	3:C:187:LYS:HA	2.43	0.43
4:E:63:ASN:HB3	4:E:64:PRO:HD2	1.99	0.43
4:E:144:ILE:HG13	4:E:145:THR:H	1.82	0.43
7:I:68:LEU:HB3	7:I:84:VAL:HG22	2.00	0.43
1:A:60:SER:C	1:A:61:ILE:HG13	2.43	0.43
1:A:819:GLY:O	1:A:822:GLU:N	2.50	0.43
1:A:900:ASP:C	1:A:906:HIS:O	2.51	0.43
1:A:1059:HIS:ND1	5:F:86:THR:HA	2.33	0.43
1:A:1132:LYS:CG	1:A:1135:ARG:HH12	2.30	0.43
2:B:25:ILE:HG22	2:B:26:THR:N	2.32	0.43
2:B:48:LEU:C	2:B:50:SER:N	2.74	0.43
2:B:57:TYR:N	2:B:57:TYR:HD1	2.16	0.43
2:B:96:TYR:N	2:B:129:PHE:O	2.44	0.43
2:B:235:SER:C	2:B:236:HIS:CD2	2.96	0.43
2:B:522:VAL:HG11	2:B:537:LYS:CB	2.43	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:36:GLU:O	4:E:38:PRO:HD3	2.17	0.43
7:I:4:PHE:H	7:I:4:PHE:HD2	1.64	0.43
1:A:371:ALA:O	1:A:435:HIS:HB3	2.18	0.43
1:A:947:PHE:CZ	4:E:203:GLU:HA	2.54	0.43
2:B:99:LYS:HA	2:B:100:PRO:HD2	1.70	0.43
2:B:168:GLY:H	2:B:450:ALA:HB1	1.83	0.43
2:B:301:ILE:HD13	2:B:382:ILE:HG21	2.01	0.43
2:B:1076:HIS:CG	9:K:40:HIS:CD2	3.04	0.43
4:E:61:GLN:CB	4:E:79:TRP:HA	2.48	0.43
6:H:77:ARG:O	6:H:78:SER:C	2.60	0.43
9:K:33:ILE:HD13	9:K:87:LEU:HD22	1.99	0.43
1:A:108:MET:N	1:A:108:MET:SD	2.92	0.43
1:A:332:LYS:H	1:A:337:ARG:HB3	1.83	0.43
1:A:903:ASN:C	1:A:907:THR:HG1	2.08	0.43
1:A:1171:GLN:HB3	1:A:1172:LEU:H	1.68	0.43
2:B:189:LEU:O	2:B:192:LEU:N	2.51	0.43
2:B:277:LYS:NZ	2:B:335:GLY:CA	2.81	0.43
2:B:633:VAL:O	2:B:694:ASP:HB2	2.19	0.43
1:A:24:PRO:HB3	1:A:237:THR:HB	2.00	0.43
1:A:33:ALA:HB1	1:A:35:ILE:HD11	2.00	0.43
1:A:253:ASN:O	1:A:254:GLU:HB2	2.16	0.43
1:A:362:ASP:OD1	1:A:459:ARG:HD3	2.17	0.43
1:A:655:PHE:O	1:A:656:TRP:C	2.61	0.43
1:A:668:ASP:CG	1:A:742:ASN:HD22	2.26	0.43
1:A:919:ILE:O	1:A:922:ASP:HB2	2.19	0.43
1:A:981:LEU:HD21	1:A:1039:LYS:HA	2.01	0.43
1:A:1104:ILE:CD1	1:A:1351:GLU:HB3	2.48	0.43
1:A:1332:PHE:CE1	1:A:1348:LEU:HD12	2.53	0.43
2:B:493:SER:HB2	2:B:751:VAL:HG11	2.00	0.43
2:B:582:VAL:HB	2:B:587:HIS:CD2	2.53	0.43
2:B:755:ILE:O	2:B:755:ILE:CG2	2.66	0.43
2:B:826:ALA:O	2:B:1011:ILE:HA	2.19	0.43
2:B:973:ILE:CG2	2:B:974:PRO:HD2	2.48	0.43
2:B:1160:VAL:HG12	2:B:1161:HIS:N	2.34	0.43
3:C:83:SER:OG	3:C:160:LYS:HB3	2.18	0.43
3:C:171:GLY:HA2	3:C:172:PRO:HD3	1.81	0.43
9:K:57:LEU:HB2	9:K:76:GLN:HG2	2.01	0.43
1:A:261:ASP:CB	1:A:323:LYS:HD2	2.46	0.43
1:A:800:VAL:HG13	1:A:812:GLU:HB3	2.01	0.43
1:A:862:ASN:HA	4:E:174:GLN:HB3	2.00	0.43
1:A:939:ASP:O	1:A:942:PHE:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1407:GLU:O	1:A:1411:GLU:HG2	2.18	0.43
2:B:226:PHE:O	2:B:228:LYS:HG3	2.19	0.43
3:C:5:GLY:O	3:C:6:PRO:C	2.62	0.43
3:C:62:PHE:O	3:C:63:ILE:C	2.62	0.43
3:C:104:PHE:HD1	3:C:152:GLU:HG3	1.83	0.43
3:C:196:ASP:HB3	3:C:199:LYS:HB2	2.00	0.43
8:J:32:GLU:CD	8:J:32:GLU:H	2.26	0.43
11:R:9:G:C2'	11:R:10:A:H5'	2.49	0.43
1:A:33:ALA:C	1:A:34:LYS:HG3	2.44	0.43
1:A:319:GLY:CA	1:A:320:ARG:NH1	2.81	0.43
1:A:379:VAL:HG12	1:A:380:VAL:N	2.34	0.43
1:A:545:GLN:HB3	1:A:549:MET:CE	2.49	0.43
1:A:893:PHE:C	1:A:893:PHE:HD2	2.26	0.43
1:A:1161:THR:HG23	1:A:1239:ARG:NH2	2.33	0.43
1:A:1208:THR:OG1	1:A:1211:GLN:HB2	2.19	0.43
2:B:274:PRO:O	2:B:275:TYR:HB2	2.19	0.43
2:B:428:ILE:HD11	2:B:448:ILE:HD13	1.99	0.43
2:B:575:PRO:HD2	2:B:576:ASP:H	1.84	0.43
2:B:802:PRO:HA	2:B:1091:TYR:CD1	2.54	0.43
2:B:1015:HIS:C	2:B:1017:ILE:H	2.27	0.43
2:B:1027:ILE:O	2:B:1029:CYS:N	2.51	0.43
3:C:79:GLN:HE21	3:C:127:ARG:HB3	1.84	0.43
4:E:68:SER:C	4:E:70:SER:H	2.25	0.43
9:K:7:PHE:C	9:K:9:LEU:H	2.27	0.43
1:A:407:ARG:HD3	1:A:413:ILE:HD13	2.01	0.43
1:A:1142:THR:O	1:A:1145:SER:OG	2.29	0.43
1:A:1198:ASP:O	1:A:1202:MET:HG2	2.19	0.43
2:B:115:GLN:HG2	2:B:193:LYS:HB2	2.01	0.43
2:B:519:TRP:CD1	2:B:519:TRP:O	2.72	0.43
2:B:766:ARG:NH2	11:R:13:C:H5'	2.34	0.43
2:B:981:ALA:HB2	2:B:987:LYS:CB	2.48	0.43
3:C:3:GLU:CG	3:C:4:GLU:N	2.73	0.43
3:C:144:ILE:HD13	3:C:144:ILE:HA	1.93	0.43
9:K:44:ASN:HA	9:K:61:TYR:CE2	2.54	0.43
1:A:254:GLU:HA	1:A:255:SER:HA	1.63	0.43
1:A:385:ILE:H	1:A:385:ILE:HG13	1.65	0.43
1:A:997:LEU:HD13	1:A:1018:PHE:HE2	1.83	0.43
1:A:1219:THR:HG21	1:A:1271:ILE:CD1	2.49	0.43
2:B:292:ILE:N	2:B:293:PRO:CD	2.82	0.43
2:B:618:ASP:O	2:B:619:ILE:C	2.61	0.43
2:B:766:ARG:HH21	2:B:1020:ARG:HB3	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:176:ILE:O	3:C:176:ILE:HG22	2.19	0.43
6:H:41:ASP:HB3	6:H:121:LEU:HD22	2.01	0.43
9:K:40:HIS:C	9:K:42:LEU:N	2.74	0.43
1:A:1384:VAL:HA	1:A:1389:PHE:CD2	2.51	0.43
3:C:99:LEU:HD23	3:C:99:LEU:N	2.33	0.43
7:I:8:ARG:O	7:I:9:ASP:CB	2.67	0.43
1:A:588:LEU:HD13	1:A:632:VAL:HG21	2.01	0.42
1:A:629:LEU:CD2	1:A:633:VAL:HG21	2.49	0.42
1:A:900:ASP:HB3	1:A:906:HIS:HB3	2.00	0.42
2:B:261:ARG:N	2:B:264:SER:HB2	2.34	0.42
2:B:973:ILE:HG22	2:B:974:PRO:HD2	2.00	0.42
7:I:20:LYS:HB2	7:I:21:GLU:H	1.49	0.42
8:J:9:SER:OG	8:J:45:CYS:HB2	2.19	0.42
9:K:47:ARG:O	9:K:50:LEU:N	2.52	0.42
1:A:53:LEU:HB3	1:A:54:ASN:H	1.50	0.42
1:A:458:HIS:NE2	1:A:478:TYR:OH	2.49	0.42
1:A:472:LEU:O	1:A:475:THR:CB	2.67	0.42
1:A:491:VAL:H	2:B:1150:ARG:HH22	1.67	0.42
1:A:526:ASP:O	1:A:529:CYS:N	2.52	0.42
1:A:567:LYS:NZ	6:H:97:MET:SD	2.92	0.42
1:A:1025:ARG:O	1:A:1035:TYR:OH	2.34	0.42
2:B:170:LEU:HG	2:B:171:PRO:O	2.18	0.42
2:B:408:LEU:O	2:B:412:LEU:HG	2.19	0.42
2:B:412:LEU:CD1	2:B:479:VAL:HG11	2.48	0.42
2:B:542:MET:HE1	2:B:743:ILE:HG21	2.01	0.42
2:B:702:LEU:HG	2:B:738:PHE:HD2	1.83	0.42
2:B:898:LEU:HD12	10:L:58:LYS:HD2	2.01	0.42
2:B:997:GLU:H	2:B:997:GLU:HG3	1.65	0.42
2:B:1006:ILE:HG22	2:B:1087:PHE:HZ	1.84	0.42
3:C:163:ILE:O	3:C:166:GLU:N	2.31	0.42
5:F:118:LEU:O	5:F:122:MET:HG3	2.19	0.42
6:H:129:TYR:C	6:H:131:ASN:H	2.27	0.42
8:J:56:LEU:O	8:J:59:LYS:N	2.40	0.42
1:A:256:GLN:HB2	1:A:257:ARG:HD2	1.66	0.42
1:A:440:ASP:O	1:A:460:VAL:HG23	2.18	0.42
1:A:532:ARG:HG3	1:A:616:VAL:CG1	2.50	0.42
1:A:550:LEU:HD13	1:A:550:LEU:HA	1.69	0.42
1:A:1254:ALA:O	1:A:1255:GLU:CB	2.67	0.42
1:A:1325:THR:HA	4:E:147:HIS:HA	2.01	0.42
1:A:1349:TYR:CA	1:A:1372:VAL:HG21	2.49	0.42
2:B:306:ASN:O	2:B:308:TRP:N	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:515:HIS:CD2	2:B:517:THR:OG1	2.73	0.42
2:B:684:LEU:HD23	2:B:689:LEU:HD12	2.01	0.42
2:B:758:PHE:CZ	2:B:1044:ALA:HA	2.55	0.42
2:B:782:LEU:HB3	2:B:784:ASN:OD1	2.19	0.42
2:B:1106:ARG:NH2	2:B:1109:GLY:H	2.17	0.42
6:H:39:THR:O	6:H:123:MET:HA	2.19	0.42
7:I:60:GLN:NE2	7:I:107:SER:OG	2.52	0.42
8:J:8:PHE:H	8:J:49:MET:HE3	1.84	0.42
1:A:532:ARG:HH22	1:A:745:GLN:HG2	1.84	0.42
1:A:1066:VAL:O	1:A:1067:LEU:C	2.61	0.42
1:A:1092:LYS:O	1:A:1093:LYS:HG3	2.19	0.42
1:A:1423:GLY:O	1:A:1424:VAL:C	2.61	0.42
2:B:124:TYR:OH	2:B:179:CYS:SG	2.59	0.42
2:B:814:PHE:O	2:B:816:GLU:N	2.52	0.42
2:B:840:ILE:HB	2:B:1011:ILE:HD12	2.02	0.42
6:H:97:MET:SD	6:H:121:LEU:HD12	2.59	0.42
9:K:46:ILE:HG21	9:K:73:LEU:HD22	2.01	0.42
1:A:23:SER:HB3	1:A:233:TRP:CE2	2.54	0.42
1:A:250:ILE:O	1:A:251:SER:OG	2.37	0.42
1:A:528:LEU:HD21	1:A:749:ALA:O	2.19	0.42
1:A:670:ILE:H	1:A:670:ILE:HG12	1.63	0.42
1:A:939:ASP:O	1:A:940:ARG:C	2.62	0.42
1:A:1130:GLN:O	1:A:1134:ILE:HG13	2.19	0.42
1:A:1161:THR:HG22	1:A:1163:ILE:H	1.85	0.42
1:A:1385:THR:O	1:A:1387:HIS:N	2.51	0.42
1:A:1391:ARG:C	1:A:1391:ARG:CD	2.82	0.42
2:B:195:CYS:HA	2:B:196:PRO:HD3	1.79	0.42
3:C:97:VAL:HG21	3:C:129:ILE:CG2	2.48	0.42
3:C:217:ASP:HA	3:C:218:PRO:HD3	1.89	0.42
7:I:54:GLU:O	7:I:55:THR:C	2.60	0.42
11:R:2:U:H2'	11:R:3:C:C6	2.54	0.42
1:A:544:ASP:HB2	9:K:47:ARG:NH2	2.35	0.42
1:A:567:LYS:C	1:A:569:LYS:N	2.78	0.42
1:A:812:GLU:O	1:A:813:PHE:C	2.63	0.42
1:A:858:ASN:ND2	1:A:858:ASN:H	2.17	0.42
1:A:965:GLN:HA	1:A:968:GLN:HG2	2.01	0.42
1:A:1151:GLU:O	1:A:1193:LEU:HA	2.20	0.42
1:A:1364:ASN:HD21	1:A:1366:ARG:CG	2.09	0.42
3:C:69:LEU:HD22	3:C:69:LEU:N	2.33	0.42
5:F:82:THR:HG22	5:F:84:TYR:HB2	2.01	0.42
1:A:32:VAL:HB	1:A:57:ARG:CB	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:442:VAL:O	1:A:457:ALA:HA	2.20	0.42
1:A:899:VAL:HG23	1:A:1029:ARG:CG	2.49	0.42
1:A:997:LEU:O	1:A:1053:PHE:CE2	2.73	0.42
2:B:25:ILE:CG2	2:B:26:THR:N	2.83	0.42
2:B:1024:ALA:O	2:B:1025:HIS:C	2.63	0.42
2:B:1027:ILE:O	2:B:1030:LEU:N	2.52	0.42
2:B:1139:ILE:H	2:B:1139:ILE:HG13	1.64	0.42
3:C:13:ALA:HA	3:C:17:ASN:O	2.20	0.42
3:C:172:PRO:C	3:C:235:VAL:HG23	2.45	0.42
3:C:219:PHE:CB	6:H:45:GLU:HG2	2.50	0.42
7:I:98:VAL:HG11	7:I:113:ASP:HB2	2.01	0.42
8:J:7:CYS:SG	8:J:7:CYS:O	2.77	0.42
1:A:380:VAL:HG11	1:A:428:TYR:N	2.35	0.42
2:B:795:ILE:HG22	2:B:796:LEU:N	2.34	0.42
2:B:863:GLU:HG3	2:B:962:LYS:HB3	2.01	0.42
3:C:27:LEU:HA	3:C:228:PHE:CZ	2.54	0.42
3:C:247:GLY:C	3:C:249:ASP:N	2.76	0.42
4:E:143:ASN:OD1	4:E:187:TYR:CE1	2.73	0.42
6:H:6:PHE:CZ	6:H:8:ASP:HB2	2.55	0.42
9:K:7:PHE:HA	9:K:10:PHE:CE2	2.55	0.42
1:A:42:ASP:HA	1:A:46:THR:O	2.19	0.42
1:A:947:PHE:CE2	1:A:954:TRP:CE2	3.07	0.42
2:B:20:ASP:O	2:B:22:SER:N	2.51	0.42
2:B:95:ILE:HD12	2:B:130:VAL:HG22	2.02	0.42
2:B:708:GLU:HG3	2:B:709:ASP:N	2.35	0.42
2:B:796:LEU:HD12	2:B:796:LEU:HA	1.74	0.42
2:B:956:THR:HG22	10:L:46:VAL:HG21	2.01	0.42
2:B:1104:HIS:CG	2:B:1122:ARG:HB2	2.55	0.42
5:F:109:VAL:HG11	5:F:123:LYS:HG2	2.01	0.42
1:A:564:ALA:O	6:H:97:MET:HB3	2.19	0.42
1:A:577:ILE:O	1:A:578:LEU:C	2.63	0.42
1:A:809:THR:HB	1:A:810:PRO:CD	2.47	0.42
1:A:1015:VAL:O	1:A:1016:THR:C	2.62	0.42
1:A:1121:GLU:O	1:A:1122:PRO:C	2.62	0.42
2:B:118:ARG:HH22	2:B:194:GLU:CD	2.28	0.42
2:B:582:VAL:HA	2:B:626:ILE:O	2.20	0.42
2:B:878:GLN:HA	2:B:885:MET:HE2	2.01	0.42
3:C:142:VAL:CG2	8:J:5:VAL:HG13	2.50	0.42
4:E:66:GLU:O	4:E:69:ILE:N	2.51	0.42
4:E:153:HIS:O	4:E:154:ILE:HD13	2.19	0.42
6:H:76:THR:O	6:H:77:ARG:O	2.37	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:98:TYR:HE1	6:H:139:ASN:HA	1.84	0.42
9:K:3:ALA:HA	9:K:4:PRO:HD3	1.79	0.42
1:A:376:TYR:CE2	1:A:377:PRO:O	2.73	0.41
1:A:726:ARG:O	1:A:727:ASP:C	2.63	0.41
1:A:733:ALA:O	1:A:737:LEU:HG	2.19	0.41
1:A:943:LEU:C	1:A:945:GLU:N	2.74	0.41
1:A:1373:ASP:O	1:A:1374:VAL:C	2.63	0.41
2:B:120:ARG:HA	2:B:963:PHE:CE2	2.54	0.41
2:B:451:LYS:HA	2:B:454:THR:HB	2.02	0.41
2:B:527:THR:OG1	2:B:528:PRO:HD2	2.19	0.41
2:B:708:GLU:C	2:B:710:LEU:H	2.28	0.41
2:B:975:GLN:HG2	2:B:976:ILE:N	2.27	0.41
2:B:992:ILE:HD12	2:B:992:ILE:HA	1.82	0.41
4:E:169:ARG:HG3	5:F:140:ASP:HB3	2.01	0.41
6:H:12:VAL:HG21	6:H:53:ASP:HB2	2.02	0.41
9:K:24:ASP:CG	9:K:74:ARG:HH11	2.28	0.41
9:K:82:ASP:HA	9:K:83:PRO:HD2	1.75	0.41
1:A:171:GLN:HE21	1:A:171:GLN:HB3	1.72	0.41
1:A:388:LEU:HD23	1:A:388:LEU:HA	1.90	0.41
1:A:549:MET:O	1:A:550:LEU:C	2.61	0.41
2:B:653:VAL:HA	2:B:657:HIS:HD2	1.85	0.41
2:B:906:SER:HB3	2:B:946:ASN:CB	2.50	0.41
2:B:1094:ARG:NH2	2:B:1098:MET:HG2	2.33	0.41
3:C:101:LEU:HD21	3:C:113:VAL:CG1	2.49	0.41
3:C:133:ILE:HD13	3:C:237:SER:HA	2.02	0.41
3:C:142:VAL:CG1	3:C:143:LEU:N	2.67	0.41
4:E:78:LEU:HD12	4:E:107:THR:HB	2.02	0.41
4:E:126:SER:C	4:E:128:PRO:HD3	2.45	0.41
7:I:62:ILE:C	7:I:64:SER:H	2.27	0.41
2:B:977:GLY:O	2:B:989:THR:HB	2.21	0.41
2:B:984:HIS:NE2	2:B:1024:ALA:HB3	2.36	0.41
3:C:118:LEU:HD23	3:C:118:LEU:HA	1.89	0.41
4:E:163:GLU:O	4:E:164:LEU:C	2.62	0.41
7:I:15:TYR:O	7:I:27:PHE:HA	2.21	0.41
8:J:6:ARG:HA	8:J:12:LYS:O	2.20	0.41
1:A:31:SER:HB2	1:A:81:PHE:O	2.21	0.41
2:B:217:ARG:NH2	2:B:405:ARG:HG3	2.35	0.41
2:B:284:ILE:H	2:B:284:ILE:HG12	1.74	0.41
2:B:323:VAL:O	2:B:324:ILE:HG13	2.20	0.41
3:C:104:PHE:CD1	3:C:152:GLU:HG3	2.55	0.41
3:C:167:HIS:HD2	3:C:169:LYS:N	2.08	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:242:GLN:HA	3:C:245:VAL:HB	2.03	0.41
5:F:89:GLU:O	5:F:93:ILE:HG12	2.20	0.41
9:K:65:HIS:CD2	9:K:67:PHE:H	2.18	0.41
10:L:26:THR:O	10:L:26:THR:HG22	2.20	0.41
2:B:226:PHE:O	2:B:227:LYS:C	2.62	0.41
2:B:279:ASP:O	2:B:280:ILE:HD13	2.20	0.41
2:B:293:PRO:C	2:B:294:ASP:O	2.63	0.41
2:B:816:GLU:O	2:B:817:LEU:HD12	2.20	0.41
2:B:860:MET:SD	2:B:861:ASP:N	2.94	0.41
2:B:1168:LEU:HD21	2:B:1214:PRO:HD2	2.02	0.41
8:J:6:ARG:N	8:J:14:VAL:HG22	2.35	0.41
11:R:3:C:H2'	11:R:4:G:H8	1.85	0.41
1:A:49:LYS:NZ	1:A:60:SER:HA	2.35	0.41
1:A:396:PRO:C	1:A:397:ASN:OD1	2.64	0.41
1:A:446:ARG:HG3	1:A:487:MET:HG2	2.01	0.41
1:A:560:ILE:H	1:A:560:ILE:HG12	1.67	0.41
1:A:658:LEU:HD12	1:A:658:LEU:O	2.21	0.41
1:A:1194:ARG:HG3	1:A:1237:ILE:CG2	2.51	0.41
2:B:757:PRO:CB	2:B:1044:ALA:HB1	2.51	0.41
2:B:890:TYR:CD2	2:B:910:VAL:HG21	2.55	0.41
2:B:1001:PHE:CZ	2:B:1073:TYR:HB2	2.56	0.41
4:E:184:VAL:O	4:E:187:TYR:HB3	2.20	0.41
7:I:102:VAL:O	7:I:104:LEU:HD23	2.21	0.41
1:A:40:THR:HG21	1:A:259:GLU:OE2	2.20	0.41
1:A:491:VAL:N	2:B:1150:ARG:NH2	2.68	0.41
1:A:697:ALA:HA	1:A:702:LEU:HB2	2.01	0.41
1:A:741:ASN:O	1:A:745:GLN:HG3	2.20	0.41
2:B:544:CYS:HB2	2:B:634:TYR:CZ	2.55	0.41
2:B:1147:LEU:O	2:B:1147:LEU:HD22	2.21	0.41
3:C:46:ILE:HA	3:C:159:ALA:HA	2.03	0.41
3:C:53:THR:O	3:C:154:LYS:N	2.42	0.41
3:C:57:VAL:HG23	8:J:57:ILE:CD1	2.51	0.41
4:E:99:HIS:CD2	4:E:99:HIS:C	2.99	0.41
1:A:44:THR:O	1:A:45:GLN:HB2	2.20	0.41
1:A:250:ILE:HB	1:A:251:SER:H	1.77	0.41
1:A:306:ASN:HD22	1:A:306:ASN:N	2.18	0.41
1:A:472:LEU:CD2	2:B:835:GLN:HB3	2.51	0.41
1:A:535:THR:HG21	1:A:616:VAL:HA	2.00	0.41
1:A:565:ILE:HG23	1:A:567:LYS:HG2	2.03	0.41
1:A:588:LEU:HA	1:A:588:LEU:HD12	1.82	0.41
1:A:858:ASN:C	1:A:858:ASN:HD22	2.28	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:474:SER:O	2:B:476:ARG:N	2.53	0.41
2:B:570:VAL:HG21	2:B:573:GLN:OE1	2.21	0.41
2:B:619:ILE:HG13	7:I:65:ASP:HB2	2.02	0.41
2:B:827:ILE:HD12	2:B:1086:PHE:CD2	2.56	0.41
2:B:1165:ILE:HB	2:B:1166:CYS:H	1.63	0.41
3:C:27:LEU:HD12	3:C:228:PHE:HE2	1.86	0.41
3:C:31:ASN:ND2	3:C:35:ARG:HD2	2.35	0.41
3:C:167:HIS:HD1	10:L:70:ARG:HB3	1.84	0.41
6:H:126:GLU:C	6:H:130:ARG:HH12	2.28	0.41
11:R:3:C:H2'	11:R:4:G:C8	2.55	0.41
12:T:26:DG:H21	12:T:27:DA:H1'	1.84	0.41
1:A:48:ALA:C	1:A:49:LYS:HG2	2.45	0.41
1:A:215:SER:O	1:A:218:ASP:HB2	2.20	0.41
1:A:525:GLN:HB2	2:B:835:GLN:OE1	2.21	0.41
1:A:545:GLN:O	1:A:548:ASN:N	2.53	0.41
1:A:574:GLY:O	1:A:575:LYS:C	2.63	0.41
1:A:777:PHE:HD2	1:A:782:ARG:CA	2.33	0.41
1:A:803:SER:OG	1:A:806:ARG:HG3	2.21	0.41
2:B:92:PHE:CD2	2:B:132:VAL:HG22	2.54	0.41
2:B:104:GLU:H	2:B:104:GLU:HG2	1.55	0.41
2:B:288:ALA:HA	2:B:331:LEU:HD12	2.02	0.41
2:B:315:LYS:HG2	7:I:13:MET:HE1	2.02	0.41
2:B:360:PHE:CD2	2:B:360:PHE:C	2.99	0.41
2:B:450:ALA:O	2:B:453:ILE:N	2.53	0.41
2:B:864:LYS:N	2:B:872:GLU:HB2	2.35	0.41
2:B:882:THR:O	2:B:883:LEU:C	2.64	0.41
3:C:85:ASP:O	3:C:86:CYS:C	2.64	0.41
3:C:162:GLY:HA3	3:C:170:TRP:CD2	2.56	0.41
3:C:227:THR:C	3:C:228:PHE:CD1	2.99	0.41
3:C:244:VAL:HG21	9:K:105:PHE:CE1	2.56	0.41
8:J:64:ASN:HB3	8:J:65:PRO:HD3	2.03	0.41
9:K:10:PHE:CD1	9:K:11:LEU:CD1	3.04	0.41
1:A:874:ASP:C	1:A:874:ASP:OD1	2.64	0.41
2:B:488:TYR:O	2:B:490:SER:N	2.54	0.41
2:B:492:LEU:HB3	2:B:751:VAL:HG21	2.03	0.41
2:B:554:ILE:HG22	2:B:558:LEU:HD11	2.02	0.41
2:B:604:ARG:HD3	2:B:691:GLU:HG2	2.02	0.41
3:C:196:ASP:O	3:C:197:SER:C	2.64	0.41
4:E:66:GLU:O	4:E:67:GLU:C	2.63	0.41
4:E:161:LYS:C	4:E:163:GLU:N	2.79	0.41
7:I:101:PHE:N	7:I:101:PHE:CD1	2.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:J:1:MET:H1	8:J:56:LEU:CB	2.33	0.41
1:A:384:ASN:O	1:A:386:ASP:N	2.54	0.40
1:A:843:LYS:HZ1	2:B:1135:ARG:NH2	2.19	0.40
1:A:1194:ARG:HH21	1:A:1237:ILE:HD13	1.86	0.40
1:A:1395:GLY:HA3	1:A:1419:ASP:OD2	2.21	0.40
2:B:458:LYS:O	2:B:462:ALA:HB2	2.21	0.40
2:B:1076:HIS:ND1	9:K:40:HIS:NE2	2.67	0.40
3:C:35:ARG:HH11	9:K:41:THR:H	1.69	0.40
6:H:58:THR:CG2	6:H:59:ILE:H	2.30	0.40
10:L:42:ARG:O	10:L:43:THR:C	2.64	0.40
10:L:53:HIS:C	10:L:55:ILE:H	2.29	0.40
1:A:101:LYS:HG2	1:A:139:TRP:CE2	2.55	0.40
1:A:737:LEU:HA	1:A:737:LEU:HD23	1.88	0.40
2:B:101:MET:CE	2:B:169:ARG:HH22	2.34	0.40
2:B:1168:LEU:HB3	2:B:1169:MET:H	1.70	0.40
2:B:1182:CYS:SG	2:B:1185:CYS:HB2	2.61	0.40
2:B:1190:ASP:O	2:B:1191:ILE:HG13	2.21	0.40
4:E:77:SER:HB2	4:E:105:PHE:HA	2.04	0.40
4:E:150:VAL:HA	4:E:151:PRO:HD3	1.94	0.40
6:H:33:GLN:H	6:H:33:GLN:HG2	1.64	0.40
9:K:33:ILE:CD1	9:K:87:LEU:HD22	2.51	0.40
1:A:381:THR:OG1	1:A:382:PRO:HD2	2.22	0.40
1:A:587:HIS:CE1	1:A:609:ASP:H	2.40	0.40
1:A:709:THR:HG22	1:A:711:ARG:H	1.87	0.40
1:A:909:ASP:O	1:A:912:LEU:N	2.51	0.40
1:A:973:ILE:HD12	1:A:973:ILE:HA	1.92	0.40
1:A:1271:ILE:HD13	1:A:1271:ILE:HA	1.89	0.40
2:B:550:ASP:HA	2:B:551:PRO:HD3	1.83	0.40
2:B:829:CYS:SG	2:B:1014:PRO:CD	3.09	0.40
2:B:1135:ARG:HG2	2:B:1139:ILE:HD11	2.02	0.40
5:F:125:LEU:C	5:F:127:GLU:N	2.78	0.40
11:R:2:U:H2'	11:R:3:C:H6	1.87	0.40
1:A:131:SER:HB3	1:A:223:GLY:HA2	2.03	0.40
1:A:251:SER:O	1:A:252:PHE:CB	2.70	0.40
1:A:321:PRO:HG3	2:B:471:LYS:NZ	2.37	0.40
1:A:322:VAL:HA	1:A:323:LYS:HD3	2.04	0.40
1:A:451:HIS:CD2	1:A:453:MET:HE2	2.57	0.40
1:A:744:LYS:O	1:A:748:MET:HG3	2.21	0.40
1:A:875:ALA:HB2	1:A:1366:ARG:HD3	2.02	0.40
1:A:947:PHE:N	1:A:947:PHE:CD1	2.89	0.40
2:B:176:SER:O	2:B:182:SER:CB	2.69	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:273:LEU:HA	2:B:274:PRO:HD2	1.67	0.40
2:B:313:MET:O	2:B:316:PRO:HD2	2.22	0.40
2:B:601:ARG:HA	2:B:615:MET:HE1	2.02	0.40
2:B:984:HIS:C	2:B:986:GLN:N	2.78	0.40
3:C:31:ASN:HD21	3:C:35:ARG:HD2	1.86	0.40
4:E:191:LYS:O	4:E:214:CYS:HB3	2.22	0.40
7:I:65:ASP:HA	7:I:66:PRO:HD3	1.76	0.40
1:A:247:ARG:NH1	1:A:263:THR:HG23	2.36	0.40
1:A:253:ASN:CG	1:A:254:GLU:H	2.29	0.40
1:A:344:ARG:NH2	12:T:21:DC:OP2	2.52	0.40
1:A:380:VAL:CG2	1:A:430:TRP:HB2	2.47	0.40
1:A:602:ASP:HB3	1:A:616:VAL:HG23	2.04	0.40
1:A:629:LEU:HD23	1:A:633:VAL:HG21	2.00	0.40
1:A:803:SER:OG	1:A:806:ARG:HD2	2.21	0.40
1:A:890:ASP:O	1:A:893:PHE:HB3	2.21	0.40
1:A:1366:ARG:HG2	1:A:1366:ARG:H	1.71	0.40
2:B:459:TYR:C	2:B:459:TYR:HD2	2.27	0.40
2:B:542:MET:SD	2:B:636:PRO:HG3	2.62	0.40
2:B:658:ILE:HD12	2:B:658:ILE:HA	1.83	0.40
4:E:58:MET:O	4:E:60:PHE:N	2.55	0.40
6:H:44:VAL:O	6:H:44:VAL:CG1	2.69	0.40
7:I:73:ARG:HB3	7:I:74:GLU:H	1.60	0.40
7:I:98:VAL:CG1	7:I:99:LEU:N	2.85	0.40
8:J:27:GLU:C	8:J:29:GLU:H	2.30	0.40

There are no symmetry-related clashes.

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
1	A	1383/1733 (80%)	1027 (74%)	248 (18%)	108 (8%)	1 12

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	1088/1224 (89%)	823 (76%)	195 (18%)	70 (6%)	1	15
3	C	264/318 (83%)	195 (74%)	51 (19%)	18 (7%)	1	14
4	E	212/215 (99%)	163 (77%)	35 (16%)	14 (7%)	1	14
5	F	82/155 (53%)	62 (76%)	15 (18%)	5 (6%)	1	15
6	H	129/146 (88%)	94 (73%)	24 (19%)	11 (8%)	0	10
7	I	117/122 (96%)	83 (71%)	23 (20%)	11 (9%)	0	9
8	J	63/70 (90%)	50 (79%)	9 (14%)	4 (6%)	1	15
9	K	112/120 (93%)	86 (77%)	21 (19%)	5 (4%)	2	19
10	L	44/70 (63%)	20 (46%)	16 (36%)	8 (18%)	0	2
All	All	3494/4173 (84%)	2603 (74%)	637 (18%)	254 (7%)	1	13

All (254) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	54	ASN
1	A	55	ASP
1	A	68	GLN
1	A	69	THR
1	A	117	GLU
1	A	226	GLU
1	A	248	PRO
1	A	250	ILE
1	A	251	SER
1	A	257	ARG
1	A	266	LEU
1	A	286	HIS
1	A	312	PRO
1	A	315	LEU
1	A	322	VAL
1	A	399	HIS
1	A	428	TYR
1	A	567	LYS
1	A	568	PRO
1	A	755	PHE
1	A	756	ILE
1	A	846	GLU
1	A	972	HIS
1	A	998	LEU
1	A	1036	ARG

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Mol	Chain	Res	Type
1	A	1171	GLN
1	A	1173	HIS
1	A	1175	SER
1	A	1223	ASP
1	A	1255	GLU
1	A	1274	ARG
1	A	1393	ASN
1	A	1394	THR
1	A	1421	CYS
2	B	45	SER
2	B	46	GLN
2	B	58	THR
2	B	67	SER
2	B	100	PRO
2	B	176	SER
2	B	229	ALA
2	B	436	VAL
2	B	466	TRP
2	B	475	SER
2	B	477	ALA
2	B	531	GLN
2	B	636	PRO
2	B	709	ASP
2	B	731	VAL
2	B	734	HIS
2	B	751	VAL
2	B	831	SER
2	B	864	LYS
2	B	879	ARG
2	B	1046	PRO
2	B	1103	ILE
2	B	1181	GLU
2	B	1223	ASP
3	C	142	VAL
3	C	174	ALA
4	E	3	GLN
4	E	59	SER
5	F	74	ILE
5	F	81	THR
6	H	32	THR
6	H	77	ARG
6	H	82	PRO

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Mol	Chain	Res	Type
6	H	90	ALA
6	H	140	ALA
7	I	20	LYS
7	I	54	GLU
7	I	107	SER
8	J	2	ILE
8	J	6	ARG
9	K	71	PHE
9	K	81	TYR
10	L	35	SER
10	L	42	ARG
10	L	43	THR
1	A	42	ASP
1	A	50	ILE
1	A	76	GLU
1	A	93	VAL
1	A	130	ASP
1	A	178	GLY
1	A	313	GLN
1	A	325	ILE
1	A	509	LEU
1	A	526	ASP
1	A	583	PRO
1	A	829	VAL
1	A	910	PRO
1	A	916	GLY
1	A	922	ASP
1	A	931	GLU
1	A	986	ILE
1	A	994	GLN
1	A	1022	LEU
1	A	1054	LEU
1	A	1172	LEU
1	A	1270	ASN
1	A	1314	SER
1	A	1386	ARG
1	A	1388	GLY
1	A	1435	PRO
1	A	1438	THR
2	B	21	GLU
2	B	307	ASP
2	B	333	PHE

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Mol	Chain	Res	Type
2	B	708	GLU
2	B	711	GLU
2	B	738	PHE
2	B	746	SER
2	B	866	TYR
2	B	883	LEU
2	B	891	ASP
2	B	981	ALA
2	B	997	GLU
2	B	1155	SER
3	C	86	CYS
3	C	110	THR
3	C	125	MET
3	C	167	HIS
4	E	67	GLU
4	E	77	SER
4	E	192	ARG
4	E	206	GLY
6	H	83	GLN
6	H	109	LYS
7	I	86	PHE
9	K	7	PHE
10	L	26	THR
10	L	45	ALA
10	L	55	ILE
1	A	56	PRO
1	A	109	HIS
1	A	131	SER
1	A	253	ASN
1	A	333	GLU
1	A	472	LEU
1	A	515	GLN
1	A	597	LEU
1	A	891	ALA
1	A	895	LYS
1	A	958	VAL
1	A	990	VAL
1	A	1157	ASP
1	A	1174	PHE
1	A	1188	GLN
1	A	1221	LYS
1	A	1233	ASP

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Mol	Chain	Res	Type
1	A	1261	LYS
1	A	1424	VAL
2	B	367	LEU
2	B	468	GLU
2	B	471	LYS
2	B	483	LEU
2	B	712	PRO
2	B	815	ARG
2	B	881	ASN
2	B	958	GLN
2	B	1157	ALA
3	C	30	ALA
3	C	227	THR
4	E	17	ARG
4	E	36	GLU
4	E	145	THR
5	F	154	ASP
6	H	62	SER
6	H	128	ASN
7	I	21	GLU
7	I	34	TYR
7	I	47	GLU
7	I	88	SER
10	L	54	ARG
1	A	39	GLU
1	A	87	ALA
1	A	314	ALA
1	A	320	ARG
1	A	418	SER
1	A	423	ASP
1	A	424	ILE
1	A	465	TYR
1	A	517	ASN
1	A	576	GLN
1	A	903	ASN
1	A	969	GLN
2	B	251	ILE
2	B	294	ASP
2	B	484	ASN
2	B	490	SER
2	B	491	THR
2	B	645	SER

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Mol	Chain	Res	Type
2	B	648	HIS
2	B	836	GLU
2	B	974	PRO
2	B	1108	ARG
2	B	1165	ILE
2	B	1222	ARG
3	C	28	ALA
3	C	90	ASP
3	C	164	ALA
3	C	172	PRO
3	C	215	GLU
4	E	115	ASN
5	F	73	ALA
5	F	104	ASN
7	I	3	THR
7	I	60	GLN
7	I	89	GLN
1	A	89	PRO
1	A	136	ALA
1	A	335	ARG
1	A	404	TYR
1	A	810	PRO
1	A	1021	LEU
2	B	552	MET
2	B	960	GLY
2	B	1166	CYS
3	C	87	PHE
3	C	213	PRO
4	E	53	PRO
4	E	124	VAL
8	J	3	VAL
9	K	4	PRO
10	L	59	ALA
1	A	324	SER
1	A	932	GLU
1	A	1107	VAL
2	B	489	SER
2	B	792	MET
2	B	976	ILE
2	B	1156	ASP
3	C	6	PRO
4	E	76	GLY

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Mol	Chain	Res	Type
9	K	39	ASP
1	A	1148	ILE
1	A	1437	GLY
2	B	467	GLY
2	B	1017	ILE
1	A	514	PRO
2	B	410	GLY
3	C	240	VAL
3	C	248	ILE
4	E	51	GLY
6	H	112	ILE
8	J	33	GLY
1	A	957	PRO
6	H	59	ILE
1	A	274	ILE
1	A	1122	PRO
2	B	555	ILE
2	B	877	PRO
1	A	610	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1218/1520 (80%)	941 (77%)	277 (23%)	1	5
2	B	960/1061 (90%)	763 (80%)	197 (20%)	1	8
3	C	234/274 (85%)	182 (78%)	52 (22%)	1	6
4	E	196/197 (100%)	165 (84%)	31 (16%)	2	15
5	F	74/137 (54%)	63 (85%)	11 (15%)	3	16
6	H	117/128 (91%)	92 (79%)	25 (21%)	1	6
7	I	113/116 (97%)	95 (84%)	18 (16%)	2	14
8	J	60/65 (92%)	45 (75%)	15 (25%)	0	4
9	K	99/102 (97%)	83 (84%)	16 (16%)	2	14

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	L	40/57 (70%)	31 (78%)	9 (22%)	1	5
All	All	3111/3657 (85%)	2460 (79%)	651 (21%)	1	7

All (651) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	SER
1	A	12	ARG
1	A	13	THR
1	A	18	GLN
1	A	26	GLU
1	A	32	VAL
1	A	40	THR
1	A	47	ARG
1	A	50	ILE
1	A	53	LEU
1	A	58	LEU
1	A	60	SER
1	A	69	THR
1	A	70	CYS
1	A	80	HIS
1	A	81	PHE
1	A	84	ILE
1	A	93	VAL
1	A	99	ILE
1	A	100	LYS
1	A	101	LYS
1	A	102	VAL
1	A	107	CYS
1	A	108	MET
1	A	110	CYS
1	A	116	ASP
1	A	120	GLU
1	A	126	LEU
1	A	130	ASP
1	A	164	ARG
1	A	169	ASN
1	A	170	THR
1	A	180	LYS
1	A	182	VAL
1	A	184	SER
1	A	185	TRP

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Mol	Chain	Res	Type
1	A	200	ARG
1	A	204	THR
1	A	206	GLU
1	A	208	LEU
1	A	221	SER
1	A	222	LEU
1	A	225	ASN
1	A	227	VAL
1	A	232	GLU
1	A	235	ILE
1	A	250	ILE
1	A	252	PHE
1	A	254	GLU
1	A	255	SER
1	A	256	GLN
1	A	257	ARG
1	A	263	THR
1	A	266	LEU
1	A	269	ILE
1	A	270	LEU
1	A	271	LYS
1	A	278	THR
1	A	282	ASN
1	A	287	HIS
1	A	295	LEU
1	A	297	GLN
1	A	302	THR
1	A	304	MET
1	A	306	ASN
1	A	307	ASP
1	A	308	ILE
1	A	313	GLN
1	A	315	LEU
1	A	316	GLN
1	A	317	LYS
1	A	320	ARG
1	A	323	LYS
1	A	330	LYS
1	A	336	ILE
1	A	337	ARG
1	A	344	ARG
1	A	370	ILE

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Mol	Chain	Res	Type
1	A	373	THR
1	A	381	THR
1	A	385	ILE
1	A	403	LYS
1	A	405	VAL
1	A	419	LYS
1	A	424	ILE
1	A	442	VAL
1	A	443	LEU
1	A	445	ASN
1	A	446	ARG
1	A	450	LEU
1	A	452	LYS
1	A	453	MET
1	A	456	MET
1	A	460	VAL
1	A	463	ILE
1	A	466	SER
1	A	469	ARG
1	A	470	LEU
1	A	471	ASN
1	A	475	THR
1	A	481	ASP
1	A	485	ASP
1	A	486	GLU
1	A	494	SER
1	A	496	GLU
1	A	507	VAL
1	A	509	LEU
1	A	513	SER
1	A	521	MET
1	A	524	VAL
1	A	527	THR
1	A	529	CYS
1	A	535	THR
1	A	545	GLN
1	A	550	LEU
1	A	553	VAL
1	A	562	THR
1	A	566	ILE
1	A	572	TRP
1	A	577	ILE

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Mol	Chain	Res	Type
1	A	589	GLN
1	A	590	ARG
1	A	612	ILE
1	A	618	GLU
1	A	621	THR
1	A	625	SER
1	A	629	LEU
1	A	630	ILE
1	A	634	THR
1	A	635	ARG
1	A	641	VAL
1	A	658	LEU
1	A	663	SER
1	A	666	ILE
1	A	670	ILE
1	A	672	ASP
1	A	675	THR
1	A	680	THR
1	A	682	THR
1	A	687	LYS
1	A	688	LYS
1	A	702	LEU
1	A	710	LEU
1	A	732	LEU
1	A	740	LEU
1	A	741	ASN
1	A	752	LYS
1	A	760	GLN
1	A	764	CYS
1	A	769	SER
1	A	771	GLU
1	A	775	ILE
1	A	783	THR
1	A	788	SER
1	A	797	LYS
1	A	801	GLU
1	A	803	SER
1	A	826	ASP
1	A	829	VAL
1	A	840	ARG
1	A	843	LYS
1	A	845	LEU

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Mol	Chain	Res	Type
1	A	848	ILE
1	A	854	ASN
1	A	855	THR
1	A	858	ASN
1	A	864	ILE
1	A	867	ILE
1	A	879	GLU
1	A	880	LYS
1	A	885	THR
1	A	886	ILE
1	A	889	SER
1	A	895	LYS
1	A	896	ARG
1	A	902	LEU
1	A	905	ASP
1	A	911	SER
1	A	918	GLU
1	A	924	LYS
1	A	927	VAL
1	A	929	LEU
1	A	938	LYS
1	A	949	ASP
1	A	960	ILE
1	A	969	GLN
1	A	973	ILE
1	A	982	THR
1	A	990	VAL
1	A	996	ASN
1	A	1000	LEU
1	A	1006	ILE
1	A	1017	LEU
1	A	1022	LEU
1	A	1025	ARG
1	A	1029	ARG
1	A	1033	GLN
1	A	1046	LEU
1	A	1048	ASN
1	A	1050	GLU
1	A	1052	GLN
1	A	1057	VAL
1	A	1058	VAL
1	A	1064	VAL

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Mol	Chain	Res	Type
1	A	1067	LEU
1	A	1093	LYS
1	A	1094	VAL
1	A	1095	THR
1	A	1104	ILE
1	A	1109	LYS
1	A	1111	MET
1	A	1112	LYS
1	A	1115	SER
1	A	1118	VAL
1	A	1120	LEU
1	A	1128	GLN
1	A	1134	ILE
1	A	1135	ARG
1	A	1145	SER
1	A	1147	THR
1	A	1159	ARG
1	A	1160	SER
1	A	1161	THR
1	A	1165	GLU
1	A	1167	GLU
1	A	1171	GLN
1	A	1172	LEU
1	A	1173	HIS
1	A	1174	PHE
1	A	1187	GLN
1	A	1219	THR
1	A	1221	LYS
1	A	1222	ASN
1	A	1230	GLU
1	A	1235	LYS
1	A	1240	CYS
1	A	1262	LYS
1	A	1264	GLU
1	A	1271	ILE
1	A	1273	LEU
1	A	1276	VAL
1	A	1279	ILE
1	A	1280	GLU
1	A	1281	ARG
1	A	1285	MET
1	A	1288	ASP

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Mol	Chain	Res	Type
1	A	1291	VAL
1	A	1299	VAL
1	A	1322	ILE
1	A	1325	THR
1	A	1329	THR
1	A	1333	ILE
1	A	1350	LYS
1	A	1351	GLU
1	A	1354	ASN
1	A	1355	VAL
1	A	1359	ASP
1	A	1364	ASN
1	A	1366	ARG
1	A	1372	VAL
1	A	1376	THR
1	A	1384	VAL
1	A	1385	THR
1	A	1391	ARG
1	A	1393	ASN
1	A	1394	THR
1	A	1398	MET
1	A	1400	CYS
1	A	1403	GLU
1	A	1404	GLU
1	A	1405	THR
1	A	1406	VAL
1	A	1407	GLU
1	A	1424	VAL
1	A	1425	SER
1	A	1428	VAL
1	A	1445	ILE
2	B	28	GLU
2	B	34	ILE
2	B	40	GLU
2	B	44	VAL
2	B	45	SER
2	B	46	GLN
2	B	57	TYR
2	B	63	ILE
2	B	66	ASP
2	B	67	SER
2	B	94	LYS

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Mol	Chain	Res	Type
2	B	97	VAL
2	B	98	THR
2	B	104	GLU
2	B	108	VAL
2	B	109	THR
2	B	112	LEU
2	B	119	LEU
2	B	128	LEU
2	B	130	VAL
2	B	134	LYS
2	B	170	LEU
2	B	178	ASN
2	B	187	SER
2	B	188	ASP
2	B	191	LYS
2	B	194	GLU
2	B	199	MET
2	B	222	ILE
2	B	225	VAL
2	B	232	SER
2	B	237	VAL
2	B	244	LEU
2	B	246	LYS
2	B	249	ARG
2	B	261	ARG
2	B	264	SER
2	B	267	ARG
2	B	268	THR
2	B	277	LYS
2	B	282	ILE
2	B	283	VAL
2	B	284	ILE
2	B	304	ASP
2	B	305	VAL
2	B	313	MET
2	B	315	LYS
2	B	319	GLU
2	B	323	VAL
2	B	324	ILE
2	B	328	GLU
2	B	347	LYS
2	B	354	ASP

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Mol	Chain	Res	Type
2	B	360	PHE
2	B	366	GLN
2	B	384	ARG
2	B	387	LEU
2	B	391	ASP
2	B	393	LYS
2	B	396	ASP
2	B	398	ARG
2	B	399	ASP
2	B	404	LYS
2	B	415	GLN
2	B	416	LEU
2	B	424	LEU
2	B	425	THR
2	B	427	ASP
2	B	429	PHE
2	B	432	MET
2	B	451	LYS
2	B	463	THR
2	B	479	VAL
2	B	482	VAL
2	B	483	LEU
2	B	487	THR
2	B	490	SER
2	B	527	THR
2	B	537	LYS
2	B	542	MET
2	B	545	ILE
2	B	552	MET
2	B	563	MET
2	B	567	GLU
2	B	570	VAL
2	B	582	VAL
2	B	591	ARG
2	B	600	LEU
2	B	601	ARG
2	B	604	ARG
2	B	612	GLU
2	B	618	ASP
2	B	626	ILE
2	B	637	LEU
2	B	641	GLU

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Mol	Chain	Res	Type
2	B	645	SER
2	B	653	VAL
2	B	664	THR
2	B	667	GLN
2	B	668	ASP
2	B	680	THR
2	B	682	SER
2	B	694	ASP
2	B	701	ILE
2	B	705	MET
2	B	710	LEU
2	B	729	ILE
2	B	731	VAL
2	B	737	THR
2	B	742	GLU
2	B	748	ILE
2	B	751	VAL
2	B	762	ASN
2	B	764	SER
2	B	790	ASP
2	B	791	THR
2	B	792	MET
2	B	794	ASN
2	B	805	THR
2	B	807	ARG
2	B	815	ARG
2	B	825	VAL
2	B	831	SER
2	B	835	GLN
2	B	843	GLN
2	B	847	ASP
2	B	848	ARG
2	B	857	ARG
2	B	864	LYS
2	B	868	MET
2	B	870	ILE
2	B	873	THR
2	B	879	ARG
2	B	880	THR
2	B	882	THR
2	B	883	LEU
2	B	886	LYS

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Mol	Chain	Res	Type
2	B	894	ASP
2	B	899	ILE
2	B	905	VAL
2	B	911	ILE
2	B	936	ASP
2	B	939	THR
2	B	943	SER
2	B	944	THR
2	B	945	GLU
2	B	948	ILE
2	B	956	THR
2	B	959	ASP
2	B	970	THR
2	B	971	THR
2	B	973	ILE
2	B	975	GLN
2	B	979	LYS
2	B	989	THR
2	B	992	ILE
2	B	997	GLU
2	B	998	ASP
2	B	999	MET
2	B	1002	THR
2	B	1007	VAL
2	B	1019	SER
2	B	1020	ARG
2	B	1022	THR
2	B	1028	GLU
2	B	1034	VAL
2	B	1050	ILE
2	B	1051	THR
2	B	1060	ARG
2	B	1061	GLU
2	B	1062	HIS
2	B	1072	MET
2	B	1082	MET
2	B	1090	THR
2	B	1092	TYR
2	B	1093	GLN
2	B	1096	ARG
2	B	1099	VAL
2	B	1104	HIS

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Mol	Chain	Res	Type
2	B	1113	VAL
2	B	1115	THR
2	B	1124	ARG
2	B	1132	GLU
2	B	1138	MET
2	B	1141	HIS
2	B	1147	LEU
2	B	1153	GLU
2	B	1156	ASP
2	B	1159	ARG
2	B	1165	ILE
2	B	1189	ILE
2	B	1191	ILE
2	B	1194	ILE
2	B	1196	ILE
2	B	1202	LEU
2	B	1221	SER
2	B	1223	ASP
3	C	4	GLU
3	C	6	PRO
3	C	10	ILE
3	C	11	ARG
3	C	15	LYS
3	C	18	VAL
3	C	25	VAL
3	C	26	ASP
3	C	27	LEU
3	C	34	ARG
3	C	36	VAL
3	C	38	ILE
3	C	41	ILE
3	C	43	THR
3	C	49	VAL
3	C	54	ASN
3	C	55	THR
3	C	56	THR
3	C	63	ILE
3	C	77	ILE
3	C	83	SER
3	C	93	ASP
3	C	97	VAL
3	C	99	LEU

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Mol	Chain	Res	Type
3	C	102	GLN
3	C	115	SER
3	C	116	LYS
3	C	119	VAL
3	C	120	ILE
3	C	129	ILE
3	C	133	ILE
3	C	138	GLU
3	C	140	ASN
3	C	142	VAL
3	C	143	LEU
3	C	145	CYS
3	C	151	GLN
3	C	154	LYS
3	C	156	THR
3	C	163	ILE
3	C	166	GLU
3	C	195	GLN
3	C	196	ASP
3	C	199	LYS
3	C	215	GLU
3	C	232	VAL
3	C	235	VAL
3	C	240	VAL
3	C	244	VAL
3	C	250	THR
3	C	254	LYS
3	C	267	GLN
4	E	9	ILE
4	E	32	GLN
4	E	33	GLU
4	E	43	LYS
4	E	48	ASP
4	E	61	GLN
4	E	65	THR
4	E	66	GLU
4	E	72	PHE
4	E	77	SER
4	E	80	VAL
4	E	83	CYS
4	E	92	THR
4	E	101	GLN

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Mol	Chain	Res	Type
4	E	104	ASN
4	E	107	THR
4	E	127	ILE
4	E	131	THR
4	E	150	VAL
4	E	152	LYS
4	E	156	LEU
4	E	158	SER
4	E	159	ASP
4	E	162	ARG
4	E	165	LEU
4	E	169	ARG
4	E	196	VAL
4	E	203	GLU
4	E	207	ARG
4	E	212	ARG
4	E	213	ILE
5	F	74	ILE
5	F	77	ASP
5	F	79	ARG
5	F	81	THR
5	F	97	ARG
5	F	107	VAL
5	F	111	LEU
5	F	112	GLU
5	F	120	ILE
5	F	123	LYS
5	F	148	VAL
6	H	2	SER
6	H	11	GLN
6	H	23	VAL
6	H	24	CYS
6	H	27	GLU
6	H	33	GLN
6	H	35	GLN
6	H	37	LYS
6	H	39	THR
6	H	55	LEU
6	H	56	THR
6	H	89	LEU
6	H	94	ASP
6	H	102	TYR

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Mol	Chain	Res	Type
6	H	103	LYS
6	H	104	PHE
6	H	106	GLU
6	H	108	SER
6	H	109	LYS
6	H	111	LEU
6	H	112	ILE
6	H	121	LEU
6	H	132	LEU
6	H	136	LYS
6	H	142	LEU
7	I	12	ASN
7	I	13	MET
7	I	15	TYR
7	I	21	GLU
7	I	28	GLU
7	I	30	ARG
7	I	31	THR
7	I	50	THR
7	I	52	ILE
7	I	62	ILE
7	I	75	CYS
7	I	78	CYS
7	I	83	ASN
7	I	95	THR
7	I	97	MET
7	I	104	LEU
7	I	118	ARG
7	I	119	THR
8	J	7	CYS
8	J	9	SER
8	J	13	VAL
8	J	27	GLU
8	J	28	ASP
8	J	31	ASP
8	J	32	GLU
8	J	34	THR
8	J	43	ARG
8	J	48	ARG
8	J	50	ILE
8	J	51	LEU
8	J	56	LEU

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Mol	Chain	Res	Type
8	J	59	LYS
8	J	64	ASN
9	K	18	LYS
9	K	20	LYS
9	K	31	VAL
9	K	33	ILE
9	K	34	THR
9	K	45	LEU
9	K	47	ARG
9	K	50	LEU
9	K	51	LEU
9	K	75	ILE
9	K	78	THR
9	K	101	LEU
9	K	102	LYS
9	K	107	THR
9	K	113	THR
9	K	114	LEU
10	L	31	CYS
10	L	46	VAL
10	L	51	CYS
10	L	55	ILE
10	L	61	THR
10	L	63	ARG
10	L	66	GLN
10	L	68	GLU
10	L	70	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (95) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	GLN
1	A	64	ASN
1	A	71	GLN
1	A	83	HIS
1	A	171	GLN
1	A	253	ASN
1	A	313	GLN
1	A	316	GLN
1	A	435	HIS
1	A	439	ASN
1	A	451	HIS

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Mol	Chain	Res	Type
1	A	503	GLN
1	A	515	GLN
1	A	517	ASN
1	A	525	GLN
1	A	545	GLN
1	A	576	GLN
1	A	654	ASN
1	A	700	ASN
1	A	736	ASN
1	A	741	ASN
1	A	742	ASN
1	A	745	GLN
1	A	757	ASN
1	A	760	GLN
1	A	851	HIS
1	A	854	ASN
1	A	858	ASN
1	A	862	ASN
1	A	877	HIS
1	A	926	GLN
1	A	965	GLN
1	A	968	GLN
1	A	996	ASN
1	A	1008	GLN
1	A	1011	GLN
1	A	1140	HIS
1	A	1222	ASN
1	A	1278	ASN
1	A	1312	ASN
1	A	1364	ASN
1	A	1393	ASN
1	A	1432	GLN
2	B	47	GLN
2	B	121	ASN
2	B	236	HIS
2	B	255	GLN
2	B	300	HIS
2	B	350	GLN
2	B	366	GLN
2	B	433	GLN
2	B	465	ASN
2	B	484	ASN

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Mol	Chain	Res	Type
2	B	515	HIS
2	B	516	ASN
2	B	518	HIS
2	B	538	ASN
2	B	572	HIS
2	B	657	HIS
2	B	706	GLN
2	B	734	HIS
2	B	744	HIS
2	B	822	ASN
2	B	842	ASN
2	B	843	GLN
2	B	957	ASN
2	B	975	GLN
2	B	984	HIS
2	B	1015	HIS
2	B	1065	GLN
2	B	1093	GLN
2	B	1097	HIS
3	C	31	ASN
3	C	73	GLN
3	C	123	ASN
3	C	167	HIS
3	C	203	GLN
4	E	32	GLN
4	E	99	HIS
4	E	115	ASN
4	E	147	HIS
4	E	174	GLN
6	H	11	GLN
6	H	33	GLN
6	H	131	ASN
6	H	134	ASN
7	I	22	ASN
7	I	60	GLN
7	I	83	ASN
7	I	116	ASN
7	I	120	GLN
8	J	53	HIS
9	K	40	HIS
9	K	65	HIS
9	K	110	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
11	R	12/24 (50%)	5 (41%)	0

All (5) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
11	R	4	G
11	R	10	A
11	R	11	U
11	R	12	G
11	R	13	C

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	1395/1733 (80%)	0.06	14 (1%) 79 59	80, 126, 198, 230	0
2	B	1106/1224 (90%)	0.10	16 (1%) 73 52	79, 120, 169, 188	0
3	C	266/318 (83%)	-0.11	3 (1%) 78 57	89, 116, 158, 167	0
4	E	214/215 (99%)	0.00	3 (1%) 73 52	113, 165, 202, 206	0
5	F	84/155 (54%)	-0.21	0 100 100	110, 133, 152, 159	0
6	H	133/146 (91%)	0.17	3 (2%) 61 43	137, 155, 178, 180	0
7	I	119/122 (97%)	0.04	2 (1%) 69 48	126, 147, 167, 181	0
8	J	65/70 (92%)	-0.07	0 100 100	86, 105, 134, 141	0
9	K	114/120 (95%)	-0.23	0 100 100	96, 118, 135, 139	0
10	L	46/70 (65%)	0.36	2 (4%) 40 30	118, 175, 189, 193	0
11	R	13/24 (54%)	0.26	1 (7%) 19 18	97, 128, 191, 203	0
12	T	28/28 (100%)	0.35	0 100 100	111, 219, 343, 346	0
13	N	14/14 (100%)	0.87	1 (7%) 22 20	308, 330, 332, 333	0
All	All	3597/4239 (84%)	0.05	45 (1%) 75 54	79, 127, 194, 346	0

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	820	GLY	5.7
11	R	13	C	5.1
2	B	335	GLY	4.3
7	I	13	MET	3.4
2	B	243	ALA	3.3
1	A	1330	ASN	3.1
13	N	1	DC	3.0
1	A	1332	PHE	2.9
2	B	821	GLN	2.9

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Mol	Chain	Res	Type	RSRZ
4	E	125	PRO	2.8
1	A	103	CYS	2.8
3	C	175	ALA	2.8
2	B	611	PRO	2.7
6	H	63	LEU	2.7
4	E	126	SER	2.6
3	C	174	ALA	2.6
2	B	446	LEU	2.5
2	B	779	GLY	2.5
1	A	816	HIS	2.5
2	B	313	MET	2.5
6	H	136	LYS	2.5
2	B	829	CYS	2.5
2	B	883	LEU	2.5
2	B	710	LEU	2.4
6	H	90	ALA	2.4
1	A	1010	ALA	2.4
10	L	43	THR	2.4
2	B	870	ILE	2.4
3	C	173	ALA	2.4
1	A	614	PHE	2.3
1	A	1108	ALA	2.3
10	L	27	LEU	2.3
1	A	997	LEU	2.3
7	I	4	PHE	2.3
1	A	1174	PHE	2.2
2	B	529	GLU	2.1
4	E	149	LEU	2.1
2	B	882	THR	2.1
1	A	1434	ALA	2.0
2	B	869	SER	2.0
2	B	305	VAL	2.0
2	B	715	ALA	2.0
1	A	3	GLY	2.0
1	A	208	LEU	2.0
1	A	1162	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
15	MG	A	1736	1/1	0.95	0.09	97,97,97,97	0
14	ZN	A	1734	1/1	0.96	0.05	181,181,181,181	0
14	ZN	I	204	1/1	0.97	0.04	148,148,148,148	0
14	ZN	A	1735	1/1	0.97	0.04	177,177,177,177	0
14	ZN	B	1307	1/1	0.98	0.03	156,156,156,156	0
14	ZN	L	105	1/1	0.99	0.03	183,183,183,183	0
14	ZN	I	203	1/1	0.99	0.02	139,139,139,139	0
14	ZN	C	319	1/1	1.00	0.01	107,107,107,107	0
14	ZN	J	101	1/1	1.00	0.04	109,109,109,109	0

6.5 Other polymers [i](#)

There are no such residues in this entry.