



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 11:26 PM UTC

PDB ID : 3GTG / pdb_00003gtg
Title : Backtracked RNA polymerase II complex with 12mer RNA
Authors : Wang, D.; Bushnell, D.A.; Huang, X.; Westover, K.D.; Levitt, M.; Kornberg, R.D.
Deposited on : 2009-03-27
Resolution : 3.78 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

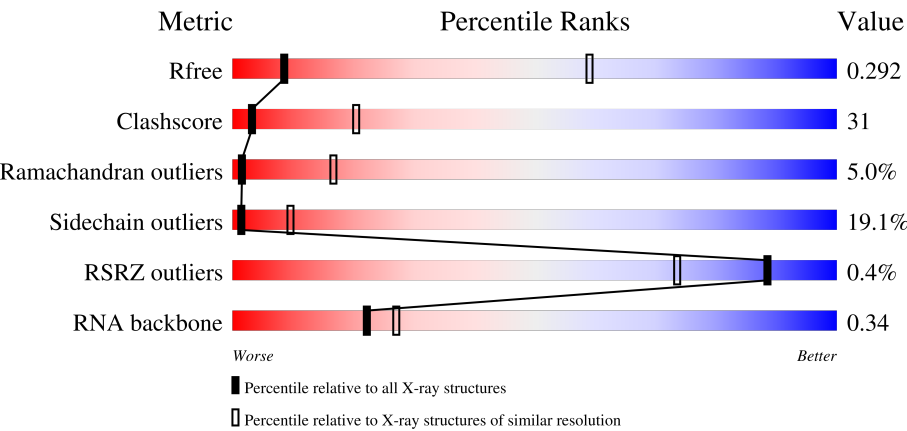
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.78 Å.

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



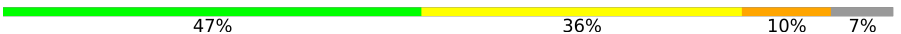
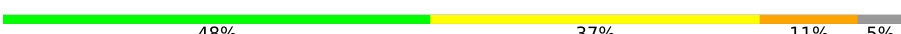
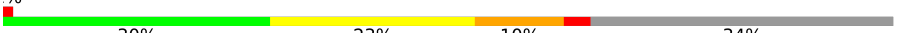
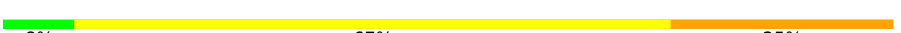
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	1085 (3.94-3.62)
Clashscore	190562	1029 (3.92-3.64)
Ramachandran outliers	187476	1064 (3.94-3.62)
Sidechain outliers	187428	1059 (3.94-3.62)
RSRZ outliers	180081	1084 (3.94-3.62)
RNA backbone	3983	1002 (4.46-3.10)

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

Mol	Chain	Length	Quality of chain
1	A	1733	35%36%10%•17%
2	B	1224	% 38%41%13%•6%
3	C	318	35%35%14%•15%
4	E	215	61%33%5%

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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	12	
12	T	29	
13	N	14	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	ZN	A	1734	-	-	X	-
14	ZN	B	1307	-	-	X	-
14	ZN	J	101	-	-	X	-

2 Entry composition [i](#)

There are 16 unique types of molecules in this entry. The entry contains 30067 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	1442	Total	C	N	O	S	0	0	0
			11332	7133	1982	2156	61			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	1153	Total	C	N	O	S	0	0	0
			9167	5794	1604	1713	56			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	271	Total	C	N	O	S	0	0	0
			2135	1344	355	423	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	215	Total	C	N	O	S	0	0	0
			1757	1114	310	322	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	85	Total	C	N	O	S	0	0	0
			684	437	116	128	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	136	Total	C	N	O	S	0	0	0
			1087	684	183	215	5			

- 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*G)-3').

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

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

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

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

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

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

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

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

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

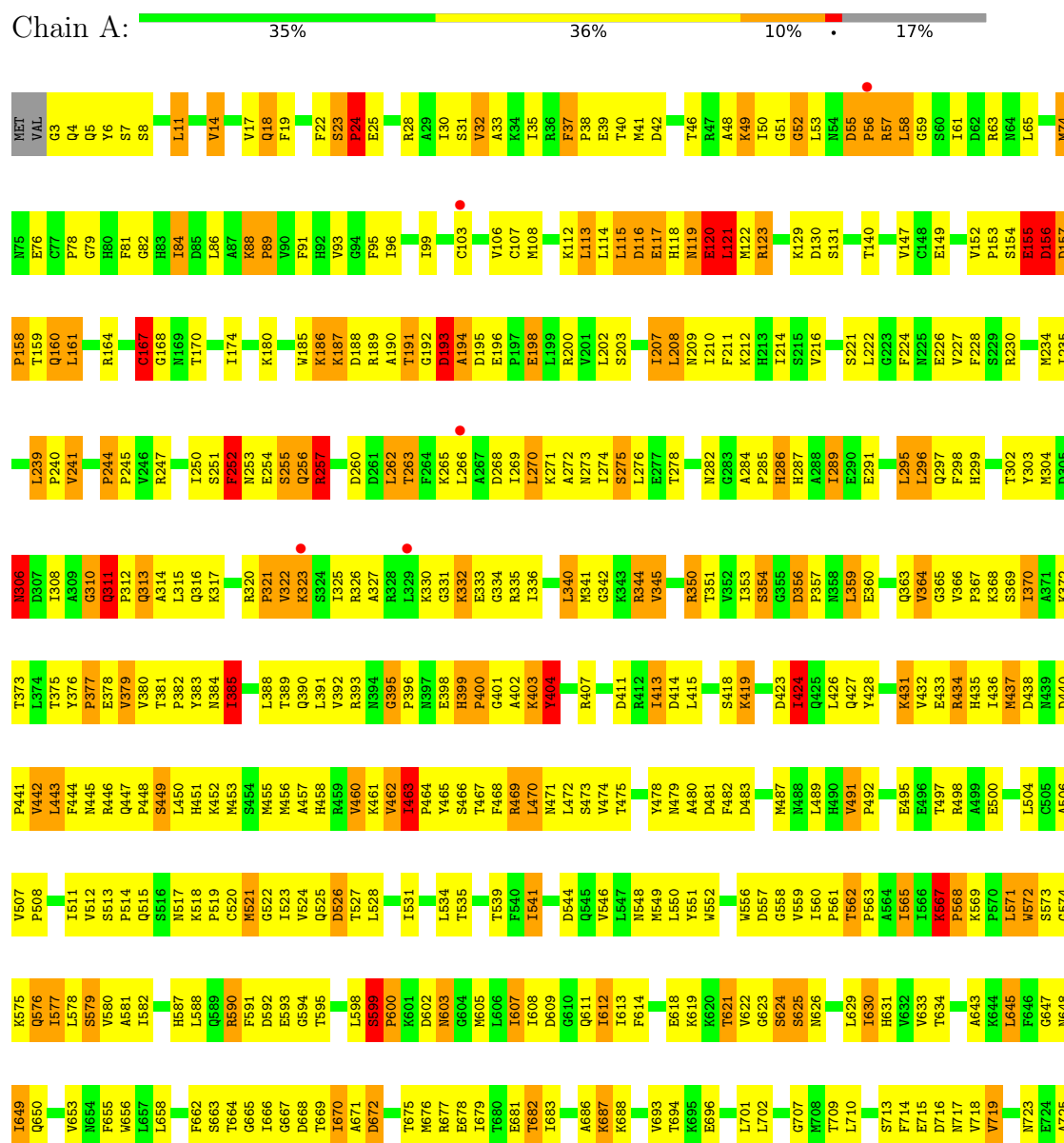
- Molecule 16 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	R	1	Total 1	O 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.

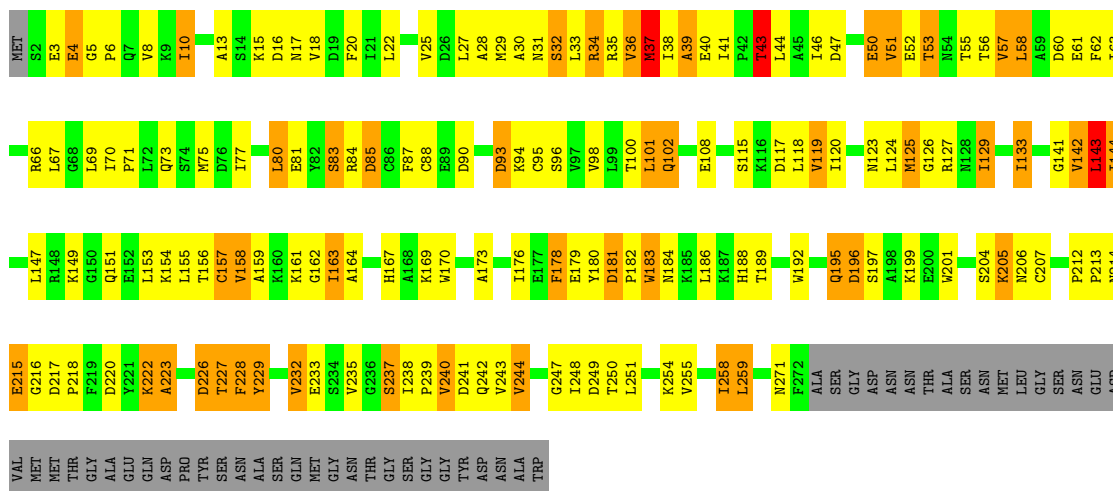
- Molecule 1: DNA-directed RNA polymerase II subunit RPB1



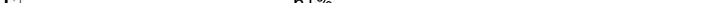


- Molecule 3: DNA-directed RNA polymerase II subunit RPB3

Chain C: 35% 35% 14% 15%

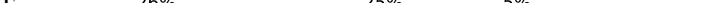


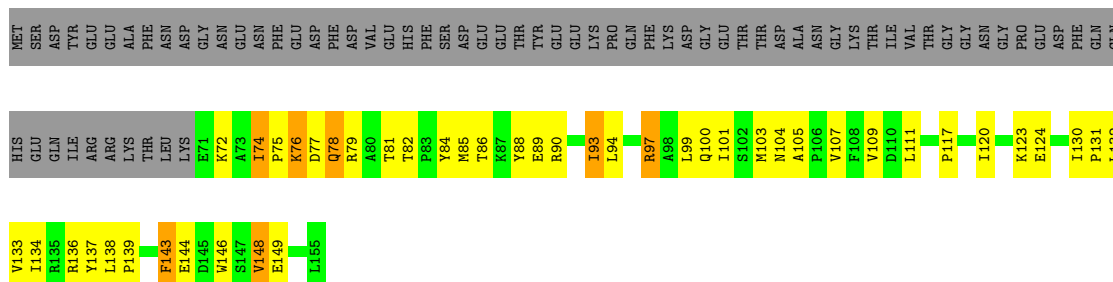
- Molecule 4: DNA-directed RNA polymerases I, II, and III subunit RPABC1

Chain E:  61% 33% 5%

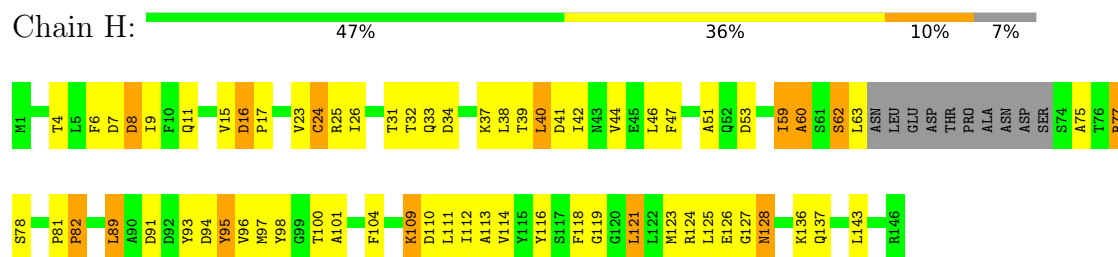


- Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC2

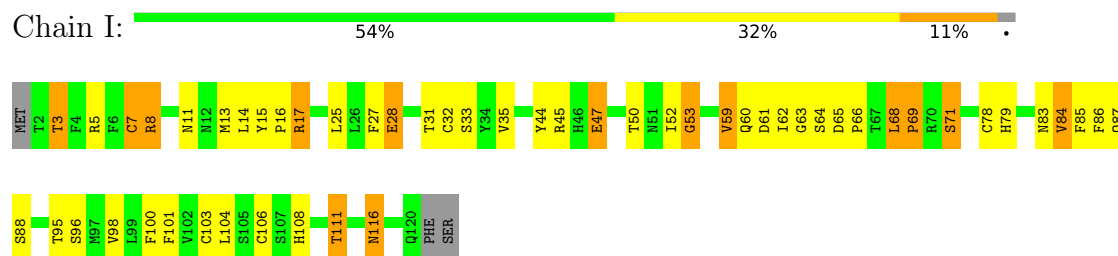
Chain F:  26% 25% 5% 45%



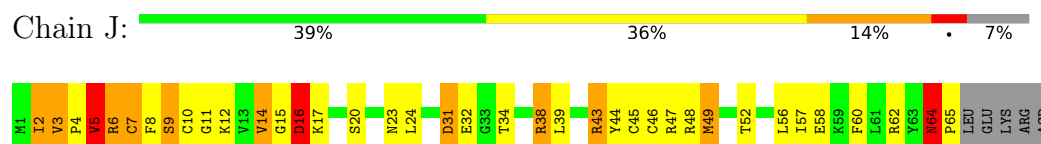
- Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC3



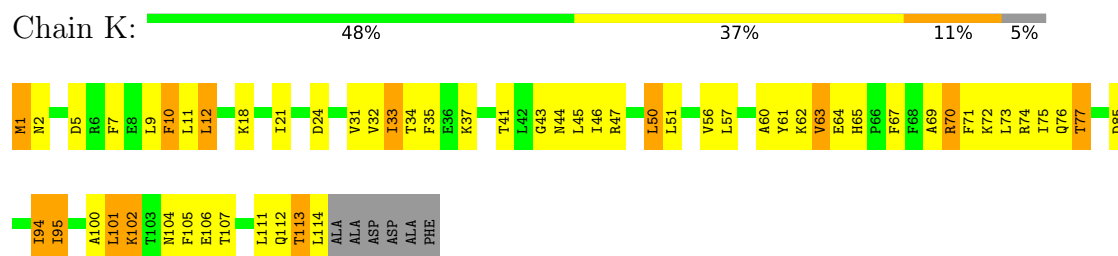
- Molecule 7: DNA-directed RNA polymerase II subunit RPB9



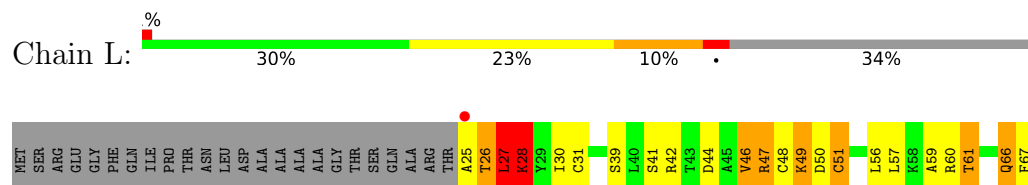
- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC5



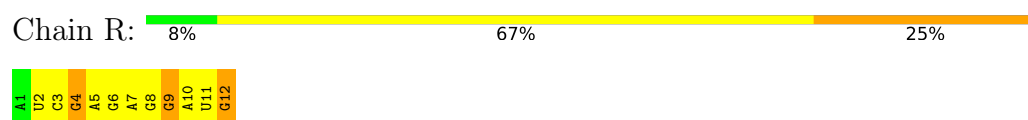
- Molecule 9: DNA-directed RNA polymerase II subunit RPB11



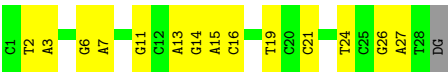
- Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC4



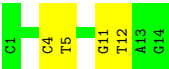
- Molecule 11: RNA (5'-R(*AP*UP*CP*GP*AP*GP*AP*GP*GP*AP*UP*G)-3')



● 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	170.96Å 223.00Å 195.41Å 90.00° 102.28° 90.00°	Depositor
Resolution (Å)	50.00 – 3.78 50.00 – 3.78	Depositor EDS
% Data completeness (in resolution range)	95.4 (50.00-3.78) 95.4 (50.00-3.78)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.47 (at 3.76Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.253 , 0.300 0.254 , 0.292	Depositor DCC
R_{free} test set	3441 reflections (4.83%)	wwPDB-VP
Wilson B-factor (Å ²)	108.9	Xtriage
Anisotropy	0.100	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 110.5	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	0.91	EDS
Total number of atoms	30067	wwPDB-VP
Average B, all atoms (Å ²)	143.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.53% 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	0.67	1/11536 (0.0%)	1.12	72/15605 (0.5%)
2	B	0.74	0/9347	1.11	47/12609 (0.4%)
3	C	0.76	1/2174 (0.0%)	1.09	5/2946 (0.2%)
4	E	0.60	0/1793	0.93	1/2413 (0.0%)
5	F	0.64	0/696	1.03	5/940 (0.5%)
6	H	0.68	0/1105	1.06	6/1495 (0.4%)
7	I	0.66	0/989	1.07	7/1331 (0.5%)
8	J	0.77	0/541	1.25	8/727 (1.1%)
9	K	0.73	1/937 (0.1%)	1.04	2/1265 (0.2%)
10	L	0.71	0/365	1.14	5/485 (1.0%)
11	R	0.76	0/292	1.13	1/455 (0.2%)
12	T	0.41	0/634	1.01	0/975
13	N	0.35	0/317	0.89	0/488
All	All	0.69	3/30726 (0.0%)	1.09	159/41734 (0.4%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	718	VAL	CA-CB	5.65	1.60	1.54
9	K	10	PHE	CA-C	5.23	1.58	1.52
3	C	43	THR	CA-CB	5.11	1.61	1.53

All (159) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	885	THR	N-CA-C	16.15	132.25	112.54
2	B	974	PRO	N-CA-C	-14.72	88.18	111.14
1	A	718	VAL	N-CA-C	13.23	122.85	110.42
2	B	296	GLU	N-CA-C	-11.61	99.64	114.04
6	H	59	ILE	CB-CA-C	-11.40	92.45	110.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	H	60	ALA	N-CA-C	-10.69	90.52	107.73
1	A	885	THR	N-CA-CB	-10.64	92.73	110.39
3	C	37	MET	N-CA-C	10.58	122.50	110.97
1	A	1204	ASP	N-CA-C	9.67	121.77	111.03
1	A	474	VAL	N-CA-C	-9.61	103.36	111.91
1	A	167	CYS	N-CA-C	-9.38	96.01	110.17
1	A	306	ASN	N-CA-C	9.35	127.40	107.67
2	B	974	PRO	CB-CA-C	9.11	123.22	111.46
1	A	88	LYS	CA-C-N	8.87	130.93	119.84
1	A	88	LYS	C-N-CA	8.87	130.93	119.84
2	B	798	TYR	CA-C-N	8.82	129.36	119.83
2	B	798	TYR	C-N-CA	8.82	129.36	119.83
2	B	1017	ILE	N-CA-CB	8.74	123.45	111.21
8	J	9	SER	N-CA-C	8.65	120.79	111.36
1	A	1176	LEU	N-CA-C	8.59	129.10	110.80
1	A	463	ILE	CA-C-N	8.54	128.58	119.78
1	A	463	ILE	C-N-CA	8.54	128.58	119.78
2	B	981	ALA	N-CA-C	8.37	128.62	110.80
2	B	763	GLN	N-CA-C	-8.36	97.41	109.96
2	B	976	ILE	N-CA-C	8.35	126.71	109.34
3	C	37	MET	CB-CA-C	-8.22	98.30	110.96
1	A	1080	THR	CB-CA-C	8.16	123.69	110.88
1	A	317	LYS	N-CA-C	-7.93	101.50	112.12
2	B	1064	TYR	N-CA-C	7.91	120.93	109.14
2	B	763	GLN	CB-CA-C	7.76	122.31	109.89
2	B	975	GLN	N-CA-C	-7.71	94.38	110.80
7	I	68	LEU	CA-C-N	7.71	129.47	119.84
7	I	68	LEU	C-N-CA	7.71	129.47	119.84
1	A	1015	VAL	CB-CA-C	-7.69	101.66	111.20
1	A	331	GLY	N-CA-C	7.65	120.74	112.33
2	B	856	PHE	N-CA-C	-7.60	97.56	109.72
1	A	793	SER	CA-C-N	7.48	129.19	119.84
1	A	793	SER	C-N-CA	7.48	129.19	119.84
7	I	53	GLY	N-CA-C	-7.39	105.06	114.37
1	A	624	SER	N-CA-C	-7.38	95.08	110.80
2	B	1021	MET	N-CA-C	7.30	121.92	113.38
4	E	49	SER	N-CA-C	7.30	123.44	113.37
8	J	31	ASP	CB-CA-C	7.29	121.83	109.50
1	A	491	VAL	CA-C-N	7.26	127.70	119.93
1	A	491	VAL	C-N-CA	7.26	127.70	119.93
9	K	9	LEU	N-CA-C	-7.17	105.14	114.04
1	A	1205	LYS	N-CA-C	-7.11	98.46	109.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	75	PRO	N-CA-C	7.08	124.81	113.12
1	A	1171	GLN	N-CA-C	-7.05	105.87	114.75
2	B	230	ALA	N-CA-C	6.96	125.20	109.81
10	L	28	LYS	N-CA-CB	-6.96	98.73	110.49
2	B	70	ILE	N-CA-C	6.94	123.78	109.34
2	B	1211	ASN	N-CA-C	6.86	125.41	110.80
3	C	39	ALA	N-CA-C	6.82	120.40	109.83
8	J	5	VAL	CB-CA-C	-6.80	101.55	111.68
1	A	919	ILE	N-CA-C	-6.79	106.42	112.12
1	A	954	TRP	CA-C-N	6.73	128.26	119.84
1	A	954	TRP	C-N-CA	6.73	128.26	119.84
1	A	1204	ASP	CB-CA-C	-6.68	100.59	110.95
2	B	638	PHE	N-CA-C	6.64	120.10	110.28
6	H	8	ASP	N-CA-C	6.62	116.79	108.45
1	A	857	ARG	N-CA-C	6.59	118.97	109.14
2	B	1094	ARG	N-CA-C	-6.57	97.57	108.34
1	A	161	LEU	N-CA-C	6.51	118.52	109.15
2	B	616	ILE	N-CA-C	6.48	116.05	106.85
5	F	138	LEU	CA-C-N	6.48	127.94	119.84
5	F	138	LEU	C-N-CA	6.48	127.94	119.84
1	A	1263	ILE	N-CA-C	6.47	118.44	111.58
2	B	1057	LYS	N-CA-C	-6.46	104.44	112.90
1	A	593	GLU	N-CA-C	6.38	124.38	110.80
2	B	64	CYS	N-CA-C	6.36	121.09	107.67
2	B	895	ASP	N-CA-C	6.33	120.74	112.89
1	A	582	ILE	CA-C-N	6.24	127.09	120.11
1	A	582	ILE	C-N-CA	6.24	127.09	120.11
9	K	9	LEU	CB-CA-C	6.22	120.22	109.15
2	B	645	SER	N-CA-C	6.21	124.04	110.80
10	L	27	LEU	CB-CA-C	-6.20	98.09	110.42
1	A	977	LYS	CA-C-N	6.18	126.54	119.92
1	A	977	LYS	C-N-CA	6.18	126.54	119.92
1	A	683	ILE	N-CA-C	-6.17	106.70	113.43
6	H	128	ASN	N-CA-C	6.17	121.66	114.62
3	C	271	ASN	N-CA-C	6.11	120.51	111.04
1	A	317	LYS	CB-CA-C	6.09	121.36	111.26
7	I	15	TYR	CA-C-N	6.07	126.08	119.89
7	I	15	TYR	C-N-CA	6.07	126.08	119.89
1	A	506	ALA	CA-C-N	6.06	124.06	120.24
1	A	506	ALA	C-N-CA	6.06	124.06	120.24
2	B	1048	THR	CB-CA-C	-6.05	100.07	110.95
1	A	24	PRO	CB-CA-C	6.04	121.53	111.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	500	THR	CA-C-N	-6.02	114.07	120.03
2	B	500	THR	C-N-CA	-6.02	114.07	120.03
1	A	306	ASN	CB-CA-C	-5.99	103.26	111.95
2	B	831	SER	N-CA-C	-5.94	98.14	110.80
1	A	625	SER	N-CA-C	-5.89	98.25	110.80
1	A	830	LYS	N-CA-C	-5.83	105.94	114.39
1	A	168	GLY	N-CA-C	5.80	126.93	113.18
7	I	71	SER	N-CA-C	5.80	118.04	109.69
1	A	590	ARG	N-CA-C	5.78	123.10	110.80
5	F	76	LYS	N-CA-CB	5.76	120.22	110.49
1	A	567	LYS	CA-C-N	5.72	127.00	119.84
1	A	567	LYS	C-N-CA	5.72	127.00	119.84
1	A	884	ASP	CB-CA-C	5.72	121.80	110.42
2	B	938	SER	N-CA-C	5.71	117.67	110.24
1	A	257	ARG	CB-CA-C	-5.69	99.10	110.42
1	A	526	ASP	CB-CA-C	-5.66	101.44	110.84
2	B	444	MET	N-CA-C	5.64	117.82	108.13
2	B	580	VAL	N-CA-C	5.62	116.09	107.77
1	A	599	SER	CA-C-N	5.62	126.87	119.84
1	A	599	SER	C-N-CA	5.62	126.87	119.84
6	H	77	ARG	N-CA-C	-5.61	100.84	109.76
10	L	46	VAL	N-CA-C	-5.61	97.67	109.34
11	R	9	G	C4'-C3'-O3'	-5.58	104.63	113.00
3	C	207	CYS	N-CA-C	5.56	119.57	112.34
1	A	1223	ASP	N-CA-C	5.56	120.37	111.81
1	A	167	CYS	CB-CA-C	-5.54	100.52	111.60
2	B	184	ALA	N-CA-C	5.53	118.67	110.48
1	A	25	GLU	N-CA-C	5.52	117.38	111.36
2	B	301	ILE	N-CA-C	5.51	120.81	109.34
10	L	42	ARG	N-CA-C	5.50	118.20	110.23
2	B	99	LYS	CA-C-N	5.47	126.68	119.84
2	B	99	LYS	C-N-CA	5.47	126.68	119.84
2	B	1093	GLN	N-CA-C	-5.46	103.28	110.33
2	B	230	ALA	CA-C-N	-5.45	116.15	121.65
2	B	230	ALA	C-N-CA	-5.45	116.15	121.65
8	J	9	SER	CB-CA-C	-5.45	101.59	110.85
2	B	491	THR	N-CA-C	-5.44	105.35	111.28
1	A	1428	VAL	N-CA-C	-5.41	105.23	110.42
2	B	226	PHE	N-CA-C	5.36	117.14	108.34
2	B	825	VAL	N-CA-C	5.36	116.70	108.71
8	J	3	VAL	CA-C-N	-5.34	114.84	120.66
8	J	3	VAL	C-N-CA	-5.34	114.84	120.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	980	PHE	N-CA-C	5.31	122.12	110.80
1	A	356	ASP	CA-C-N	5.29	125.61	119.47
1	A	356	ASP	C-N-CA	5.29	125.61	119.47
1	A	23	SER	CA-C-N	5.29	126.45	119.84
1	A	23	SER	C-N-CA	5.29	126.45	119.84
6	H	59	ILE	N-CA-C	-5.27	100.27	108.86
1	A	37	PHE	CA-C-N	5.25	126.41	119.84
1	A	37	PHE	C-N-CA	5.25	126.41	119.84
5	F	143	PHE	N-CA-C	5.25	116.78	108.96
1	A	1311	VAL	N-CA-C	5.23	116.23	107.18
10	L	67	PHE	N-CA-C	5.20	117.92	109.24
1	A	594	GLY	N-CA-C	-5.18	100.90	113.18
1	A	1177	LEU	CA-C-N	5.18	131.02	121.70
1	A	1177	LEU	C-N-CA	5.18	131.02	121.70
2	B	729	ILE	N-CA-C	5.17	114.74	106.88
2	B	570	VAL	CA-C-N	5.17	124.79	119.05
2	B	570	VAL	C-N-CA	5.17	124.79	119.05
2	B	839	MET	N-CA-C	5.15	116.90	109.07
1	A	156	ASP	N-CA-C	-5.14	99.85	110.80
1	A	1169	ILE	CA-C-N	5.13	130.93	121.70
1	A	1169	ILE	C-N-CA	5.13	130.93	121.70
8	J	64	ASN	N-CA-C	5.12	121.13	109.81
1	A	607	ILE	N-CA-C	5.09	115.18	107.75
1	A	286	HIS	CA-C-N	5.07	130.83	121.70
1	A	286	HIS	C-N-CA	5.07	130.83	121.70
8	J	49	MET	N-CA-C	-5.05	106.97	113.23
2	B	196	PRO	N-CA-C	-5.03	109.44	114.68
7	I	35	VAL	N-CA-C	5.03	115.69	107.24

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	11332	0	11392	801	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	9167	0	9178	677	0
3	C	2135	0	2090	164	1
4	E	1757	0	1781	58	0
5	F	684	0	703	28	0
6	H	1087	0	1062	50	0
7	I	971	0	929	33	0
8	J	532	0	545	57	0
9	K	919	0	929	60	0
10	L	363	0	387	28	0
11	R	260	0	132	21	0
12	T	566	0	316	15	0
13	N	284	0	161	3	0
14	A	2	0	0	3	0
14	B	1	0	0	2	0
14	C	1	0	0	0	0
14	I	2	0	0	0	0
14	J	1	0	0	2	0
14	L	1	0	0	0	0
15	A	1	0	0	0	0
16	R	1	0	0	0	0
All	All	30067	0	29605	1834	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 31.

All (1834) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:399:HIS:CG	1:A:400:PRO:HD3	1.52	1.43
2:B:439:ALA:CB	2:B:440:HIS:HA	1.41	1.42
1:A:399:HIS:CD2	1:A:400:PRO:HD3	1.62	1.34
1:A:1081:LEU:CD2	1:A:1082:ASN:H	1.47	1.27
2:B:439:ALA:HB3	2:B:440:HIS:CA	1.66	1.24
2:B:636:PRO:CB	2:B:637:LEU:HA	1.66	1.23
1:A:1081:LEU:HD22	1:A:1082:ASN:N	1.53	1.23
1:A:115:LEU:HD12	1:A:122:MET:CE	1.73	1.18
2:B:636:PRO:HB3	2:B:637:LEU:HA	1.22	1.14
1:A:49:LYS:HB3	1:A:55:ASP:OD2	1.46	1.14
2:B:995:ARG:HB3	2:B:997:GLU:OE2	1.49	1.13
2:B:863:GLU:HA	2:B:864:LYS:HB2	1.25	1.13
10:L:48:CYS:HB3	10:L:51:CYS:SG	1.88	1.13

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:399:HIS:CG	1:A:400:PRO:CD	2.33	1.12
1:A:399:HIS:CB	1:A:400:PRO:HD3	1.79	1.11
1:A:868:TYR:CE1	1:A:1064:VAL:HG11	1.85	1.11
2:B:955:THR:HG22	2:B:956:THR:H	0.95	1.10
1:A:49:LYS:HB2	1:A:50:ILE:C	1.75	1.09
1:A:115:LEU:HD12	1:A:122:MET:HE3	1.31	1.09
2:B:636:PRO:CB	2:B:637:LEU:CA	2.30	1.09
1:A:567:LYS:HB2	1:A:568:PRO:HD2	1.25	1.09
1:A:399:HIS:CB	1:A:400:PRO:CD	2.30	1.09
1:A:272:ALA:C	1:A:296:LEU:HD11	1.77	1.09
1:A:666:ILE:HD11	2:B:1026:LEU:HB3	1.13	1.08
1:A:1081:LEU:HD22	1:A:1082:ASN:H	0.95	1.08
2:B:77:HIS:CA	2:B:78:THR:HB	1.84	1.08
2:B:77:HIS:HA	2:B:78:THR:HB	1.17	1.08
2:B:636:PRO:HB2	2:B:637:LEU:HB3	1.34	1.08
1:A:399:HIS:HB3	1:A:400:PRO:CD	1.84	1.07
1:A:630:ILE:H	1:A:630:ILE:HD12	1.13	1.07
1:A:886:ILE:HD11	1:A:943:LEU:HB3	1.35	1.07
2:B:878:GLN:HG2	2:B:879:ARG:H	1.17	1.06
1:A:50:ILE:HG12	1:A:51:GLY:H	1.16	1.06
1:A:120:GLU:HA	1:A:120:GLU:OE2	1.54	1.06
2:B:636:PRO:HB2	2:B:637:LEU:CB	1.86	1.05
2:B:973:ILE:HG22	2:B:974:PRO:HD2	1.39	1.04
1:A:252:PHE:HD1	1:A:256:GLN:HG2	1.19	1.03
3:C:3:GLU:HG3	3:C:4:GLU:H	1.20	1.03
2:B:979:LYS:HD3	2:B:1097:HIS:HD2	1.19	1.03
1:A:115:LEU:CD1	1:A:122:MET:HB2	1.88	1.02
2:B:769:TYR:OH	11:R:12:G:H2'	1.59	1.02
1:A:256:GLN:HG3	1:A:256:GLN:O	1.59	1.02
1:A:1081:LEU:HD13	1:A:1082:ASN:N	1.73	1.02
1:A:40:THR:H	1:A:41:MET:HB2	1.22	1.01
1:A:310:GLY:N	1:A:311:GLN:HB3	1.75	1.01
2:B:636:PRO:HB2	2:B:637:LEU:CA	1.90	1.01
10:L:26:THR:C	10:L:27:LEU:HG	1.84	0.99
1:A:353:ILE:HD13	1:A:487:MET:HE2	1.45	0.99
1:A:254:GLU:HG2	2:B:918:ILE:HD12	1.42	0.99
1:A:666:ILE:HD11	2:B:1026:LEU:CB	1.94	0.98
1:A:107:CYS:HG	14:A:1734:ZN:ZN	0.66	0.98
3:C:3:GLU:HB3	9:K:104:ASN:HD21	1.27	0.97
2:B:906:SER:HA	2:B:946:ASN:CB	1.94	0.97
2:B:635:ARG:HB2	2:B:636:PRO:HD2	1.44	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:666:ILE:CD1	2:B:1026:LEU:HB3	1.94	0.97
12:T:15:DA:H2''	12:T:16:DC:H5''	1.46	0.97
10:L:25:ALA:O	10:L:27:LEU:HG	1.64	0.97
2:B:863:GLU:HA	2:B:864:LYS:CB	1.93	0.96
2:B:973:ILE:CG2	2:B:974:PRO:HD2	1.95	0.96
2:B:955:THR:CG2	2:B:956:THR:H	1.78	0.96
1:A:320:ARG:HB3	1:A:321:PRO:HD2	1.48	0.96
2:B:955:THR:HG22	2:B:956:THR:N	1.79	0.96
1:A:1084:PHE:HD1	1:A:1084:PHE:H	0.96	0.95
2:B:60:GLN:O	2:B:63:ILE:HG22	1.67	0.95
2:B:979:LYS:HD3	2:B:1097:HIS:CD2	2.02	0.95
2:B:638:PHE:CD1	2:B:743:ILE:HD13	2.00	0.95
1:A:187:LYS:O	1:A:189:ARG:HG3	1.66	0.94
1:A:455:MET:HE1	2:B:1130:PHE:CE1	2.02	0.94
2:B:994:TYR:HB2	2:B:999:MET:CE	1.98	0.94
2:B:1187:ASN:HD21	2:B:1190:ASP:HB2	1.30	0.94
1:A:160:GLN:HE21	1:A:160:GLN:HA	1.29	0.94
1:A:1431:GLY:O	2:B:1152:MET:HE2	1.68	0.94
11:R:4:G:H2'	11:R:5:A:H8	1.33	0.93
1:A:155:GLU:OE2	1:A:155:GLU:HA	1.67	0.93
2:B:863:GLU:CA	2:B:864:LYS:HB2	1.98	0.93
1:A:678:GLU:HA	1:A:681:GLU:HG2	1.50	0.93
1:A:901:LEU:H	1:A:926:GLN:HE21	1.15	0.93
1:A:1062:GLU:HG2	5:F:88:TYR:OH	1.67	0.92
1:A:916:GLY:O	1:A:919:ILE:HB	1.69	0.92
1:A:310:GLY:CA	1:A:311:GLN:HB3	2.00	0.92
1:A:767:GLN:HG3	1:A:799:PHE:HB2	1.52	0.92
1:A:446:ARG:HD2	1:A:480:ALA:HB2	1.52	0.92
1:A:399:HIS:CD2	1:A:400:PRO:CD	2.49	0.91
2:B:78:THR:HG23	2:B:78:THR:O	1.68	0.91
1:A:1192:LEU:HG	1:A:1193:LEU:H	1.36	0.91
1:A:49:LYS:HB2	1:A:50:ILE:CA	2.01	0.91
1:A:252:PHE:HD1	1:A:256:GLN:CG	1.84	0.90
1:A:1084:PHE:HD1	1:A:1084:PHE:N	1.69	0.90
9:K:65:HIS:CD2	9:K:67:PHE:HB2	2.07	0.90
1:A:668:ASP:HB3	1:A:743:VAL:HG23	1.54	0.90
1:A:1386:ARG:HA	1:A:1390:ASN:HD21	1.35	0.90
2:B:784:ASN:ND2	2:B:788:ARG:HD2	1.87	0.90
2:B:906:SER:HA	2:B:946:ASN:HB3	1.54	0.89
1:A:455:MET:HE1	2:B:1130:PHE:HE1	1.37	0.89
1:A:1081:LEU:CG	1:A:1082:ASN:H	1.86	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:55:ASP:H	1:A:56:PRO:HD2	1.38	0.89
1:A:253:ASN:HA	1:A:255:SER:H	1.36	0.89
8:J:46:CYS:HG	14:J:101:ZN:ZN	0.65	0.89
1:A:356:ASP:HB3	1:A:359:LEU:HD12	1.55	0.88
1:A:120:GLU:O	1:A:122:MET:N	2.05	0.88
1:A:272:ALA:CB	1:A:296:LEU:CD1	2.51	0.88
1:A:1084:PHE:N	1:A:1084:PHE:CD1	2.38	0.88
2:B:549:THR:HG22	2:B:550:ASP:H	1.38	0.88
1:A:115:LEU:CD1	1:A:122:MET:HE3	2.03	0.87
2:B:439:ALA:CB	2:B:440:HIS:CA	2.30	0.87
2:B:999:MET:HG3	2:B:1000:PRO:HD2	1.55	0.87
1:A:834:THR:HG21	1:A:1077:THR:HA	1.53	0.87
1:A:1386:ARG:HH22	12:T:15:DA:H8	1.21	0.87
1:A:160:GLN:NE2	1:A:160:GLN:H	1.73	0.86
1:A:252:PHE:CD1	1:A:256:GLN:HG2	2.09	0.86
2:B:994:TYR:HB2	2:B:999:MET:HE1	1.55	0.86
1:A:470:LEU:HD21	1:A:487:MET:CE	2.05	0.86
1:A:115:LEU:CD1	1:A:122:MET:CB	2.53	0.86
2:B:638:PHE:CE1	2:B:743:ILE:HD13	2.10	0.86
2:B:879:ARG:HA	2:B:879:ARG:CZ	2.05	0.86
2:B:577:ALA:HB1	2:B:589:VAL:HG11	1.56	0.86
2:B:878:GLN:CG	2:B:879:ARG:H	1.88	0.86
9:K:43:GLY:HA2	9:K:71:PHE:CE1	2.10	0.86
1:A:399:HIS:HB3	1:A:400:PRO:HD2	1.58	0.86
1:A:1085:HIS:HD2	1:A:1086:PHE:N	1.73	0.86
3:C:186:LEU:HB3	3:C:188:HIS:HD2	1.40	0.86
2:B:715:ALA:H	2:B:716:ASN:HA	1.40	0.85
1:A:1081:LEU:CD1	1:A:1082:ASN:N	2.39	0.85
2:B:956:THR:HA	2:B:961:LEU:O	1.77	0.85
2:B:1185:CYS:HG	14:B:1307:ZN:ZN	0.56	0.84
2:B:825:VAL:HG23	2:B:1010:LEU:HG	1.58	0.84
1:A:272:ALA:O	1:A:296:LEU:HD21	1.77	0.84
8:J:32:GLU:CD	8:J:32:GLU:H	1.85	0.84
1:A:118:HIS:HB2	1:A:123:ARG:HG2	1.60	0.84
1:A:399:HIS:HB3	1:A:400:PRO:HD3	1.51	0.84
1:A:1386:ARG:NH2	12:T:15:DA:H8	1.75	0.84
1:A:272:ALA:HB1	1:A:296:LEU:HD13	1.57	0.83
1:A:567:LYS:CB	1:A:568:PRO:HD2	2.08	0.83
1:A:272:ALA:HB1	1:A:296:LEU:CD1	2.07	0.83
1:A:1081:LEU:CD2	1:A:1082:ASN:N	2.26	0.83
1:A:1084:PHE:CE2	1:A:1086:PHE:O	2.31	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1106:ARG:HG3	2:B:1107:ALA:N	1.92	0.83
2:B:76:GLN:O	2:B:77:HIS:HB2	1.78	0.83
1:A:39:GLU:HB3	1:A:41:MET:HB2	1.60	0.83
1:A:192:GLY:O	1:A:193:ASP:HB3	1.74	0.83
1:A:286:HIS:HB3	1:A:287:HIS:HB2	1.61	0.83
2:B:878:GLN:HG2	2:B:879:ARG:N	1.90	0.83
2:B:906:SER:HA	2:B:946:ASN:HB2	1.60	0.83
9:K:1:MET:O	9:K:1:MET:HE2	1.78	0.83
1:A:588:LEU:HB3	1:A:607:ILE:HB	1.59	0.83
2:B:85:SER:HA	2:B:86:ARG:HB3	1.58	0.83
2:B:71:LEU:HG	2:B:72:GLU:N	1.92	0.83
1:A:668:ASP:HB3	1:A:743:VAL:CG2	2.08	0.82
9:K:43:GLY:CA	9:K:71:PHE:CE1	2.62	0.82
1:A:1085:HIS:CD2	1:A:1086:PHE:N	2.47	0.82
1:A:253:ASN:HB3	1:A:254:GLU:HA	1.61	0.82
1:A:419:LYS:NZ	1:A:419:LYS:HB3	1.95	0.82
9:K:47:ARG:HD2	9:K:60:ALA:HA	1.62	0.82
1:A:160:GLN:HA	1:A:160:GLN:NE2	1.94	0.82
2:B:604:ARG:HD3	2:B:691:GLU:OE2	1.79	0.82
2:B:78:THR:H	2:B:79:THR:HB	1.44	0.82
1:A:272:ALA:O	1:A:296:LEU:HD11	1.80	0.82
2:B:784:ASN:CG	2:B:788:ARG:HD2	2.04	0.82
10:L:46:VAL:HG12	10:L:47:ARG:H	1.43	0.82
8:J:9:SER:OG	8:J:45:CYS:HB2	1.79	0.81
1:A:160:GLN:NE2	1:A:160:GLN:CA	2.43	0.81
1:A:310:GLY:H	1:A:311:GLN:HB3	1.43	0.81
1:A:115:LEU:CD1	1:A:122:MET:CG	2.59	0.81
1:A:276:LEU:HD13	1:A:296:LEU:CD2	2.11	0.81
2:B:77:HIS:HA	2:B:78:THR:CB	1.97	0.81
1:A:115:LEU:HD12	1:A:122:MET:CG	2.11	0.81
2:B:973:ILE:HG22	2:B:974:PRO:CD	2.10	0.81
1:A:320:ARG:HB3	1:A:321:PRO:CD	2.10	0.81
4:E:15:ALA:O	4:E:19:VAL:HG23	1.81	0.81
1:A:1189:SER:HB3	1:A:1241:ARG:HB3	1.63	0.80
1:A:351:THR:HG22	1:A:468:PHE:CD1	2.17	0.80
1:A:793:SER:HB2	1:A:794:PRO:HD2	1.64	0.80
2:B:849:GLY:HA2	2:B:852:ARG:HG3	1.64	0.80
1:A:254:GLU:CG	2:B:918:ILE:HD12	2.10	0.79
1:A:470:LEU:HD21	1:A:487:MET:HE3	1.61	0.79
1:A:445:ASN:HB3	1:A:455:MET:HG2	1.64	0.79
1:A:821:ARG:O	1:A:825:ILE:HG12	1.82	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:57:VAL:HG23	8:J:57:ILE:HD11	1.64	0.79
1:A:50:ILE:HG12	1:A:51:GLY:N	1.94	0.79
1:A:345:VAL:HG12	2:B:1154:ALA:O	1.82	0.79
2:B:1002:THR:HG23	2:B:1004:GLU:H	1.46	0.79
2:B:526:GLU:OE2	2:B:752:ALA:HB3	1.82	0.79
2:B:803:LEU:N	2:B:822:ASN:HD21	1.81	0.79
1:A:868:TYR:HE1	1:A:1064:VAL:HG11	1.43	0.79
1:A:160:GLN:NE2	1:A:160:GLN:N	2.31	0.79
1:A:49:LYS:CB	1:A:55:ASP:OD2	2.30	0.78
1:A:208:LEU:HB2	1:A:235:ILE:HD11	1.65	0.78
1:A:370:ILE:HG23	2:B:1105:ALA:HB2	1.64	0.78
1:A:507:VAL:HG13	1:A:521:MET:HE1	1.63	0.78
3:C:124:LEU:C	3:C:126:GLY:H	1.90	0.78
2:B:445:LYS:HA	2:B:447:ALA:H	1.47	0.78
1:A:58:LEU:HD11	1:A:244:PRO:HD2	1.66	0.78
2:B:1174:LYS:HB2	2:B:1179:GLN:O	1.84	0.78
2:B:581:PHE:HA	2:B:585:VAL:O	1.84	0.77
2:B:603:LEU:HB3	2:B:609:ILE:HG12	1.65	0.77
1:A:994:GLN:HE22	1:A:1023:ARG:HE	1.33	0.77
3:C:167:HIS:HD2	3:C:169:LYS:H	1.32	0.77
8:J:20:SER:O	8:J:24:LEU:HG	1.84	0.77
1:A:107:CYS:SG	14:A:1734:ZN:ZN	1.74	0.77
1:A:497:THR:HG23	2:B:1146:PHE:HD1	1.49	0.77
1:A:192:GLY:O	1:A:193:ASP:CB	2.33	0.77
1:A:630:ILE:H	1:A:630:ILE:CD1	1.89	0.77
1:A:378:GLU:OE1	1:A:434:ARG:HD3	1.85	0.77
1:A:573:SER:O	1:A:576:GLN:HB2	1.83	0.77
2:B:516:ASN:HD22	2:B:516:ASN:H	1.31	0.77
1:A:157:ASP:OD1	1:A:158:PRO:HD3	1.85	0.76
1:A:875:ALA:HB2	1:A:1366:ARG:HD3	1.64	0.76
2:B:807:ARG:HG2	2:B:1045:SER:OG	1.85	0.76
2:B:486:TYR:OH	2:B:1096:ARG:HG2	1.86	0.76
9:K:70:ARG:O	9:K:70:ARG:HG3	1.85	0.76
3:C:3:GLU:HG3	3:C:4:GLU:N	1.98	0.76
2:B:78:THR:H	2:B:79:THR:CB	1.99	0.76
10:L:25:ALA:O	10:L:27:LEU:CG	2.33	0.76
1:A:115:LEU:CD1	1:A:122:MET:HG2	2.15	0.76
1:A:1118:VAL:HG23	1:A:1306:LEU:HB2	1.66	0.75
1:A:203:SER:O	1:A:207:ILE:HD11	1.87	0.75
7:I:7:CYS:SG	7:I:8:ARG:O	2.44	0.75
1:A:115:LEU:HD13	1:A:122:MET:CB	2.15	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:361:LEU:HD21	2:B:377:PHE:CD2	2.22	0.75
5:F:74:ILE:HD13	5:F:74:ILE:H	1.51	0.75
1:A:821:ARG:HH12	2:B:514:LEU:HD13	1.50	0.75
10:L:48:CYS:CB	10:L:51:CYS:SG	2.64	0.75
3:C:101:LEU:HD13	3:C:117:ASP:O	1.87	0.75
3:C:186:LEU:HB3	3:C:188:HIS:CD2	2.21	0.75
6:H:109:LYS:HB3	6:H:111:LEU:H	1.52	0.75
1:A:917:SER:O	1:A:918:GLU:HG3	1.86	0.74
2:B:744:HIS:HD2	2:B:746:SER:OG	1.70	0.74
1:A:185:TRP:HB2	1:A:198:GLU:HG3	1.68	0.74
1:A:1431:GLY:HA3	2:B:1152:MET:HE2	1.70	0.74
1:A:356:ASP:OD2	9:K:65:HIS:HE1	1.70	0.74
1:A:1390:ASN:C	1:A:1392:SER:H	1.95	0.74
2:B:655:LYS:O	2:B:658:ILE:HG22	1.86	0.74
2:B:634:TYR:CE1	2:B:692:TYR:CD1	2.76	0.74
3:C:124:LEU:O	3:C:126:GLY:N	2.20	0.74
11:R:11:U:C5	11:R:12:G:C5	2.75	0.74
1:A:195:ASP:CG	1:A:196:GLU:H	1.95	0.74
3:C:27:LEU:HD12	3:C:228:PHE:HE2	1.53	0.74
1:A:58:LEU:C	1:A:58:LEU:HD22	2.11	0.74
2:B:941:LEU:HD13	2:B:942:ARG:H	1.53	0.73
3:C:67:LEU:HA	3:C:70:ILE:HD12	1.69	0.73
3:C:31:ASN:O	3:C:35:ARG:HG3	1.87	0.73
2:B:78:THR:N	2:B:79:THR:HB	2.03	0.73
2:B:898:LEU:HD13	2:B:952:VAL:HG11	1.70	0.73
2:B:483:LEU:HD23	2:B:484:ASN:H	1.53	0.73
2:B:762:ASN:OD1	2:B:984:HIS:HD2	1.72	0.73
1:A:91:PHE:H	1:A:297:GLN:HE22	1.34	0.73
2:B:591:ARG:O	2:B:592:ASN:HB3	1.87	0.73
2:B:1084:GLN:H	2:B:1084:GLN:CD	1.97	0.73
1:A:767:GLN:HG3	1:A:799:PHE:CB	2.19	0.73
1:A:50:ILE:CG1	1:A:51:GLY:H	1.99	0.73
1:A:55:ASP:H	1:A:56:PRO:CD	2.02	0.72
1:A:272:ALA:CB	1:A:296:LEU:HD11	2.19	0.72
1:A:497:THR:CG2	2:B:1146:PHE:HD1	2.02	0.72
1:A:534:LEU:O	1:A:574:GLY:HA3	1.89	0.72
2:B:827:ILE:CD1	2:B:1086:PHE:HD2	2.02	0.72
1:A:1431:GLY:HA3	2:B:1152:MET:CE	2.20	0.72
1:A:1081:LEU:CD1	1:A:1082:ASN:H	1.99	0.72
10:L:25:ALA:O	10:L:27:LEU:CD2	2.38	0.72
10:L:26:THR:O	10:L:27:LEU:HG	1.90	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:745:PRO:O	2:B:748:ILE:HG12	1.90	0.72
1:A:519:PRO:O	1:A:624:SER:HB2	1.90	0.72
1:A:49:LYS:H	1:A:50:ILE:HA	1.55	0.72
1:A:630:ILE:HD12	1:A:630:ILE:N	1.98	0.72
1:A:1085:HIS:CD2	1:A:1086:PHE:HB2	2.25	0.72
1:A:24:PRO:O	1:A:28:ARG:HB2	1.89	0.71
1:A:49:LYS:HB2	1:A:50:ILE:O	1.90	0.71
2:B:1115:THR:HB	2:B:1117:GLN:H	1.55	0.71
2:B:85:SER:CA	2:B:86:ARG:HB3	2.20	0.71
1:A:526:ASP:HB2	2:B:835:GLN:CD	2.16	0.71
1:A:875:ALA:HA	1:A:878:ILE:HD12	1.72	0.71
2:B:32:ALA:HB3	2:B:658:ILE:HD11	1.72	0.71
2:B:843:GLN:HG2	2:B:993:THR:HB	1.71	0.71
2:B:981:ALA:HB2	2:B:987:LYS:HA	1.71	0.71
8:J:56:LEU:O	8:J:60:PHE:HD2	1.72	0.71
2:B:78:THR:HA	2:B:79:THR:O	1.90	0.71
2:B:493:SER:HA	2:B:751:VAL:HG11	1.73	0.71
2:B:373:ARG:HA	2:B:566:LEU:HD23	1.73	0.71
6:H:109:LYS:HA	6:H:110:ASP:CB	2.19	0.71
1:A:115:LEU:HD13	1:A:122:MET:HG2	1.71	0.71
3:C:62:PHE:O	3:C:66:ARG:HG3	1.90	0.71
2:B:77:HIS:CB	2:B:78:THR:HB	2.21	0.71
2:B:115:GLN:OE1	2:B:115:GLN:HA	1.90	0.71
3:C:67:LEU:HA	3:C:70:ILE:CD1	2.20	0.71
8:J:5:VAL:HA	8:J:15:GLY:H	1.55	0.71
1:A:443:LEU:HD12	2:B:1146:PHE:CZ	2.26	0.70
1:A:793:SER:CB	1:A:794:PRO:HD2	2.19	0.70
8:J:17:LYS:HB3	8:J:39:LEU:HD23	1.73	0.70
1:A:1383:SER:O	1:A:1388:GLY:HA3	1.91	0.70
2:B:530:GLY:HA3	11:R:12:G:H22	1.55	0.70
3:C:238:ILE:CG2	3:C:242:GLN:HB2	2.21	0.70
2:B:176:SER:O	2:B:182:SER:HB3	1.91	0.70
2:B:464:GLY:HA2	2:B:480:SER:HB3	1.73	0.70
1:A:565:ILE:HG13	6:H:97:MET:HG2	1.74	0.70
2:B:439:ALA:HB3	2:B:440:HIS:HA	0.71	0.70
2:B:796:LEU:O	2:B:799:PRO:HD3	1.91	0.70
2:B:498:THR:HG22	2:B:499:ASN:N	2.06	0.70
1:A:567:LYS:HB2	1:A:568:PRO:CD	2.13	0.70
3:C:124:LEU:C	3:C:126:GLY:N	2.48	0.70
1:A:115:LEU:HD12	1:A:122:MET:HB2	1.70	0.70
8:J:6:ARG:HG2	8:J:11:GLY:O	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:L:26:THR:O	10:L:27:LEU:CG	2.40	0.70
1:A:40:THR:N	1:A:41:MET:HB2	2.01	0.69
1:A:679:ILE:O	1:A:682:THR:HG22	1.92	0.69
1:A:1192:LEU:HG	1:A:1193:LEU:N	2.06	0.69
6:H:109:LYS:CB	6:H:111:LEU:H	2.05	0.69
7:I:106:CYS:SG	7:I:108:HIS:HB3	2.31	0.69
1:A:115:LEU:O	1:A:116:ASP:CG	2.36	0.69
9:K:43:GLY:HA2	9:K:71:PHE:HE1	1.58	0.69
2:B:644:GLU:HG3	2:B:654:ARG:HH22	1.56	0.69
1:A:39:GLU:O	1:A:53:LEU:HD13	1.91	0.69
1:A:544:ASP:HB2	9:K:47:ARG:HH21	1.58	0.69
2:B:634:TYR:HE1	2:B:692:TYR:CD1	2.10	0.69
2:B:973:ILE:CG2	2:B:974:PRO:CD	2.68	0.69
8:J:7:CYS:SG	8:J:10:CYS:HB2	2.33	0.69
12:T:2:DT:H2"	12:T:3:DA:C8	2.27	0.69
2:B:905:VAL:N	2:B:947:GLY:O	2.25	0.69
1:A:253:ASN:HA	1:A:255:SER:N	2.06	0.69
2:B:78:THR:O	2:B:78:THR:CG2	2.41	0.69
2:B:1185:CYS:SG	14:B:1307:ZN:ZN	1.75	0.69
1:A:457:ALA:O	1:A:507:VAL:HG23	1.92	0.69
1:A:398:GLU:O	1:A:399:HIS:C	2.35	0.68
1:A:1081:LEU:HD13	1:A:1082:ASN:CA	2.22	0.68
2:B:577:ALA:HB1	2:B:589:VAL:CG1	2.21	0.68
1:A:899:VAL:HB	1:A:929:LEU:HD11	1.73	0.68
2:B:1156:ASP:HB3	2:B:1198:TYR:H	1.59	0.68
1:A:167:CYS:SG	14:A:1734:ZN:ZN	1.82	0.68
1:A:365:GLY:O	1:A:468:PHE:HA	1.92	0.68
3:C:93:ASP:O	3:C:127:ARG:NH2	2.27	0.68
2:B:596:LEU:O	2:B:600:LEU:HD23	1.94	0.68
8:J:46:CYS:SG	14:J:101:ZN:ZN	1.79	0.68
1:A:354:SER:O	1:A:469:ARG:HA	1.94	0.68
1:A:847:ASP:HB3	1:A:1424:VAL:HG23	1.76	0.68
2:B:864:LYS:HE2	2:B:864:LYS:HA	1.75	0.68
5:F:82:THR:HG22	5:F:84:TYR:H	1.59	0.68
7:I:71:SER:HB3	7:I:85:PHE:HE2	1.58	0.68
2:B:25:ILE:HD11	2:B:653:VAL:HB	1.74	0.68
1:A:392:VAL:HG11	1:A:424:ILE:HG21	1.76	0.67
3:C:46:ILE:HG23	3:C:157:CYS:HB3	1.76	0.67
3:C:167:HIS:CD2	3:C:169:LYS:H	2.12	0.67
3:C:178:PHE:HD2	3:C:178:PHE:C	2.02	0.67
1:A:41:MET:HG3	1:A:42:ASP:H	1.58	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:251:SER:O	1:A:252:PHE:HB3	1.93	0.67
1:A:765:VAL:CG2	1:A:800:VAL:HB	2.24	0.67
3:C:142:VAL:O	3:C:143:LEU:HB2	1.95	0.67
2:B:1077:THR:HG23	2:B:1079:LYS:H	1.59	0.67
1:A:185:TRP:HB2	1:A:198:GLU:CG	2.23	0.67
1:A:886:ILE:HD11	1:A:943:LEU:CB	2.21	0.67
10:L:26:THR:O	10:L:27:LEU:HD12	1.95	0.67
2:B:516:ASN:H	2:B:516:ASN:ND2	1.91	0.67
2:B:1152:MET:O	2:B:1157:ALA:HB2	1.95	0.67
3:C:51:VAL:HG13	3:C:155:LEU:HD21	1.75	0.67
3:C:162:GLY:HA3	3:C:170:TRP:CE2	2.30	0.67
1:A:889:SER:C	1:A:891:ALA:H	2.02	0.67
2:B:706:GLN:O	2:B:710:LEU:HB2	1.95	0.67
3:C:73:GLN:HE21	3:C:75:MET:H	1.43	0.67
1:A:669:THR:CG2	1:A:761:MET:HE3	2.25	0.67
2:B:911:ILE:O	2:B:912:ILE:HG13	1.94	0.67
4:E:89:GLY:HA2	4:E:117:THR:OG1	1.95	0.67
1:A:120:GLU:OE2	1:A:120:GLU:CA	2.36	0.66
1:A:1013:ASP:HA	1:A:1016:THR:OG1	1.95	0.66
1:A:1116:LEU:HB2	1:A:1308:THR:HB	1.77	0.66
1:A:1312:ASN:O	1:A:1316:VAL:HG23	1.95	0.66
2:B:827:ILE:CD1	2:B:1086:PHE:CD2	2.78	0.66
3:C:10:ILE:HB	9:K:112:GLN:HE21	1.60	0.66
3:C:51:VAL:HG13	3:C:155:LEU:CD2	2.25	0.66
2:B:57:TYR:O	2:B:58:THR:C	2.38	0.66
11:R:8:G:H2'	11:R:9:G:H8	1.60	0.66
1:A:356:ASP:CB	1:A:359:LEU:HD12	2.26	0.66
1:A:470:LEU:HD21	1:A:487:MET:HE1	1.76	0.66
1:A:665:GLY:O	1:A:668:ASP:HB2	1.94	0.66
1:A:890:ASP:H	1:A:1296:GLY:HA3	1.60	0.66
1:A:1017:LEU:HB2	4:E:205:SER:HA	1.77	0.66
2:B:759:PRO:HB3	2:B:767:ASN:OD1	1.95	0.66
2:B:1033:LYS:HA	2:B:1089:PRO:HG2	1.76	0.66
1:A:1169:ILE:H	1:A:1170:ILE:HG22	1.60	0.66
3:C:13:ALA:HA	3:C:17:ASN:O	1.95	0.66
9:K:44:ASN:HA	9:K:61:TYR:CE2	2.30	0.66
2:B:872:GLU:CD	2:B:916:THR:HB	2.21	0.66
1:A:575:LYS:HB3	1:A:612:ILE:HD11	1.76	0.66
1:A:306:ASN:H	1:A:306:ASN:HD22	1.44	0.66
2:B:31:TRP:CE3	2:B:34:ILE:HD12	2.31	0.66
1:A:341:MET:HE1	1:A:843:LYS:NZ	2.10	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1342:GLU:HG3	4:E:198:ILE:HD13	1.77	0.66
2:B:762:ASN:HB2	2:B:767:ASN:ND2	2.11	0.66
3:C:108:GLU:OE1	3:C:149:LYS:HE2	1.96	0.66
8:J:38:ARG:HB2	8:J:38:ARG:HH11	1.61	0.66
1:A:48:ALA:C	1:A:49:LYS:HD2	2.21	0.65
1:A:445:ASN:HD21	1:A:447:GLN:NE2	1.94	0.65
3:C:220:ASP:OD2	3:C:223:ALA:HB2	1.97	0.65
1:A:115:LEU:HD12	1:A:122:MET:CB	2.26	0.65
1:A:269:ILE:HG13	1:A:299:HIS:HB3	1.78	0.65
1:A:1072:ILE:HD11	1:A:1368:MET:HG2	1.77	0.65
3:C:178:PHE:C	3:C:178:PHE:CD2	2.73	0.65
1:A:1431:GLY:C	2:B:1152:MET:HE2	2.22	0.65
2:B:728:ARG:HH21	2:B:1048:THR:H	1.44	0.65
2:B:778:MET:CE	2:B:1094:ARG:HD3	2.27	0.65
3:C:8:VAL:CG2	9:K:101:LEU:HD21	2.25	0.65
5:F:74:ILE:N	5:F:74:ILE:CD1	2.59	0.65
1:A:155:GLU:OE2	1:A:155:GLU:CA	2.43	0.65
1:A:1119:TYR:CD1	1:A:1326:ARG:HB3	2.31	0.65
2:B:58:THR:O	2:B:59:LEU:C	2.40	0.65
2:B:716:ASN:O	2:B:717:GLU:HB2	1.96	0.65
3:C:47:ASP:HA	10:L:69:ALA:HB3	1.77	0.65
1:A:120:GLU:C	1:A:122:MET:H	2.03	0.65
1:A:1111:MET:HG3	1:A:1114:PRO:HG3	1.78	0.65
2:B:361:LEU:HD21	2:B:377:PHE:HD2	1.58	0.65
3:C:178:PHE:HD2	3:C:179:GLU:N	1.93	0.65
1:A:272:ALA:O	1:A:296:LEU:CD2	2.43	0.65
1:A:360:GLU:HB2	1:A:363:GLN:CD	2.21	0.65
2:B:778:MET:HE1	2:B:1094:ARG:HD3	1.78	0.65
3:C:66:ARG:HH12	8:J:4:PRO:HA	1.61	0.65
1:A:157:ASP:N	1:A:158:PRO:HD2	2.12	0.65
1:A:719:VAL:O	1:A:723:ASN:ND2	2.29	0.65
1:A:1111:MET:HE2	1:A:1114:PRO:HA	1.78	0.65
3:C:58:LEU:CD2	8:J:57:ILE:HD13	2.27	0.65
6:H:116:TYR:HB2	6:H:123:MET:HB3	1.79	0.65
2:B:976:ILE:O	2:B:990:ILE:HB	1.97	0.64
2:B:701:ILE:HD11	2:B:703:ILE:HD11	1.80	0.64
4:E:213:ILE:HG12	4:E:214:CYS:H	1.63	0.64
8:J:7:CYS:SG	8:J:10:CYS:N	2.62	0.64
1:A:284:ALA:N	1:A:285:PRO:HD3	2.11	0.64
1:A:436:ILE:HD11	1:A:491:VAL:HG11	1.79	0.64
3:C:8:VAL:HG21	9:K:101:LEU:CD2	2.28	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:255:SER:HB2	1:A:257:ARG:HA	1.80	0.64
1:A:419:LYS:HB3	1:A:419:LYS:HZ3	1.59	0.64
1:A:445:ASN:HB3	1:A:455:MET:CG	2.27	0.64
1:A:1081:LEU:CG	1:A:1082:ASN:N	2.48	0.64
1:A:272:ALA:O	1:A:296:LEU:CD1	2.45	0.64
1:A:115:LEU:HD12	1:A:122:MET:SD	2.37	0.64
1:A:156:ASP:OD2	1:A:160:GLN:HG2	1.97	0.64
1:A:834:THR:CG2	1:A:1077:THR:HA	2.27	0.64
1:A:160:GLN:N	1:A:160:GLN:CD	2.55	0.64
1:A:1434:ALA:O	1:A:1436:ILE:N	2.31	0.64
2:B:58:THR:O	2:B:61:ASP:N	2.30	0.64
2:B:77:HIS:CA	2:B:78:THR:CB	2.66	0.64
2:B:796:LEU:HB3	2:B:799:PRO:HG3	1.80	0.64
1:A:115:LEU:HD13	1:A:122:MET:CG	2.26	0.64
1:A:1390:ASN:O	1:A:1392:SER:N	2.30	0.64
1:A:118:HIS:O	1:A:120:GLU:N	2.30	0.64
1:A:306:ASN:HD22	1:A:306:ASN:N	1.96	0.64
1:A:364:VAL:HG13	1:A:366:VAL:HG23	1.78	0.64
1:A:497:THR:HG23	2:B:1146:PHE:CD1	2.33	0.64
1:A:507:VAL:CG1	1:A:521:MET:HE1	2.27	0.64
2:B:168:GLY:H	2:B:450:ALA:HB1	1.63	0.64
3:C:43:THR:HG23	3:C:44:LEU:H	1.63	0.64
11:R:4:G:H2'	11:R:5:A:C8	2.24	0.64
1:A:40:THR:H	1:A:41:MET:CB	2.05	0.63
1:A:58:LEU:HD22	1:A:59:GLY:N	2.13	0.63
1:A:252:PHE:CD1	1:A:256:GLN:CG	2.76	0.63
2:B:117:ALA:HA	2:B:122:LEU:HB2	1.80	0.63
1:A:157:ASP:N	1:A:158:PRO:CD	2.58	0.63
2:B:635:ARG:CB	2:B:636:PRO:HD2	2.11	0.63
2:B:417:PHE:HE1	2:B:453:ILE:HG21	1.63	0.63
3:C:226:ASP:O	3:C:227:THR:CB	2.47	0.63
8:J:6:ARG:HA	8:J:12:LYS:O	1.98	0.63
2:B:1097:HIS:NE2	11:R:9:G:H4'	2.14	0.63
1:A:272:ALA:HB3	1:A:296:LEU:CD1	2.27	0.63
1:A:353:ILE:HD13	1:A:487:MET:CE	2.26	0.63
1:A:440:ASP:H	1:A:460:VAL:HG23	1.63	0.63
2:B:122:LEU:HD22	2:B:958:GLN:HE21	1.63	0.63
2:B:213:ILE:HD11	2:B:481:GLN:OE1	1.98	0.63
1:A:147:VAL:HG12	1:A:170:THR:HG22	1.81	0.63
1:A:779:PHE:CE1	1:A:785:PRO:HD3	2.33	0.63
1:A:1089:VAL:HG13	1:A:1090:ALA:N	2.15	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:822:ASN:HD22	8:J:52:THR:HG21	1.64	0.62
2:B:827:ILE:HD12	2:B:1086:PHE:CD2	2.34	0.62
1:A:188:ASP:O	1:A:189:ARG:HG2	2.00	0.62
1:A:544:ASP:HB2	9:K:47:ARG:NH2	2.14	0.62
1:A:886:ILE:CD1	1:A:943:LEU:HB3	2.22	0.62
2:B:757:PRO:HG3	2:B:983:ARG:CZ	2.29	0.62
2:B:762:ASN:HB2	2:B:767:ASN:HD21	1.65	0.62
2:B:1169:MET:HE1	2:B:1205:GLN:HG3	1.81	0.62
10:L:26:THR:OG1	10:L:27:LEU:N	2.30	0.62
2:B:769:TYR:OH	11:R:12:G:C2'	2.43	0.62
1:A:381:THR:HG22	1:A:384:ASN:ND2	2.14	0.62
3:C:226:ASP:O	3:C:227:THR:HB	2.00	0.62
1:A:1431:GLY:CA	2:B:1152:MET:HE2	2.30	0.62
2:B:979:LYS:CD	2:B:1097:HIS:HD2	2.04	0.62
4:E:88:VAL:HG23	4:E:116:ILE:HA	1.82	0.62
1:A:399:HIS:CG	1:A:400:PRO:N	2.67	0.62
1:A:1441:PHE:CZ	5:F:89:GLU:HA	2.34	0.62
2:B:168:GLY:N	2:B:450:ALA:HB1	2.14	0.62
2:B:436:VAL:HA	2:B:437:GLU:C	2.25	0.62
1:A:310:GLY:HA2	1:A:311:GLN:HB3	1.81	0.62
1:A:1189:SER:CB	1:A:1241:ARG:HB3	2.29	0.62
1:A:807:GLY:HA3	2:B:728:ARG:HH11	1.65	0.61
1:A:18:GLN:HG2	1:A:1418:LEU:HD12	1.82	0.61
1:A:55:ASP:N	1:A:56:PRO:CD	2.62	0.61
1:A:575:LYS:NZ	1:A:602:ASP:OD2	2.31	0.61
2:B:526:GLU:C	2:B:527:THR:HG22	2.26	0.61
2:B:637:LEU:CD1	2:B:740:HIS:HB3	2.29	0.61
3:C:3:GLU:CG	3:C:4:GLU:H	2.04	0.61
3:C:8:VAL:HG21	9:K:101:LEU:HD21	1.83	0.61
10:L:26:THR:O	10:L:27:LEU:CD1	2.48	0.61
2:B:492:LEU:HB3	2:B:751:VAL:HG21	1.82	0.61
2:B:861:ASP:OD2	2:B:914:LYS:HE2	1.99	0.61
3:C:228:PHE:N	3:C:228:PHE:CD1	2.66	0.61
11:R:11:U:H5	11:R:12:G:C4	2.18	0.61
1:A:49:LYS:HB2	1:A:50:ILE:HA	1.81	0.61
1:A:1377:THR:HB	4:E:176:PRO:HA	1.83	0.61
2:B:1115:THR:O	2:B:1198:TYR:HD2	1.81	0.61
3:C:142:VAL:HG23	8:J:15:GLY:HA3	1.82	0.61
1:A:254:GLU:HG2	2:B:918:ILE:CD1	2.24	0.61
1:A:313:GLN:HB2	1:A:314:ALA:CA	2.29	0.61
1:A:356:ASP:OD2	9:K:65:HIS:CE1	2.53	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:399:HIS:O	1:A:401:GLY:N	2.33	0.61
2:B:77:HIS:ND1	2:B:78:THR:HB	2.15	0.61
2:B:471:LYS:HB2	2:B:472:ALA:HA	1.81	0.61
2:B:619:ILE:HG21	7:I:62:ILE:HA	1.81	0.61
3:C:57:VAL:CG2	8:J:57:ILE:HD11	2.29	0.61
8:J:6:ARG:H	8:J:14:VAL:H	1.48	0.61
3:C:73:GLN:HE21	3:C:75:MET:N	1.97	0.61
6:H:110:ASP:HB3	6:H:111:LEU:HD12	1.82	0.61
1:A:526:ASP:HB2	2:B:835:GLN:NE2	2.16	0.61
2:B:287:ARG:NH2	2:B:294:ASP:OD2	2.34	0.61
2:B:769:TYR:HE1	11:R:12:G:HO2'	1.47	0.61
1:A:313:GLN:HB2	1:A:314:ALA:HA	1.82	0.61
1:A:456:MET:HE2	1:A:478:TYR:CE1	2.36	0.61
2:B:408:LEU:HD23	2:B:545:ILE:HG21	1.82	0.61
2:B:979:LYS:HG2	2:B:1095:LEU:HD12	1.82	0.61
2:B:1051:THR:O	2:B:1055:ILE:HG12	2.00	0.61
1:A:513:SER:C	1:A:515:GLN:H	2.07	0.61
2:B:530:GLY:HA3	11:R:12:G:N2	2.16	0.61
2:B:1156:ASP:CB	2:B:1198:TYR:H	2.13	0.61
1:A:55:ASP:O	1:A:57:ARG:N	2.34	0.61
4:E:19:VAL:O	4:E:23:VAL:HG23	2.00	0.61
6:H:104:PHE:HE1	6:H:136:LYS:HG2	1.66	0.61
10:L:60:ARG:HG3	10:L:61:THR:H	1.66	0.60
1:A:741:ASN:HD22	1:A:744:LYS:H	1.49	0.60
2:B:439:ALA:HB1	2:B:440:HIS:HA	1.70	0.60
3:C:55:THR:OG1	3:C:151:GLN:HA	2.00	0.60
8:J:7:CYS:HG	8:J:10:CYS:H	1.46	0.60
1:A:1085:HIS:CD2	1:A:1085:HIS:C	2.78	0.60
3:C:3:GLU:CB	9:K:104:ASN:HD21	2.08	0.60
6:H:104:PHE:CE1	6:H:136:LYS:HG2	2.35	0.60
1:A:946:VAL:HG22	4:E:201:LYS:HB3	1.82	0.60
1:A:91:PHE:H	1:A:297:GLN:NE2	1.99	0.60
1:A:446:ARG:CD	1:A:480:ALA:HB2	2.30	0.60
2:B:33:VAL:HG11	2:B:638:PHE:CZ	2.37	0.60
2:B:635:ARG:O	2:B:636:PRO:C	2.44	0.60
1:A:185:TRP:O	1:A:186:LYS:HG2	2.01	0.60
1:A:889:SER:C	1:A:891:ALA:N	2.59	0.60
1:A:1177:LEU:H	1:A:1178:ASP:HB3	1.66	0.60
1:A:265:LYS:HA	1:A:268:ASP:HB2	1.84	0.60
1:A:1449:SER:HA	1:A:1450:LEU:C	2.27	0.60
2:B:861:ASP:OD1	2:B:862:GLN:N	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:978:ASP:HB2	2:B:980:PHE:HE1	1.67	0.60
3:C:32:SER:O	3:C:36:VAL:HG12	2.01	0.60
9:K:43:GLY:HA3	9:K:71:PHE:CE1	2.37	0.60
2:B:773:MET:HE1	2:B:985:GLY:HA2	1.83	0.60
3:C:235:VAL:HG11	8:J:6:ARG:HH21	1.67	0.60
7:I:63:GLY:HA3	7:I:104:LEU:HD11	1.82	0.60
9:K:46:ILE:O	9:K:50:LEU:HB2	2.02	0.60
10:L:41:SER:O	10:L:44:ASP:HB2	2.01	0.60
2:B:1115:THR:O	2:B:1198:TYR:CD2	2.55	0.60
1:A:316:GLN:HG2	1:A:322:VAL:HG13	1.83	0.59
2:B:973:ILE:HG23	2:B:974:PRO:HD2	1.83	0.59
1:A:185:TRP:HH2	1:A:200:ARG:HH11	1.48	0.59
1:A:623:GLY:O	1:A:625:SER:N	2.36	0.59
1:A:1370:LEU:O	1:A:1374:VAL:HG23	2.02	0.59
1:A:1386:ARG:NH2	12:T:15:DA:C8	2.64	0.59
2:B:822:ASN:ND2	8:J:52:THR:HG21	2.17	0.59
1:A:252:PHE:O	1:A:256:GLN:HG2	2.02	0.59
1:A:1236:LEU:C	1:A:1237:ILE:HG13	2.26	0.59
2:B:441:ASP:O	2:B:443:ASN:N	2.34	0.59
1:A:262:LEU:O	1:A:266:LEU:HD23	2.03	0.59
1:A:451:HIS:HB3	1:A:453:MET:H	1.68	0.59
1:A:663:SER:O	1:A:742:ASN:CG	2.46	0.59
1:A:767:GLN:CG	1:A:799:PHE:HB2	2.29	0.59
1:A:195:ASP:O	1:A:196:GLU:C	2.46	0.59
2:B:20:ASP:O	2:B:21:GLU:HG2	2.02	0.59
2:B:301:ILE:HG22	2:B:302:CYS:N	2.18	0.59
1:A:424:ILE:O	1:A:424:ILE:HG23	2.03	0.59
1:A:1021:LEU:CD1	1:A:1025:ARG:HE	2.16	0.59
2:B:745:PRO:O	2:B:747:MET:N	2.35	0.59
6:H:38:LEU:HD13	6:H:125:LEU:HD13	1.83	0.59
2:B:762:ASN:OD1	2:B:984:HIS:CD2	2.53	0.59
2:B:977:GLY:O	2:B:1099:VAL:HG13	2.02	0.59
2:B:978:ASP:O	2:B:980:PHE:HD1	1.85	0.59
4:E:198:ILE:HD11	4:E:212:ARG:HD2	1.82	0.59
1:A:599:SER:HB2	1:A:603:ASN:H	1.68	0.59
2:B:274:PRO:O	2:B:275:TYR:HB2	2.03	0.59
2:B:474:SER:O	2:B:475:SER:O	2.21	0.59
2:B:745:PRO:C	2:B:747:MET:H	2.11	0.59
5:F:74:ILE:H	5:F:74:ILE:CD1	2.14	0.59
1:A:377:PRO:HB3	1:A:431:LYS:HD3	1.84	0.59
1:A:902:LEU:HG	1:A:926:GLN:HG3	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:8:VAL:CG2	9:K:101:LEU:CD2	2.80	0.59
3:C:43:THR:CG2	3:C:44:LEU:N	2.65	0.59
1:A:364:VAL:HG13	1:A:364:VAL:O	2.01	0.58
2:B:77:HIS:ND1	2:B:78:THR:HG21	2.18	0.58
2:B:211:VAL:CG2	2:B:483:LEU:HG	2.33	0.58
2:B:715:ALA:N	2:B:716:ASN:HA	2.10	0.58
1:A:1151:GLU:HG3	1:A:1194:ARG:HB3	1.85	0.58
1:A:1168:GLU:HG2	1:A:1171:GLN:HB3	1.85	0.58
1:A:819:GLY:O	1:A:820:GLY:C	2.47	0.58
2:B:806:THR:HG23	2:B:1046:PRO:HD3	1.84	0.58
2:B:878:GLN:O	2:B:879:ARG:NH2	2.36	0.58
2:B:402:GLY:CA	2:B:695:ALA:HB3	2.33	0.58
2:B:978:ASP:OD1	2:B:1099:VAL:HG22	2.03	0.58
1:A:224:PHE:HZ	1:A:234:MET:HE3	1.68	0.58
1:A:451:HIS:NE2	1:A:1074:GLU:HG3	2.18	0.58
1:A:483:ASP:HB3	2:B:837:ASP:HB3	1.85	0.58
6:H:38:LEU:HD12	6:H:124:ARG:O	2.04	0.58
1:A:915:SER:O	1:A:917:SER:O	2.21	0.58
4:E:31:THR:HG23	4:E:34:GLU:HB2	1.86	0.58
4:E:23:VAL:HB	4:E:30:ILE:HD11	1.86	0.58
6:H:95:TYR:HE2	6:H:97:MET:HG3	1.69	0.58
6:H:114:VAL:HG22	6:H:125:LEU:HB3	1.86	0.58
2:B:202:TYR:CD1	2:B:209:GLU:HB3	2.39	0.58
2:B:547:VAL:HG12	2:B:612:GLU:OE2	2.04	0.58
2:B:555:ILE:HA	2:B:558:LEU:HD12	1.86	0.58
4:E:16:PHE:CE2	4:E:20:LYS:HE2	2.39	0.58
7:I:17:ARG:NH1	7:I:28:GLU:HG2	2.18	0.58
2:B:354:ASP:HA	2:B:357:GLN:HB2	1.86	0.57
2:B:487:THR:HG22	2:B:488:TYR:N	2.19	0.57
1:A:670:ILE:HG22	1:A:671:ALA:H	1.69	0.57
3:C:58:LEU:HD23	8:J:57:ILE:HD13	1.86	0.57
4:E:78:LEU:HD12	4:E:107:THR:HB	1.85	0.57
1:A:402:ALA:O	1:A:415:LEU:HD12	2.04	0.57
1:A:1029:ARG:O	1:A:1033:GLN:HB2	2.04	0.57
2:B:361:LEU:HD11	2:B:381:MET:HE1	1.87	0.57
6:H:109:LYS:HG2	6:H:111:LEU:HB2	1.85	0.57
2:B:638:PHE:CE1	2:B:743:ILE:CD1	2.85	0.57
2:B:975:GLN:NE2	2:B:976:ILE:HG22	2.20	0.57
2:B:983:ARG:HD2	2:B:1091:TYR:HD2	1.68	0.57
1:A:848:ILE:HG21	1:A:1370:LEU:HD11	1.86	0.57
2:B:77:HIS:ND1	2:B:78:THR:CB	2.67	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:459:TYR:C	2:B:459:TYR:CD2	2.82	0.57
2:B:980:PHE:CE2	2:B:1094:ARG:HG3	2.39	0.57
1:A:567:LYS:NZ	6:H:46:LEU:HB2	2.20	0.57
2:B:79:THR:HG22	2:B:80:GLU:H	1.69	0.57
1:A:464:PRO:C	1:A:465:TYR:HD1	2.13	0.57
1:A:726:ARG:O	1:A:730:GLY:N	2.36	0.57
2:B:487:THR:HG22	2:B:488:TYR:H	1.69	0.57
3:C:142:VAL:HG13	3:C:143:LEU:H	1.69	0.57
1:A:186:LYS:NZ	1:A:194:ALA:HB1	2.20	0.57
1:A:1349:TYR:O	1:A:1350:LYS:C	2.46	0.57
2:B:860:MET:SD	2:B:861:ASP:N	2.78	0.57
8:J:10:CYS:SG	8:J:43:ARG:HD2	2.44	0.57
10:L:28:LYS:HG3	10:L:39:SER:OG	2.04	0.57
1:A:1085:HIS:HD2	1:A:1086:PHE:H	1.52	0.57
2:B:792:MET:O	2:B:793:ALA:HB2	2.03	0.57
8:J:48:ARG:O	8:J:52:THR:OG1	2.23	0.57
1:A:676:MET:HA	1:A:679:ILE:HD12	1.86	0.57
6:H:89:LEU:HB2	6:H:91:ASP:OD1	2.05	0.57
2:B:636:PRO:CB	2:B:637:LEU:HB3	2.23	0.56
1:A:577:ILE:HG13	1:A:578:LEU:N	2.18	0.56
1:A:658:LEU:HD13	2:B:831:SER:N	2.20	0.56
1:A:915:SER:HB3	1:A:919:ILE:HG13	1.86	0.56
2:B:766:ARG:HE	2:B:1020:ARG:HB2	1.70	0.56
13:N:4:DC:H2"	13:N:5:DT:OP2	2.05	0.56
1:A:419:LYS:HB3	1:A:419:LYS:HZ2	1.70	0.56
1:A:549:MET:HE1	1:A:656:TRP:HD1	1.70	0.56
1:A:669:THR:HG21	1:A:761:MET:HE3	1.87	0.56
1:A:1089:VAL:HG13	1:A:1090:ALA:H	1.69	0.56
2:B:216:GLU:N	2:B:499:ASN:O	2.36	0.56
2:B:417:PHE:CE1	2:B:453:ILE:HG21	2.40	0.56
2:B:488:TYR:C	2:B:490:SER:H	2.13	0.56
2:B:765:PRO:O	2:B:769:TYR:HB2	2.05	0.56
2:B:898:LEU:HD13	2:B:952:VAL:CG1	2.36	0.56
9:K:102:LYS:O	9:K:106:GLU:HG2	2.06	0.56
2:B:308:TRP:HA	2:B:311:LEU:HD12	1.87	0.56
2:B:591:ARG:O	2:B:592:ASN:CB	2.52	0.56
2:B:1159:ARG:HD3	2:B:1193:GLN:CG	2.35	0.56
3:C:162:GLY:HA3	3:C:170:TRP:CD2	2.40	0.56
1:A:579:SER:HB3	1:A:611:GLN:HA	1.87	0.56
1:A:910:PRO:HA	1:A:916:GLY:HA3	1.87	0.56
2:B:827:ILE:HD11	2:B:1086:PHE:CD2	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:986:GLN:OE1	2:B:986:GLN:HA	2.06	0.56
1:A:244:PRO:HB2	1:A:245:PRO:HD3	1.86	0.56
3:C:46:ILE:CG2	3:C:157:CYS:HB3	2.34	0.56
1:A:901:LEU:N	1:A:926:GLN:HE21	1.94	0.56
1:A:868:TYR:CZ	1:A:1064:VAL:HG11	2.38	0.56
2:B:1032:SER:O	2:B:1033:LYS:C	2.49	0.56
6:H:95:TYR:HD2	6:H:95:TYR:C	2.12	0.56
1:A:330:LYS:O	1:A:334:GLY:HA3	2.06	0.56
1:A:679:ILE:HG23	1:A:729:ALA:HB1	1.88	0.56
2:B:386:LEU:C	2:B:388:CYS:H	2.12	0.56
3:C:248:ILE:CD1	9:K:101:LEU:HD13	2.36	0.56
1:A:341:MET:HE1	1:A:843:LYS:HZ1	1.70	0.56
1:A:942:PHE:C	1:A:942:PHE:CD2	2.84	0.56
2:B:964:VAL:HG12	2:B:965:LYS:N	2.21	0.56
1:A:14:VAL:HB	1:A:1432:GLN:HE22	1.72	0.55
1:A:775:ILE:HB	1:A:797:LYS:C	2.31	0.55
1:A:803:SER:OG	1:A:806:ARG:HG3	2.06	0.55
2:B:239:GLU:HG2	2:B:255:GLN:HG2	1.87	0.55
2:B:839:MET:HG2	2:B:989:THR:O	2.07	0.55
3:C:238:ILE:HG23	3:C:242:GLN:HB2	1.87	0.55
1:A:447:GLN:HB3	1:A:448:PRO:HA	1.87	0.55
1:A:1243:VAL:HG13	1:A:1244:ARG:HB2	1.87	0.55
2:B:498:THR:CG2	2:B:499:ASN:N	2.69	0.55
2:B:856:PHE:HB3	2:B:967:ARG:HD2	1.88	0.55
8:J:45:CYS:O	8:J:48:ARG:HG3	2.06	0.55
2:B:1159:ARG:HD3	2:B:1193:GLN:HG3	1.89	0.55
1:A:157:ASP:CB	1:A:158:PRO:HD3	2.36	0.55
1:A:195:ASP:CG	1:A:196:GLU:N	2.64	0.55
1:A:715:GLU:O	1:A:719:VAL:HG23	2.06	0.55
2:B:1033:LYS:CA	2:B:1089:PRO:HG2	2.36	0.55
4:E:157:SER:OG	4:E:160:GLU:HB2	2.06	0.55
1:A:1407:GLU:HA	1:A:1410:PHE:HB2	1.87	0.55
2:B:648:HIS:CD2	2:B:649:LYS:H	2.24	0.55
2:B:795:ILE:HG22	2:B:796:LEU:H	1.71	0.55
2:B:825:VAL:O	2:B:1087:PHE:HA	2.06	0.55
6:H:95:TYR:C	6:H:95:TYR:CD2	2.84	0.55
1:A:874:ASP:N	1:A:1058:VAL:HG23	2.21	0.55
2:B:525:ALA:O	2:B:527:THR:HG22	2.06	0.55
4:E:205:SER:O	4:E:206:GLY:C	2.49	0.55
9:K:69:ALA:O	9:K:70:ARG:HB3	2.06	0.55
1:A:203:SER:O	1:A:207:ILE:CD1	2.54	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1100:ARG:HH21	1:A:1351:GLU:CG	2.20	0.55
2:B:315:LYS:HD2	7:I:13:MET:HE1	1.89	0.55
2:B:383:ASN:O	2:B:387:LEU:HB2	2.07	0.55
6:H:109:LYS:HA	6:H:110:ASP:HB3	1.88	0.55
1:A:672:ASP:H	1:A:736:ASN:HD21	1.55	0.55
1:A:1119:TYR:HD1	1:A:1326:ARG:HB3	1.70	0.55
2:B:710:LEU:HD13	2:B:733:HIS:HB3	1.89	0.55
2:B:782:LEU:HB3	2:B:784:ASN:OD1	2.07	0.55
2:B:826:ALA:O	2:B:1011:ILE:HA	2.07	0.55
7:I:59:VAL:HB	7:I:61:ASP:H	1.72	0.55
1:A:1100:ARG:HH21	1:A:1351:GLU:HG2	1.72	0.55
1:A:18:GLN:NE2	1:A:228:PHE:CD1	2.75	0.55
2:B:73:GLN:HG3	2:B:86:ARG:HG3	1.89	0.55
2:B:785:TYR:CD1	2:B:785:TYR:C	2.84	0.55
2:B:983:ARG:HG3	2:B:1093:GLN:OE1	2.06	0.54
2:B:1150:ARG:O	2:B:1151:LEU:HD12	2.07	0.54
1:A:1390:ASN:C	1:A:1392:SER:N	2.59	0.54
2:B:617:ARG:HA	2:B:624:LEU:HD12	1.88	0.54
5:F:81:THR:HG23	5:F:144:GLU:OE1	2.07	0.54
8:J:10:CYS:HG	8:J:46:CYS:HG	1.55	0.54
1:A:187:LYS:O	1:A:189:ARG:CG	2.50	0.54
1:A:527:THR:HG21	1:A:650:GLN:HG2	1.89	0.54
2:B:77:HIS:CG	2:B:78:THR:HB	2.42	0.54
2:B:634:TYR:CD1	2:B:692:TYR:HB3	2.42	0.54
2:B:849:GLY:CA	2:B:852:ARG:HG3	2.36	0.54
2:B:998:ASP:OD2	3:C:35:ARG:NH2	2.39	0.54
1:A:901:LEU:HD12	1:A:926:GLN:HG2	1.88	0.54
2:B:728:ARG:NH2	2:B:1048:THR:H	2.05	0.54
1:A:203:SER:O	1:A:207:ILE:CG1	2.55	0.54
1:A:541:ILE:HG21	1:A:549:MET:HE3	1.89	0.54
2:B:118:ARG:HA	2:B:207:GLY:HA2	1.89	0.54
3:C:142:VAL:HG22	3:C:143:LEU:N	2.21	0.54
2:B:469:GLN:O	2:B:470:LYS:HB2	2.07	0.54
2:B:879:ARG:HA	2:B:879:ARG:NE	2.21	0.54
8:J:16:ASP:N	8:J:16:ASP:OD1	2.41	0.54
1:A:350:ARG:O	1:A:351:THR:HB	2.07	0.54
1:A:470:LEU:CD2	1:A:487:MET:HE1	2.37	0.54
2:B:976:ILE:O	2:B:990:ILE:O	2.24	0.54
1:A:49:LYS:HD2	1:A:49:LYS:N	2.22	0.54
1:A:399:HIS:O	1:A:400:PRO:C	2.51	0.54
1:A:696:GLU:HG2	1:A:701:LEU:HB2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:56:ASP:HB3	2:B:57:TYR:CD1	2.42	0.54
2:B:878:GLN:CG	2:B:879:ARG:N	2.59	0.54
1:A:901:LEU:H	1:A:926:GLN:NE2	1.95	0.54
1:A:1086:PHE:HE1	1:A:1092:LYS:HG2	1.73	0.54
1:A:1429:ILE:O	1:A:1429:ILE:HG22	2.06	0.54
2:B:363:HIS:O	2:B:364:ILE:HB	2.08	0.54
2:B:1153:GLU:OE2	2:B:1153:GLU:N	2.41	0.54
3:C:36:VAL:HA	3:C:40:GLU:HB2	1.90	0.54
3:C:63:ILE:O	3:C:66:ARG:N	2.40	0.54
1:A:455:MET:CE	2:B:1130:PHE:HE1	2.16	0.54
1:A:567:LYS:O	1:A:569:LYS:N	2.41	0.54
2:B:57:TYR:O	2:B:59:LEU:N	2.40	0.54
1:A:253:ASN:CB	1:A:254:GLU:HA	2.32	0.53
2:B:167:ILE:HG22	2:B:453:ILE:HD12	1.90	0.53
2:B:363:HIS:C	2:B:365:THR:H	2.16	0.53
2:B:681:TRP:HA	2:B:684:LEU:HD12	1.90	0.53
2:B:863:GLU:HA	2:B:864:LYS:CG	2.37	0.53
2:B:1175:LEU:HD23	2:B:1176:ASN:H	1.73	0.53
1:A:302:THR:HG21	1:A:314:ALA:HB3	1.89	0.53
2:B:1154:ALA:O	2:B:1155:SER:HB2	2.07	0.53
3:C:178:PHE:CD2	3:C:179:GLU:N	2.76	0.53
8:J:7:CYS:SG	8:J:7:CYS:O	2.54	0.53
1:A:563:PRO:HB3	1:A:572:TRP:CE2	2.44	0.53
1:A:1402:PHE:CD2	1:A:1403:GLU:HB2	2.43	0.53
2:B:706:GLN:HB2	2:B:710:LEU:HD23	1.91	0.53
2:B:1084:GLN:HG2	3:C:201:TRP:CZ2	2.43	0.53
2:B:1132:GLU:O	2:B:1133:MET:C	2.50	0.53
8:J:10:CYS:HB2	8:J:46:CYS:SG	2.49	0.53
11:R:6:G:H2'	11:R:7:A:H8	1.73	0.53
1:A:836:TYR:CZ	1:A:840:ARG:HD2	2.43	0.53
2:B:986:GLN:HE21	2:B:1022:THR:HG21	1.74	0.53
9:K:61:TYR:HA	9:K:72:LYS:O	2.08	0.53
1:A:32:VAL:HB	1:A:57:ARG:HB2	1.90	0.53
1:A:528:LEU:HA	1:A:531:ILE:HG22	1.90	0.53
1:A:1146:VAL:O	1:A:1197:LEU:HD22	2.08	0.53
2:B:978:ASP:HB2	2:B:980:PHE:CE1	2.43	0.53
1:A:115:LEU:CG	1:A:122:MET:HE3	2.39	0.53
1:A:956:LEU:HD23	1:A:957:PRO:CD	2.39	0.53
2:B:1001:PHE:CE2	2:B:1073:TYR:HB2	2.44	0.53
1:A:118:HIS:O	1:A:119:ASN:C	2.52	0.53
1:A:255:SER:HA	1:A:256:GLN:C	2.34	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:364:VAL:O	1:A:364:VAL:CG1	2.57	0.53
1:A:468:PHE:CE2	1:A:489:LEU:HD13	2.44	0.53
1:A:1086:PHE:HE1	1:A:1092:LYS:CG	2.21	0.53
2:B:486:TYR:CZ	2:B:1096:ARG:HG2	2.43	0.53
1:A:49:LYS:N	1:A:50:ILE:HA	2.14	0.53
1:A:571:LEU:C	1:A:572:TRP:CE3	2.87	0.53
3:C:229:TYR:N	3:C:229:TYR:CD1	2.76	0.53
9:K:65:HIS:O	9:K:67:PHE:N	2.42	0.53
1:A:819:GLY:O	1:A:822:GLU:N	2.40	0.53
1:A:1080:THR:CG2	1:A:1098:VAL:HG23	2.38	0.53
1:A:419:LYS:NZ	1:A:419:LYS:CB	2.70	0.53
1:A:447:GLN:HG3	1:A:449:SER:OG	2.09	0.53
1:A:458:HIS:NE2	1:A:507:VAL:HG21	2.24	0.53
1:A:849:MET:CE	1:A:1061:GLY:HA2	2.39	0.53
6:H:8:ASP:CG	6:H:9:ILE:H	2.17	0.53
6:H:95:TYR:HD2	6:H:96:VAL:N	2.07	0.53
1:A:18:GLN:HB3	2:B:1215:ARG:HB2	1.91	0.52
1:A:956:LEU:HD11	1:A:1017:LEU:HD22	1.91	0.52
3:C:228:PHE:N	3:C:228:PHE:HD1	2.08	0.52
5:F:74:ILE:HD13	5:F:74:ILE:N	2.19	0.52
6:H:37:LYS:H	6:H:126:GLU:HB3	1.74	0.52
1:A:1063:MET:SD	1:A:1436:ILE:HG12	2.50	0.52
1:A:1213:GLY:HA2	1:A:1216:ILE:HD12	1.91	0.52
2:B:773:MET:C	2:B:775:LYS:H	2.17	0.52
1:A:208:LEU:CB	1:A:235:ILE:HD11	2.37	0.52
1:A:534:LEU:HA	1:A:539:THR:HG21	1.90	0.52
1:A:815:PHE:O	1:A:818:MET:HB2	2.09	0.52
1:A:1128:GLN:HB3	1:A:1304:TRP:CE2	2.45	0.52
1:A:1389:PHE:O	1:A:1390:ASN:OD1	2.27	0.52
2:B:232:SER:C	2:B:261:ARG:HH21	2.18	0.52
4:E:79:TRP:NE1	4:E:81:GLU:HG3	2.25	0.52
5:F:132:LEU:O	5:F:148:VAL:HG23	2.09	0.52
7:I:17:ARG:HH12	7:I:28:GLU:HG2	1.75	0.52
1:A:962:ARG:O	1:A:966:ASN:HB2	2.09	0.52
1:A:1323:ASP:OD1	1:A:1325:THR:HG22	2.09	0.52
2:B:57:TYR:CD1	2:B:57:TYR:N	2.76	0.52
2:B:745:PRO:C	2:B:747:MET:N	2.67	0.52
3:C:80:LEU:HD21	3:C:95:CYS:O	2.09	0.52
1:A:11:LEU:HA	2:B:1193:GLN:O	2.08	0.52
1:A:55:ASP:HA	1:A:58:LEU:O	2.10	0.52
1:A:873:MET:HG2	1:A:957:PRO:HG3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:48:LEU:O	2:B:49:ASP:C	2.52	0.52
1:A:74:MET:HG3	1:A:74:MET:O	2.10	0.52
1:A:1015:VAL:HG12	1:A:1019:CYS:SG	2.49	0.52
2:B:230:ALA:HB3	2:B:231:PRO:HD3	1.91	0.52
2:B:827:ILE:HD12	2:B:1086:PHE:HD2	1.71	0.52
1:A:304:MET:SD	2:B:1210:MET:HG3	2.50	0.52
1:A:512:VAL:HA	1:A:519:PRO:HA	1.90	0.52
1:A:667:GLY:HA2	1:A:670:ILE:CG1	2.40	0.52
2:B:95:ILE:HG23	2:B:95:ILE:O	2.10	0.52
2:B:273:LEU:HB2	2:B:276:ILE:HD12	1.92	0.52
2:B:915:THR:HB	2:B:934:LYS:HB3	1.91	0.52
2:B:1112:GLN:HG2	2:B:1119:VAL:HG12	1.90	0.52
2:B:1149:GLU:C	2:B:1151:LEU:H	2.18	0.52
3:C:220:ASP:OD2	3:C:223:ALA:CB	2.57	0.52
1:A:663:SER:O	1:A:742:ASN:OD1	2.27	0.52
2:B:115:GLN:HG2	2:B:193:LYS:HB2	1.91	0.52
2:B:476:ARG:C	2:B:478:GLY:H	2.18	0.52
2:B:1008:PRO:HG3	2:B:1087:PHE:CE1	2.45	0.52
1:A:380:VAL:HG12	1:A:428:TYR:HA	1.91	0.52
2:B:58:THR:O	2:B:60:GLN:N	2.43	0.52
2:B:498:THR:HG22	2:B:499:ASN:H	1.74	0.52
2:B:764:SER:HB2	2:B:765:PRO:HD3	1.92	0.52
2:B:911:ILE:CG2	2:B:912:ILE:HG13	2.40	0.52
2:B:1074:ASN:HB3	2:B:1077:THR:HG22	1.92	0.52
1:A:469:ARG:NH2	2:B:991:GLY:O	2.43	0.52
1:A:664:THR:OG1	2:B:1014:PRO:HB2	2.10	0.52
2:B:784:ASN:OD1	2:B:784:ASN:N	2.42	0.52
11:R:5:A:H2'	11:R:6:G:C8	2.45	0.52
1:A:1308:THR:HG22	1:A:1309:ASP:N	2.24	0.51
2:B:56:ASP:HB3	2:B:57:TYR:CE1	2.45	0.51
2:B:827:ILE:HD11	2:B:1086:PHE:HD2	1.73	0.51
7:I:85:PHE:HB3	7:I:101:PHE:CD2	2.44	0.51
9:K:11:LEU:C	9:K:12:LEU:HG	2.35	0.51
1:A:446:ARG:NH1	1:A:478:TYR:O	2.42	0.51
1:A:686:ALA:HB1	1:A:725:ALA:HB2	1.92	0.51
2:B:1060:ARG:HD2	2:B:1064:TYR:O	2.10	0.51
1:A:1198:ASP:O	1:A:1202:MET:HG2	2.11	0.51
2:B:402:GLY:HA3	2:B:695:ALA:HB3	1.90	0.51
2:B:497:ARG:HE	2:B:538:ASN:HD21	1.57	0.51
5:F:81:THR:CG2	5:F:144:GLU:OE1	2.58	0.51
7:I:100:PHE:CE2	7:I:111:THR:HG23	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:669:THR:HG22	1:A:761:MET:HE3	1.92	0.51
1:A:886:ILE:O	1:A:944:ARG:NH2	2.39	0.51
2:B:386:LEU:C	2:B:388:CYS:N	2.69	0.51
2:B:1030:LEU:O	2:B:1031:LEU:C	2.53	0.51
3:C:46:ILE:HD13	3:C:159:ALA:HB2	1.93	0.51
3:C:144:ILE:HD13	3:C:144:ILE:N	2.25	0.51
1:A:915:SER:HB3	1:A:919:ILE:CG1	2.41	0.51
1:A:1062:GLU:HG2	5:F:88:TYR:CZ	2.44	0.51
1:A:1086:PHE:O	1:A:1087:ALA:HB3	2.11	0.51
2:B:874:PHE:CZ	2:B:964:VAL:HG23	2.44	0.51
2:B:1115:THR:HG22	2:B:1117:GLN:HG3	1.93	0.51
3:C:71:PRO:HB2	3:C:133:ILE:HD12	1.90	0.51
4:E:64:PRO:HG3	4:E:76:GLY:HA2	1.91	0.51
4:E:191:LYS:HG2	4:E:192:ARG:H	1.75	0.51
12:T:26:DG:N2	12:T:27:DA:H1'	2.25	0.51
1:A:354:SER:OG	1:A:467:THR:HG21	2.11	0.51
2:B:449:ASN:C	2:B:451:LYS:H	2.17	0.51
3:C:35:ARG:HB3	3:C:35:ARG:HH11	1.75	0.51
2:B:994:TYR:CB	2:B:999:MET:CE	2.81	0.51
3:C:123:ASN:ND2	3:C:125:MET:HG2	2.25	0.51
11:R:11:U:H5	11:R:12:G:C5	2.23	0.51
1:A:821:ARG:NH1	2:B:514:LEU:HD13	2.22	0.51
2:B:349:ILE:O	2:B:353:LYS:N	2.39	0.51
2:B:1002:THR:HG21	2:B:1006:ILE:HG13	1.92	0.51
3:C:173:ALA:O	3:C:233:GLU:O	2.28	0.51
4:E:88:VAL:HG21	4:E:116:ILE:HD13	1.91	0.51
8:J:32:GLU:CD	8:J:32:GLU:N	2.62	0.51
1:A:556:TRP:O	1:A:558:GLY:N	2.43	0.51
1:A:572:TRP:HE3	1:A:572:TRP:N	2.08	0.51
1:A:578:LEU:O	1:A:581:ALA:HB3	2.11	0.51
1:A:647:GLY:O	1:A:648:ASN:C	2.54	0.51
3:C:88:CYS:O	3:C:88:CYS:SG	2.69	0.51
5:F:82:THR:O	5:F:136:ARG:NH1	2.44	0.51
1:A:403:LYS:HG3	1:A:404:TYR:CE1	2.46	0.51
2:B:984:HIS:CE1	2:B:1025:HIS:HA	2.45	0.51
3:C:39:ALA:HA	3:C:164:ALA:HB3	1.93	0.51
4:E:79:TRP:HE1	4:E:81:GLU:HG3	1.75	0.51
12:T:11:DG:H1	13:N:4:DC:H42	1.59	0.51
2:B:731:VAL:O	2:B:732:SER:CB	2.59	0.50
4:E:12:LEU:HD11	4:E:58:MET:HE1	1.92	0.50
1:A:37:PHE:HB2	1:A:52:GLY:HA3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:118:HIS:C	1:A:120:GLU:N	2.70	0.50
1:A:326:ARG:HE	1:A:1406:VAL:HG21	1.75	0.50
1:A:444:PHE:CZ	1:A:470:LEU:HD23	2.46	0.50
1:A:1081:LEU:HD13	1:A:1082:ASN:CB	2.41	0.50
2:B:773:MET:C	2:B:775:LYS:N	2.66	0.50
2:B:780:VAL:HG12	2:B:817:LEU:HD23	1.93	0.50
2:B:1204:PHE:O	2:B:1208:MET:HG3	2.11	0.50
6:H:41:ASP:CB	6:H:121:LEU:HB3	2.41	0.50
1:A:39:GLU:HB3	1:A:41:MET:CB	2.35	0.50
1:A:278:THR:HG23	1:A:282:ASN:HD22	1.76	0.50
1:A:320:ARG:CB	1:A:321:PRO:CD	2.81	0.50
1:A:572:TRP:CE3	1:A:572:TRP:N	2.79	0.50
2:B:85:SER:CA	2:B:86:ARG:CB	2.84	0.50
2:B:114:PRO:HG2	2:B:181:LEU:HD21	1.94	0.50
2:B:345:LYS:HG2	2:B:348:ARG:NH2	2.26	0.50
2:B:642:ASP:C	2:B:644:GLU:H	2.20	0.50
9:K:100:ALA:O	9:K:101:LEU:C	2.54	0.50
1:A:1075:PRO:O	1:A:1076:ALA:C	2.54	0.50
2:B:25:ILE:HG22	2:B:26:THR:N	2.26	0.50
2:B:459:TYR:C	2:B:459:TYR:HD2	2.19	0.50
2:B:529:GLU:HA	2:B:533:CYS:HB2	1.92	0.50
2:B:603:LEU:HB3	2:B:609:ILE:CG1	2.38	0.50
2:B:758:PHE:HZ	2:B:1031:LEU:HD22	1.75	0.50
2:B:911:ILE:C	2:B:912:ILE:HG13	2.35	0.50
2:B:1187:ASN:ND2	2:B:1190:ASP:HB2	2.12	0.50
6:H:109:LYS:CA	6:H:111:LEU:H	2.24	0.50
1:A:193:ASP:O	1:A:194:ALA:O	2.30	0.50
2:B:78:THR:HA	2:B:79:THR:C	2.36	0.50
2:B:472:ALA:HB1	2:B:476:ARG:H	1.77	0.50
2:B:840:ILE:HD12	2:B:1011:ILE:HD12	1.93	0.50
4:E:179:GLN:O	4:E:182:ASP:HB2	2.11	0.50
4:E:180:ARG:HB2	4:E:215:MET:OXT	2.12	0.50
1:A:6:TYR:O	2:B:1175:LEU:HD21	2.11	0.50
1:A:157:ASP:CG	1:A:158:PRO:HD3	2.36	0.50
1:A:158:PRO:HA	1:A:159:THR:OG1	2.12	0.50
1:A:376:TYR:CZ	1:A:498:ARG:HD2	2.46	0.50
1:A:668:ASP:OD2	1:A:742:ASN:HB2	2.12	0.50
1:A:1177:LEU:HB3	1:A:1178:ASP:HB2	1.94	0.50
1:A:1391:ARG:O	1:A:1391:ARG:HG3	2.12	0.50
1:A:403:LYS:HG3	1:A:404:TYR:HE1	1.77	0.50
1:A:567:LYS:C	1:A:569:LYS:H	2.20	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:870:GLU:OE1	4:E:202:SER:HB2	2.12	0.50
2:B:126:SER:HB2	2:B:172:ILE:HD11	1.92	0.50
2:B:174:LEU:HD11	2:B:204:ILE:HD13	1.93	0.50
2:B:731:VAL:O	2:B:732:SER:HB3	2.11	0.50
3:C:35:ARG:HB3	3:C:35:ARG:NH1	2.27	0.50
3:C:96:SER:HB2	3:C:158:VAL:HG12	1.93	0.50
3:C:100:THR:HG22	3:C:119:VAL:HG12	1.94	0.50
1:A:58:LEU:C	1:A:58:LEU:CD2	2.83	0.50
1:A:106:VAL:HG11	1:A:214:ILE:HD11	1.94	0.50
1:A:306:ASN:HB2	1:A:313:GLN:OE1	2.10	0.50
2:B:680:THR:O	2:B:683:SER:OG	2.30	0.50
2:B:978:ASP:O	2:B:980:PHE:CD1	2.63	0.50
6:H:98:TYR:C	6:H:118:PHE:HD2	2.20	0.50
7:I:14:LEU:HB3	7:I:27:PHE:HB3	1.94	0.50
1:A:103:CYS:HB3	1:A:174:ILE:HD13	1.94	0.50
1:A:185:TRP:CH2	1:A:200:ARG:HD2	2.47	0.50
1:A:195:ASP:OD1	1:A:196:GLU:N	2.45	0.50
1:A:313:GLN:HB2	1:A:314:ALA:HB2	1.94	0.50
1:A:451:HIS:HB3	1:A:453:MET:N	2.27	0.50
1:A:453:MET:HG2	1:A:520:CYS:SG	2.52	0.50
1:A:524:VAL:HG12	1:A:525:GLN:HG3	1.94	0.50
1:A:814:PHE:O	1:A:817:ALA:HB3	2.11	0.50
1:A:1088:GLY:O	1:A:1089:VAL:HG12	2.12	0.50
1:A:114:LEU:O	1:A:115:LEU:O	2.30	0.49
1:A:185:TRP:O	1:A:186:LYS:CG	2.60	0.49
1:A:256:GLN:O	1:A:256:GLN:CG	2.43	0.49
2:B:1108:ARG:HG2	2:B:1109:GLY:H	1.76	0.49
3:C:63:ILE:O	3:C:66:ARG:HB2	2.12	0.49
1:A:272:ALA:CA	1:A:296:LEU:HD11	2.40	0.49
1:A:573:SER:H	1:A:576:GLN:HG3	1.76	0.49
1:A:768:GLN:HG2	1:A:816:HIS:HA	1.92	0.49
1:A:1436:ILE:O	1:A:1438:THR:N	2.44	0.49
2:B:127:GLY:HA2	2:B:169:ARG:HG2	1.93	0.49
2:B:519:TRP:HZ2	2:B:705:MET:HE1	1.75	0.49
2:B:640:VAL:HG13	2:B:650:GLU:O	2.12	0.49
2:B:911:ILE:O	2:B:911:ILE:HG23	2.11	0.49
2:B:911:ILE:HG22	2:B:912:ILE:HG13	1.94	0.49
2:B:1132:GLU:O	2:B:1134:GLU:N	2.45	0.49
3:C:53:THR:O	3:C:153:LEU:HA	2.12	0.49
4:E:124:VAL:HB	4:E:125:PRO:HD3	1.95	0.49
1:A:367:PRO:HA	1:A:463:ILE:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:53:GLN:HG2	2:B:547:VAL:HG22	1.93	0.49
2:B:386:LEU:O	2:B:388:CYS:N	2.46	0.49
2:B:628:THR:O	2:B:628:THR:HG22	2.12	0.49
2:B:635:ARG:O	2:B:636:PRO:O	2.30	0.49
2:B:1084:GLN:NE2	3:C:192:TRP:H	2.10	0.49
3:C:127:ARG:HG3	3:C:129:ILE:HG21	1.94	0.49
6:H:47:PHE:HB3	6:H:95:TYR:CD1	2.47	0.49
1:A:22:PHE:HB2	2:B:1211:ASN:OD1	2.13	0.49
1:A:403:LYS:C	1:A:404:TYR:CD1	2.91	0.49
1:A:441:PRO:HD3	1:A:498:ARG:NH2	2.27	0.49
1:A:451:HIS:CE1	1:A:1074:GLU:HG3	2.48	0.49
1:A:956:LEU:CD2	1:A:957:PRO:HD2	2.42	0.49
1:A:1341:ILE:HG23	1:A:1342:GLU:N	2.28	0.49
2:B:77:HIS:ND1	2:B:78:THR:CG2	2.75	0.49
2:B:581:PHE:N	2:B:581:PHE:CD1	2.80	0.49
2:B:1065:GLN:OE1	2:B:1065:GLN:HA	2.12	0.49
1:A:224:PHE:HZ	1:A:234:MET:CE	2.25	0.49
1:A:401:GLY:C	1:A:435:HIS:CD2	2.90	0.49
1:A:413:ILE:N	1:A:413:ILE:CD1	2.76	0.49
1:A:468:PHE:HE2	1:A:489:LEU:HD13	1.76	0.49
1:A:1017:LEU:HB2	4:E:206:GLY:H	1.78	0.49
1:A:1187:GLN:HB3	1:A:1188:GLN:HA	1.94	0.49
1:A:1220:PHE:O	1:A:1221:LYS:HB2	2.13	0.49
2:B:976:ILE:HG23	2:B:977:GLY:H	1.76	0.49
2:B:1175:LEU:HD23	2:B:1176:ASN:N	2.28	0.49
3:C:258:ILE:O	3:C:259:LEU:C	2.55	0.49
4:E:199:ILE:O	4:E:199:ILE:HG22	2.12	0.49
9:K:35:PHE:N	9:K:35:PHE:CD1	2.81	0.49
1:A:78:PRO:O	2:B:1201:LYS:HE2	2.12	0.49
1:A:369:SER:HB2	9:K:2:ASN:OD1	2.13	0.49
3:C:167:HIS:CD2	3:C:169:LYS:HG2	2.47	0.49
1:A:567:LYS:CB	1:A:568:PRO:CD	2.80	0.49
1:A:840:ARG:HG2	1:A:1402:PHE:HZ	1.76	0.49
2:B:531:GLN:HG2	2:B:531:GLN:O	2.11	0.49
2:B:986:GLN:NE2	2:B:1022:THR:HG21	2.27	0.49
1:A:118:HIS:O	1:A:122:MET:HB3	2.13	0.49
1:A:272:ALA:O	1:A:275:SER:HB3	2.13	0.49
1:A:456:MET:HE3	1:A:507:VAL:HG22	1.94	0.49
1:A:464:PRO:O	1:A:465:TYR:HB2	2.13	0.49
1:A:807:GLY:HA3	2:B:728:ARG:NH1	2.28	0.49
2:B:95:ILE:HG13	2:B:130:VAL:HG22	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:364:ILE:O	2:B:365:THR:HB	2.12	0.49
2:B:530:GLY:CA	11:R:12:G:H22	2.23	0.49
2:B:807:ARG:O	2:B:810:GLU:HB3	2.13	0.49
1:A:443:LEU:O	1:A:489:LEU:HA	2.12	0.49
1:A:626:ASN:O	1:A:631:HIS:ND1	2.45	0.49
1:A:716:ASP:O	1:A:717:ASN:C	2.56	0.49
1:A:1064:VAL:O	1:A:1064:VAL:HG12	2.13	0.49
1:A:1094:VAL:HA	1:A:1113:THR:HG21	1.95	0.49
3:C:35:ARG:NH1	9:K:41:THR:OG1	2.45	0.49
10:L:60:ARG:HG3	10:L:61:THR:N	2.27	0.49
1:A:649:ILE:O	1:A:653:VAL:HG23	2.13	0.49
2:B:515:HIS:H	2:B:518:HIS:CD2	2.30	0.49
2:B:879:ARG:O	2:B:880:THR:OG1	2.27	0.49
9:K:7:PHE:HA	9:K:10:PHE:CE2	2.47	0.49
1:A:800:VAL:HG13	1:A:812:GLU:CD	2.38	0.48
1:A:900:ASP:HA	1:A:926:GLN:HE22	1.77	0.48
2:B:899:ILE:H	2:B:899:ILE:HD12	1.77	0.48
8:J:57:ILE:O	8:J:58:GLU:C	2.56	0.48
1:A:398:GLU:O	1:A:399:HIS:O	2.30	0.48
1:A:513:SER:O	1:A:515:GLN:N	2.46	0.48
1:A:666:ILE:HD12	1:A:666:ILE:N	2.27	0.48
1:A:909:ASP:HB3	1:A:912:LEU:HG	1.95	0.48
2:B:874:PHE:CE1	2:B:964:VAL:HG23	2.47	0.48
4:E:191:LYS:O	4:E:214:CYS:HB3	2.14	0.48
6:H:42:ILE:HG23	6:H:95:TYR:HE1	1.78	0.48
1:A:33:ALA:HB3	1:A:82:GLY:HA3	1.95	0.48
1:A:49:LYS:CB	1:A:50:ILE:HA	2.35	0.48
2:B:792:MET:O	2:B:793:ALA:CB	2.61	0.48
2:B:857:ARG:NH2	2:B:942:ARG:NH2	2.62	0.48
3:C:52:GLU:HB3	3:C:154:LYS:HB3	1.94	0.48
8:J:44:TYR:HA	8:J:47:ARG:HB2	1.95	0.48
1:A:56:PRO:O	1:A:57:ARG:HB2	2.11	0.48
1:A:341:MET:HE1	1:A:843:LYS:HZ3	1.78	0.48
1:A:360:GLU:HB2	1:A:363:GLN:OE1	2.13	0.48
1:A:871:ASP:OD1	1:A:1366:ARG:NH2	2.45	0.48
1:A:1169:ILE:HB	1:A:1170:ILE:HB	1.94	0.48
2:B:256:VAL:HG11	2:B:382:ILE:CD1	2.44	0.48
2:B:636:PRO:O	2:B:692:TYR:HA	2.13	0.48
2:B:977:GLY:HA2	2:B:990:ILE:O	2.13	0.48
2:B:979:LYS:HB2	2:B:1097:HIS:HB2	1.95	0.48
4:E:62:ALA:N	4:E:78:LEU:O	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:492:PRO:HB3	1:A:497:THR:HG22	1.94	0.48
2:B:525:ALA:O	2:B:768:THR:HG23	2.14	0.48
2:B:541:LEU:HB2	2:B:747:MET:HE3	1.95	0.48
3:C:58:LEU:HB3	3:C:62:PHE:HD2	1.78	0.48
3:C:238:ILE:HG22	3:C:239:PRO:O	2.13	0.48
3:C:251:LEU:O	3:C:255:VAL:HG23	2.13	0.48
1:A:188:ASP:C	1:A:189:ARG:HG2	2.39	0.48
1:A:351:THR:HG22	1:A:468:PHE:HD1	1.70	0.48
1:A:1344:GLY:O	1:A:1345:ARG:C	2.56	0.48
1:A:1353:TYR:C	1:A:1355:VAL:H	2.21	0.48
2:B:414:ALA:C	2:B:416:LEU:H	2.22	0.48
2:B:498:THR:CG2	2:B:499:ASN:H	2.26	0.48
2:B:604:ARG:CD	2:B:691:GLU:OE2	2.58	0.48
2:B:1051:THR:HB	2:B:1054:GLY:H	1.77	0.48
3:C:58:LEU:HD21	8:J:57:ILE:HD13	1.96	0.48
1:A:266:LEU:HD21	1:A:303:TYR:CE1	2.49	0.48
1:A:492:PRO:HA	2:B:1149:GLU:OE1	2.14	0.48
1:A:676:MET:O	1:A:677:ARG:C	2.56	0.48
2:B:377:PHE:O	2:B:380:TYR:N	2.42	0.48
2:B:706:GLN:H	2:B:710:LEU:HG	1.79	0.48
2:B:893:LEU:HD11	2:B:910:VAL:HG12	1.95	0.48
3:C:222:LYS:O	3:C:223:ALA:HB2	2.12	0.48
4:E:161:LYS:HD2	4:E:195:VAL:HG23	1.96	0.48
5:F:85:MET:HE2	5:F:90:ARG:HA	1.95	0.48
10:L:30:ILE:O	10:L:56:LEU:HD23	2.14	0.48
1:A:152:VAL:CG2	1:A:153:PRO:HD2	2.43	0.48
1:A:568:PRO:HD3	6:H:94:ASP:O	2.14	0.48
1:A:598:LEU:HB3	6:H:25:ARG:HH12	1.78	0.48
1:A:900:ASP:HA	1:A:926:GLN:NE2	2.29	0.48
3:C:163:ILE:HD13	9:K:10:PHE:CE1	2.49	0.48
6:H:6:PHE:CG	6:H:7:ASP:N	2.82	0.48
1:A:360:GLU:HA	1:A:360:GLU:OE2	2.14	0.48
1:A:471:ASN:HD22	1:A:473:SER:H	1.62	0.48
1:A:1280:GLU:O	1:A:1281:ARG:C	2.57	0.48
1:A:1383:SER:C	1:A:1388:GLY:HA3	2.38	0.48
1:A:388:LEU:HA	1:A:391:LEU:HD12	1.96	0.48
1:A:549:MET:O	1:A:552:TRP:HB2	2.14	0.48
2:B:215:GLN:HE22	2:B:499:ASN:HB3	1.78	0.48
2:B:440:HIS:C	2:B:442:PHE:N	2.70	0.48
6:H:6:PHE:HD2	6:H:59:ILE:HG12	1.79	0.48
1:A:38:PRO:HG3	1:A:274:ILE:CD1	2.43	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1135:ARG:O	2:B:1139:ILE:HG13	2.13	0.47
2:B:1142:GLY:HA3	5:F:88:TYR:HE2	1.78	0.47
2:B:1166:CYS:SG	2:B:1167:GLY:N	2.87	0.47
2:B:1196:ILE:HG13	2:B:1200:ALA:HB3	1.96	0.47
3:C:34:ARG:O	3:C:38:ILE:HG12	2.14	0.47
6:H:41:ASP:HB3	6:H:121:LEU:HB3	1.96	0.47
1:A:535:THR:O	1:A:575:LYS:HE2	2.14	0.47
1:A:901:LEU:HB2	1:A:926:GLN:HG2	1.96	0.47
2:B:211:VAL:HG21	2:B:483:LEU:HG	1.96	0.47
2:B:636:PRO:CB	2:B:637:LEU:CB	2.71	0.47
2:B:779:GLY:O	2:B:795:ILE:HG23	2.15	0.47
2:B:795:ILE:H	2:B:795:ILE:HD12	1.80	0.47
2:B:810:GLU:HG3	2:B:811:TYR:CD2	2.50	0.47
2:B:1024:ALA:O	2:B:1027:ILE:N	2.47	0.47
2:B:1025:HIS:ND1	2:B:1025:HIS:C	2.72	0.47
3:C:102:GLN:HB3	3:C:154:LYS:HE2	1.96	0.47
3:C:127:ARG:HG3	3:C:129:ILE:CG2	2.44	0.47
1:A:156:ASP:OD1	1:A:156:ASP:N	2.32	0.47
2:B:85:SER:N	2:B:86:ARG:HB3	2.30	0.47
2:B:1016:ALA:O	2:B:1017:ILE:HD13	2.14	0.47
2:B:1073:TYR:OH	3:C:179:GLU:HG3	2.13	0.47
3:C:27:LEU:C	3:C:29:MET:H	2.22	0.47
3:C:227:THR:C	3:C:228:PHE:CD1	2.92	0.47
6:H:113:ALA:HA	6:H:125:LEU:O	2.13	0.47
1:A:513:SER:C	1:A:515:GLN:N	2.72	0.47
1:A:546:VAL:O	1:A:550:LEU:HD22	2.13	0.47
1:A:663:SER:HA	2:B:1014:PRO:HG3	1.97	0.47
1:A:861:GLY:HA3	4:E:174:GLN:HE21	1.79	0.47
1:A:1081:LEU:CD1	1:A:1082:ASN:ND2	2.78	0.47
1:A:1168:GLU:HA	1:A:1171:GLN:HB2	1.94	0.47
2:B:979:LYS:CD	2:B:1097:HIS:CD2	2.87	0.47
3:C:84:ARG:HD2	9:K:11:LEU:HD21	1.97	0.47
1:A:40:THR:HB	1:A:41:MET:HA	1.96	0.47
1:A:1287:TYR:CD2	1:A:1305:VAL:HG21	2.50	0.47
2:B:90:ILE:CG2	2:B:91:SER:N	2.77	0.47
2:B:549:THR:HG22	2:B:550:ASP:N	2.20	0.47
2:B:906:SER:O	2:B:907:GLY:C	2.57	0.47
2:B:1070:GLU:O	2:B:1071:VAL:C	2.57	0.47
3:C:29:MET:O	3:C:30:ALA:C	2.57	0.47
9:K:24:ASP:OD1	9:K:74:ARG:NH1	2.47	0.47
1:A:107:CYS:SG	1:A:167:CYS:SG	3.11	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154:SER:O	1:A:156:ASP:N	2.48	0.47
1:A:447:GLN:HA	1:A:448:PRO:C	2.40	0.47
1:A:608:ILE:HB	1:A:613:ILE:HD11	1.96	0.47
1:A:1434:ALA:HA	1:A:1435:PRO:HD2	1.70	0.47
2:B:1155:SER:HB3	2:B:1156:ASP:H	1.55	0.47
3:C:37:MET:HG2	3:C:176:ILE:HD11	1.96	0.47
7:I:62:ILE:C	7:I:64:SER:H	2.22	0.47
1:A:666:ILE:HG22	1:A:670:ILE:HD11	1.97	0.47
2:B:190:TYR:CE1	8:J:62:ARG:HD3	2.50	0.47
2:B:202:TYR:C	2:B:203:PHE:CD1	2.93	0.47
2:B:440:HIS:C	2:B:442:PHE:H	2.23	0.47
2:B:520:GLY:C	2:B:521:LEU:HG	2.39	0.47
2:B:1210:MET:HG2	2:B:1210:MET:O	2.15	0.47
3:C:84:ARG:HG3	3:C:85:ASP:OD1	2.15	0.47
3:C:183:TRP:CD1	3:C:183:TRP:H	2.32	0.47
4:E:198:ILE:N	4:E:210:SER:O	2.44	0.47
10:L:46:VAL:HG12	10:L:47:ARG:N	2.21	0.47
1:A:276:LEU:HD13	1:A:296:LEU:HD23	1.95	0.47
1:A:424:ILE:O	1:A:424:ILE:CG2	2.62	0.47
1:A:1227:ILE:HG22	1:A:1228:TRP:H	1.80	0.47
1:A:1407:GLU:O	1:A:1411:GLU:HG2	2.15	0.47
2:B:334:ILE:HG22	2:B:334:ILE:O	2.14	0.47
2:B:583:ASN:HD21	2:B:628:THR:HB	1.79	0.47
2:B:637:LEU:O	2:B:690:VAL:HA	2.13	0.47
4:E:100:ILE:HG23	4:E:105:PHE:HB2	1.97	0.47
6:H:62:SER:O	6:H:63:LEU:C	2.58	0.47
9:K:32:VAL:HA	9:K:73:LEU:O	2.15	0.47
9:K:65:HIS:HD2	9:K:67:PHE:HB2	1.72	0.47
1:A:115:LEU:CD1	1:A:122:MET:CE	2.65	0.47
1:A:313:GLN:HB2	1:A:314:ALA:CB	2.45	0.47
1:A:804:TYR:OH	2:B:763:GLN:HB2	2.15	0.47
2:B:121:ASN:N	2:B:121:ASN:HD22	2.13	0.47
2:B:304:ASP:C	2:B:306:ASN:H	2.22	0.47
1:A:265:LYS:HB2	1:A:265:LYS:NZ	2.30	0.47
2:B:370:PHE:HD2	2:B:373:ARG:HG3	1.79	0.47
2:B:809:MET:HA	2:B:812:LEU:HD12	1.97	0.47
3:C:37:MET:HE3	3:C:37:MET:HB2	1.68	0.47
3:C:142:VAL:HG23	8:J:5:VAL:HG13	1.96	0.47
9:K:7:PHE:CD1	9:K:7:PHE:C	2.93	0.47
1:A:342:GLY:HA3	2:B:1131:GLY:HA2	1.96	0.46
1:A:413:ILE:N	1:A:413:ILE:HD12	2.29	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:492:PRO:HB3	1:A:497:THR:CG2	2.45	0.46
1:A:809:THR:HG23	1:A:812:GLU:OE1	2.14	0.46
2:B:203:PHE:C	2:B:204:ILE:HD12	2.39	0.46
2:B:820:GLY:O	2:B:821:GLN:HG3	2.15	0.46
3:C:248:ILE:HD13	9:K:101:LEU:HD13	1.96	0.46
4:E:29:PHE:C	4:E:30:ILE:HG13	2.40	0.46
12:T:26:DG:C2	12:T:27:DA:H1'	2.50	0.46
1:A:760:GLN:HE21	1:A:765:VAL:HA	1.80	0.46
1:A:917:SER:C	1:A:919:ILE:H	2.24	0.46
1:A:1021:LEU:HD11	1:A:1025:ARG:HE	1.80	0.46
1:A:1044:TRP:O	1:A:1045:VAL:C	2.59	0.46
1:A:1097:GLY:C	1:A:1099:PRO:HD2	2.41	0.46
1:A:1341:ILE:HD13	1:A:1380:GLY:HA2	1.96	0.46
1:A:1376:THR:CG2	4:E:212:ARG:HH22	2.29	0.46
1:A:1436:ILE:O	1:A:1437:GLY:C	2.57	0.46
4:E:185:ALA:HB1	4:E:190:LEU:HD23	1.96	0.46
1:A:106:VAL:HG11	1:A:214:ILE:CD1	2.46	0.46
1:A:465:TYR:HD2	2:B:976:ILE:HB	1.80	0.46
1:A:655:PHE:O	1:A:656:TRP:C	2.57	0.46
1:A:946:VAL:HG12	1:A:947:PHE:N	2.29	0.46
1:A:956:LEU:HD23	1:A:957:PRO:HD2	1.96	0.46
2:B:60:GLN:OE1	2:B:95:ILE:HG22	2.15	0.46
2:B:1132:GLU:C	2:B:1134:GLU:N	2.72	0.46
3:C:37:MET:HB3	3:C:38:ILE:H	1.61	0.46
1:A:3:GLY:C	1:A:4:GLN:HG3	2.41	0.46
1:A:95:PHE:HB3	1:A:234:MET:SD	2.56	0.46
1:A:320:ARG:O	1:A:321:PRO:C	2.59	0.46
1:A:1444:MET:HB2	5:F:133:VAL:CG1	2.45	0.46
2:B:173:MET:HB2	2:B:203:PHE:CZ	2.50	0.46
2:B:1096:ARG:O	2:B:1097:HIS:C	2.57	0.46
1:A:310:GLY:CA	1:A:311:GLN:CB	2.80	0.46
1:A:353:ILE:HG21	1:A:487:MET:HE3	1.97	0.46
1:A:465:TYR:N	1:A:465:TYR:CD1	2.84	0.46
2:B:488:TYR:HE2	2:B:812:LEU:O	1.97	0.46
2:B:515:HIS:HD2	2:B:517:THR:H	1.63	0.46
2:B:549:THR:CG2	2:B:550:ASP:H	2.18	0.46
2:B:1074:ASN:HB3	2:B:1077:THR:CG2	2.45	0.46
2:B:1131:GLY:N	2:B:1134:GLU:OE1	2.49	0.46
3:C:69:LEU:HD12	8:J:6:ARG:CD	2.46	0.46
3:C:204:SER:O	3:C:206:ASN:N	2.48	0.46
1:A:118:HIS:CB	1:A:123:ARG:HB3	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:370:ILE:CG2	2:B:1105:ALA:HB2	2.42	0.46
1:A:508:PRO:HB3	1:A:643:ALA:HB2	1.98	0.46
1:A:1100:ARG:HH12	1:A:1111:MET:HE3	1.81	0.46
1:A:1101:LEU:O	1:A:1105:LEU:HD12	2.16	0.46
2:B:313:MET:HA	2:B:313:MET:HE2	1.97	0.46
2:B:796:LEU:O	2:B:797:TYR:C	2.59	0.46
2:B:1110:PRO:HB2	2:B:1119:VAL:CG2	2.46	0.46
6:H:93:TYR:CD1	6:H:143:LEU:HD23	2.50	0.46
7:I:52:ILE:HG13	7:I:53:GLY:H	1.81	0.46
7:I:84:VAL:CG2	7:I:85:PHE:N	2.78	0.46
1:A:55:ASP:O	1:A:56:PRO:C	2.58	0.46
1:A:112:LYS:HG2	1:A:113:LEU:N	2.30	0.46
1:A:190:ALA:O	1:A:191:THR:OG1	2.30	0.46
1:A:368:LYS:O	1:A:372:LYS:N	2.49	0.46
1:A:667:GLY:HA2	1:A:670:ILE:HG13	1.97	0.46
1:A:731:ARG:HG3	1:A:755:PHE:CZ	2.51	0.46
1:A:1086:PHE:CE1	1:A:1092:LYS:HG2	2.51	0.46
2:B:636:PRO:O	2:B:691:GLU:O	2.33	0.46
2:B:754:SER:O	2:B:806:THR:OG1	2.27	0.46
2:B:1093:GLN:H	2:B:1093:GLN:HG2	1.52	0.46
4:E:27:GLY:O	4:E:65:THR:HG22	2.14	0.46
8:J:57:ILE:O	8:J:60:PHE:HB2	2.15	0.46
1:A:4:GLN:O	1:A:5:GLN:HG3	2.15	0.46
1:A:563:PRO:HB3	1:A:572:TRP:CD2	2.51	0.46
2:B:289:LEU:O	2:B:327:ARG:NH2	2.47	0.46
2:B:1115:THR:CG2	2:B:1117:GLN:HG3	2.45	0.46
3:C:69:LEU:HD12	8:J:6:ARG:HD3	1.98	0.46
8:J:10:CYS:CB	8:J:46:CYS:SG	3.03	0.46
1:A:120:GLU:O	1:A:121:LEU:C	2.59	0.46
1:A:466:SER:HB3	2:B:1103:ILE:CD1	2.46	0.46
1:A:841:LEU:HD21	1:A:1105:LEU:HD22	1.97	0.46
1:A:1344:GLY:O	1:A:1347:ALA:N	2.46	0.46
3:C:15:LYS:HE3	9:K:114:LEU:HD22	1.98	0.46
3:C:142:VAL:CG2	8:J:5:VAL:HG13	2.46	0.46
6:H:16:ASP:HA	6:H:17:PRO:HD3	1.83	0.46
8:J:43:ARG:HB2	8:J:45:CYS:SG	2.56	0.46
9:K:21:ILE:HD12	9:K:33:ILE:HG12	1.98	0.46
1:A:323:LYS:HD3	1:A:323:LYS:HA	1.70	0.46
1:A:353:ILE:HG22	1:A:468:PHE:HB2	1.98	0.46
1:A:890:ASP:OD2	1:A:1296:GLY:HA2	2.16	0.46
1:A:1308:THR:CG2	1:A:1309:ASP:N	2.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:748:ILE:HG12	2:B:748:ILE:H	1.49	0.46
2:B:860:MET:O	2:B:861:ASP:HB2	2.15	0.46
3:C:176:ILE:O	3:C:176:ILE:HG22	2.14	0.46
3:C:244:VAL:HG21	9:K:105:PHE:CE1	2.51	0.46
8:J:5:VAL:HA	8:J:15:GLY:N	2.28	0.46
1:A:495:GLU:O	1:A:498:ARG:HB2	2.16	0.45
1:A:523:ILE:HG22	1:A:528:LEU:HB2	1.97	0.45
1:A:1008:GLN:HA	1:A:1011:GLN:HB3	1.98	0.45
1:A:1011:GLN:O	1:A:1015:VAL:HG23	2.16	0.45
3:C:241:ASP:O	3:C:244:VAL:HG13	2.17	0.45
1:A:208:LEU:HD13	1:A:209:ASN:N	2.32	0.45
1:A:265:LYS:HE2	1:A:303:TYR:HA	1.98	0.45
1:A:525:GLN:HB3	2:B:1015:HIS:HD2	1.81	0.45
1:A:779:PHE:CZ	2:B:517:THR:HA	2.51	0.45
2:B:1188:LYS:HB2	2:B:1189:ILE:HD12	1.98	0.45
3:C:235:VAL:HG11	8:J:6:ARG:NH2	2.29	0.45
4:E:28:TYR:CE1	4:E:78:LEU:HD13	2.50	0.45
6:H:31:THR:C	6:H:33:GLN:H	2.24	0.45
9:K:57:LEU:HD12	9:K:76:GLN:HG2	1.98	0.45
12:T:6:DG:H2'	12:T:7:DA:C8	2.51	0.45
1:A:491:VAL:HA	1:A:492:PRO:HD2	1.61	0.45
1:A:939:ASP:O	1:A:940:ARG:C	2.58	0.45
2:B:41:LYS:HB3	2:B:45:SER:HB3	1.97	0.45
2:B:797:TYR:HE1	2:B:854:LEU:HG	1.81	0.45
2:B:874:PHE:CE1	2:B:964:VAL:CG2	3.00	0.45
2:B:879:ARG:HA	2:B:879:ARG:NH1	2.30	0.45
1:A:55:ASP:CA	1:A:58:LEU:O	2.65	0.45
2:B:795:ILE:HD12	2:B:795:ILE:N	2.31	0.45
2:B:1106:ARG:NH1	2:B:1110:PRO:HD2	2.31	0.45
3:C:33:LEU:O	3:C:37:MET:HE3	2.17	0.45
7:I:68:LEU:HA	7:I:69:PRO:HD2	1.56	0.45
7:I:96:SER:HB2	7:I:98:VAL:HG23	1.97	0.45
2:B:78:THR:N	2:B:79:THR:CB	2.72	0.45
2:B:635:ARG:NH2	2:B:742:GLU:OE2	2.47	0.45
2:B:728:ARG:NH1	2:B:760:ASP:OD2	2.49	0.45
2:B:1202:LEU:O	2:B:1205:GLN:HB2	2.16	0.45
3:C:15:LYS:C	3:C:16:ASP:OD2	2.60	0.45
3:C:142:VAL:HG13	3:C:144:ILE:CD1	2.46	0.45
4:E:28:TYR:HA	4:E:64:PRO:HA	1.98	0.45
5:F:93:ILE:O	5:F:94:LEU:C	2.58	0.45
5:F:136:ARG:HD2	5:F:146:TRP:CD1	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:109:LYS:HB3	6:H:111:LEU:N	2.27	0.45
1:A:88:LYS:HA	1:A:89:PRO:HD2	1.54	0.45
1:A:399:HIS:CD2	1:A:400:PRO:CG	2.99	0.45
1:A:500:GLU:OE1	2:B:1145:SER:N	2.49	0.45
1:A:912:LEU:HD22	1:A:1036:ARG:NH2	2.32	0.45
2:B:721:LEU:HA	2:B:722:ASP:HA	1.77	0.45
2:B:999:MET:HG2	2:B:1008:PRO:HD2	1.98	0.45
2:B:1081:LEU:HD23	2:B:1081:LEU:HA	1.81	0.45
2:B:1084:GLN:CD	2:B:1084:GLN:N	2.71	0.45
8:J:44:TYR:CD1	8:J:44:TYR:C	2.94	0.45
1:A:247:ARG:NH1	1:A:263:THR:HG23	2.31	0.45
1:A:571:LEU:C	1:A:572:TRP:HE3	2.23	0.45
2:B:273:LEU:CB	2:B:276:ILE:HD12	2.47	0.45
2:B:333:PHE:C	2:B:335:GLY:H	2.25	0.45
2:B:554:ILE:O	2:B:557:PHE:HB3	2.17	0.45
2:B:1164:GLY:HA3	2:B:1190:ASP:HB3	1.99	0.45
2:B:1206:GLU:O	2:B:1207:LEU:C	2.59	0.45
3:C:41:ILE:HD11	3:C:243:VAL:HG13	1.97	0.45
3:C:44:LEU:HD22	3:C:129:ILE:HG13	1.99	0.45
3:C:242:GLN:OE1	3:C:242:GLN:HA	2.16	0.45
1:A:129:LYS:O	1:A:130:ASP:HB2	2.16	0.45
1:A:160:GLN:H	1:A:160:GLN:CD	2.17	0.45
1:A:590:ARG:NH2	1:A:621:THR:HA	2.32	0.45
1:A:811:GLN:O	1:A:812:GLU:C	2.60	0.45
2:B:344:LYS:HG2	2:B:347:LYS:HD2	1.98	0.45
2:B:422:LYS:O	2:B:425:THR:HG22	2.17	0.45
2:B:488:TYR:C	2:B:490:SER:N	2.75	0.45
2:B:1168:LEU:HD13	2:B:1208:MET:HE3	1.97	0.45
3:C:5:GLY:HA3	3:C:6:PRO:HD2	1.77	0.45
3:C:176:ILE:HG12	3:C:232:VAL:HG13	1.98	0.45
5:F:77:ASP:OD1	5:F:78:GLN:HG3	2.17	0.45
7:I:7:CYS:O	7:I:11:ASN:HA	2.17	0.45
1:A:41:MET:HG3	1:A:42:ASP:N	2.29	0.45
1:A:315:LEU:HD22	1:A:315:LEU:H	1.81	0.45
1:A:344:ARG:CZ	2:B:1120:GLU:HG3	2.47	0.45
1:A:511:ILE:HG12	1:A:521:MET:HG3	1.97	0.45
1:A:541:ILE:HG21	1:A:549:MET:CE	2.47	0.45
1:A:1389:PHE:O	1:A:1390:ASN:CG	2.60	0.45
2:B:192:LEU:O	2:B:193:LYS:HB2	2.16	0.45
2:B:376:PHE:CE2	2:B:569:TYR:HD2	2.34	0.45
2:B:439:ALA:HB3	2:B:440:HIS:CG	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:662:MET:C	2:B:664:THR:H	2.24	0.45
7:I:32:CYS:SG	7:I:33:SER:N	2.87	0.45
1:A:278:THR:O	1:A:282:ASN:HB2	2.17	0.45
1:A:464:PRO:C	1:A:465:TYR:CD1	2.94	0.45
2:B:345:LYS:HE2	2:B:348:ARG:HH22	1.81	0.45
2:B:364:ILE:HD13	2:B:585:VAL:HG13	1.99	0.45
2:B:604:ARG:HD3	2:B:691:GLU:CD	2.41	0.45
2:B:953:LEU:HA	10:L:56:LEU:O	2.17	0.45
6:H:23:VAL:CG1	6:H:24:CYS:N	2.80	0.45
6:H:110:ASP:O	6:H:128:ASN:ND2	2.50	0.45
1:A:438:ASP:OD1	1:A:461:LYS:HA	2.17	0.44
1:A:567:LYS:C	1:A:569:LYS:N	2.76	0.44
1:A:1431:GLY:HA3	2:B:1152:MET:SD	2.57	0.44
2:B:471:LYS:CB	2:B:472:ALA:HA	2.47	0.44
2:B:964:VAL:HG12	2:B:965:LYS:H	1.81	0.44
1:A:389:THR:HA	1:A:426:LEU:HD12	2.00	0.44
1:A:472:LEU:HD13	2:B:835:GLN:NE2	2.32	0.44
1:A:714:PHE:O	1:A:715:GLU:C	2.58	0.44
1:A:1085:HIS:O	1:A:1086:PHE:CG	2.71	0.44
1:A:1383:SER:OG	1:A:1388:GLY:N	2.51	0.44
2:B:121:ASN:HD21	2:B:965:LYS:HE3	1.83	0.44
2:B:221:ASN:OD1	2:B:242:SER:HA	2.17	0.44
2:B:634:TYR:HA	2:B:693:ILE:O	2.16	0.44
2:B:905:VAL:HG12	2:B:906:SER:N	2.32	0.44
2:B:975:GLN:HE21	2:B:975:GLN:HB3	1.52	0.44
2:B:996:ARG:HG3	2:B:1007:VAL:HG21	2.00	0.44
2:B:1162:ILE:HG22	2:B:1163:CYS:N	2.32	0.44
4:E:213:ILE:HG12	4:E:214:CYS:N	2.30	0.44
5:F:101:ILE:HB	5:F:117:PRO:HB3	1.99	0.44
1:A:326:ARG:HG2	1:A:1406:VAL:HG21	2.00	0.44
2:B:440:HIS:O	2:B:442:PHE:N	2.50	0.44
2:B:515:HIS:O	2:B:516:ASN:C	2.61	0.44
2:B:530:GLY:HA2	2:B:533:CYS:HB2	2.00	0.44
2:B:698:GLU:O	2:B:701:ILE:HD13	2.16	0.44
2:B:765:PRO:O	2:B:769:TYR:N	2.49	0.44
2:B:857:ARG:NH2	12:T:24:DT:OP1	2.51	0.44
3:C:43:THR:CG2	3:C:44:LEU:H	2.26	0.44
10:L:26:THR:O	10:L:27:LEU:O	2.34	0.44
1:A:118:HIS:HB2	1:A:123:ARG:CG	2.40	0.44
1:A:375:THR:OG1	1:A:433:GLU:HB3	2.17	0.44
1:A:380:VAL:HG11	1:A:427:GLN:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1152:ILE:HB	7:I:44:TYR:HB3	1.98	0.44
2:B:40:GLU:HG3	2:B:681:TRP:HB3	1.99	0.44
2:B:215:GLN:NE2	2:B:499:ASN:HB3	2.32	0.44
2:B:363:HIS:C	2:B:365:THR:N	2.75	0.44
2:B:365:THR:HG21	2:B:370:PHE:CG	2.53	0.44
2:B:589:VAL:HG12	2:B:590:HIS:N	2.32	0.44
2:B:640:VAL:HG12	2:B:641:GLU:N	2.32	0.44
2:B:773:MET:HA	2:B:776:GLN:NE2	2.33	0.44
2:B:1033:LYS:N	2:B:1089:PRO:HG2	2.33	0.44
4:E:160:GLU:O	4:E:163:GLU:HB3	2.18	0.44
4:E:213:ILE:CG1	4:E:214:CYS:H	2.28	0.44
7:I:45:ARG:HE	7:I:47:GLU:HG3	1.81	0.44
10:L:41:SER:O	10:L:44:ASP:CB	2.66	0.44
1:A:442:VAL:O	1:A:457:ALA:HA	2.17	0.44
1:A:599:SER:HA	1:A:600:PRO:HD2	1.71	0.44
1:A:645:LEU:O	1:A:649:ILE:HG13	2.17	0.44
1:A:1021:LEU:HD12	1:A:1025:ARG:HE	1.80	0.44
2:B:466:TRP:HA	2:B:466:TRP:CE3	2.52	0.44
2:B:657:HIS:CE1	2:B:689:LEU:HD11	2.53	0.44
2:B:739:THR:HB	2:B:740:HIS:ND1	2.31	0.44
2:B:797:TYR:HB3	2:B:798:TYR:CD1	2.53	0.44
2:B:1092:TYR:C	2:B:1093:GLN:O	2.57	0.44
9:K:113:THR:O	9:K:114:LEU:HB2	2.18	0.44
12:T:14:DG:H2'	12:T:15:DA:C4	2.52	0.44
1:A:185:TRP:HB2	1:A:198:GLU:HG2	1.99	0.44
1:A:323:LYS:HG3	1:A:327:ALA:CB	2.47	0.44
1:A:367:PRO:HB3	1:A:465:TYR:O	2.18	0.44
1:A:531:ILE:O	1:A:531:ILE:HG12	2.17	0.44
1:A:824:LEU:HD22	2:B:529:GLU:OE1	2.18	0.44
2:B:212:LEU:HD23	2:B:212:LEU:HA	1.66	0.44
2:B:809:MET:HE1	2:B:983:ARG:HH21	1.83	0.44
3:C:51:VAL:HG13	3:C:155:LEU:HD23	1.98	0.44
5:F:93:ILE:HD11	5:F:134:ILE:HD11	1.98	0.44
7:I:85:PHE:O	7:I:86:PHE:HB3	2.17	0.44
1:A:120:GLU:C	1:A:122:MET:N	2.63	0.44
1:A:1189:SER:HB2	1:A:1242:VAL:O	2.17	0.44
2:B:781:PHE:HE2	2:B:785:TYR:HB2	1.82	0.44
2:B:1110:PRO:HB2	2:B:1119:VAL:HG22	1.99	0.44
7:I:78:CYS:O	7:I:79:HIS:HB2	2.18	0.44
11:R:5:A:H2'	11:R:6:G:H8	1.82	0.44
1:A:662:PHE:HD2	2:B:829:CYS:SG	2.40	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:709:THR:HG22	1:A:710:LEU:N	2.33	0.44
2:B:64:CYS:HA	2:B:67:SER:HB3	1.99	0.44
2:B:414:ALA:C	2:B:416:LEU:N	2.76	0.44
2:B:473:MET:HA	2:B:474:SER:HA	1.84	0.44
2:B:1156:ASP:OD2	2:B:1156:ASP:N	2.49	0.44
3:C:167:HIS:CD2	3:C:167:HIS:C	2.96	0.44
1:A:399:HIS:CE1	1:A:462:VAL:HG21	2.52	0.44
1:A:407:ARG:HD3	1:A:413:ILE:HD11	1.99	0.44
1:A:447:GLN:CB	1:A:448:PRO:HA	2.47	0.44
1:A:1156:PRO:O	1:A:1158:PRO:HD3	2.18	0.44
2:B:293:PRO:O	2:B:297:ILE:HG12	2.17	0.44
2:B:349:ILE:C	2:B:351:TYR:H	2.25	0.44
2:B:522:VAL:HG12	2:B:523:CYS:N	2.32	0.44
2:B:986:GLN:HG3	2:B:1025:HIS:CD2	2.52	0.44
3:C:115:SER:OG	3:C:141:GLY:HA3	2.18	0.44
10:L:30:ILE:C	10:L:56:LEU:HD23	2.43	0.44
1:A:23:SER:HA	1:A:24:PRO:HD2	1.67	0.43
1:A:49:LYS:CB	1:A:50:ILE:O	2.64	0.43
1:A:116:ASP:O	1:A:117:GLU:O	2.36	0.43
1:A:154:SER:O	1:A:155:GLU:C	2.61	0.43
1:A:340:LEU:HD22	1:A:1429:ILE:HG23	2.00	0.43
1:A:548:ASN:HA	9:K:60:ALA:HB1	1.99	0.43
1:A:667:GLY:HA2	1:A:670:ILE:HG12	1.99	0.43
1:A:858:ASN:C	1:A:858:ASN:HD22	2.26	0.43
1:A:1173:HIS:CG	1:A:1173:HIS:O	2.70	0.43
1:A:1331:SER:OG	1:A:1333:ILE:HG23	2.18	0.43
2:B:260:GLY:O	2:B:267:ARG:HD3	2.18	0.43
5:F:86:THR:OG1	5:F:89:GLU:HG3	2.18	0.43
6:H:98:TYR:C	6:H:98:TYR:CD2	2.96	0.43
8:J:9:SER:HB3	8:J:48:ARG:HH21	1.84	0.43
1:A:440:ASP:HB2	1:A:460:VAL:HG21	1.99	0.43
1:A:473:SER:OG	1:A:522:GLY:O	2.28	0.43
1:A:605:MET:HE3	1:A:614:PHE:O	2.18	0.43
1:A:852:TYR:CE2	1:A:1060:PRO:HB2	2.53	0.43
1:A:916:GLY:C	1:A:917:SER:O	2.59	0.43
2:B:401:PHE:O	2:B:404:LYS:HG3	2.18	0.43
2:B:764:SER:CB	2:B:765:PRO:HD3	2.47	0.43
9:K:10:PHE:CD2	9:K:10:PHE:N	2.86	0.43
13:N:11:DG:H2"	13:N:12:DT:H5"	2.00	0.43
1:A:11:LEU:HD13	2:B:1195:HIS:HD2	1.82	0.43
1:A:86:LEU:HD23	1:A:273:ASN:ND2	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:381:THR:OG1	1:A:382:PRO:HD2	2.18	0.43
1:A:1084:PHE:CD2	1:A:1086:PHE:O	2.69	0.43
2:B:20:ASP:O	2:B:20:ASP:CG	2.60	0.43
2:B:430:ARG:HA	2:B:433:GLN:HE21	1.83	0.43
2:B:822:ASN:HD22	8:J:52:THR:CG2	2.29	0.43
4:E:9:ILE:HG23	4:E:10:SER:H	1.82	0.43
6:H:26:ILE:HG22	6:H:40:LEU:O	2.18	0.43
7:I:87:GLN:O	7:I:88:SER:C	2.61	0.43
10:L:25:ALA:C	10:L:26:THR:CG2	2.91	0.43
11:R:7:A:C2	11:R:8:G:C4	3.06	0.43
12:T:13:DA:H2''	12:T:14:DG:C8	2.53	0.43
1:A:365:GLY:N	1:A:469:ARG:O	2.43	0.43
1:A:810:PRO:HA	2:B:1047:PHE:CE2	2.53	0.43
4:E:24:LYS:HB3	4:E:30:ILE:HD12	2.00	0.43
9:K:35:PHE:HD1	9:K:35:PHE:H	1.66	0.43
1:A:185:TRP:O	1:A:186:LYS:CB	2.67	0.43
2:B:174:LEU:HD22	2:B:202:TYR:CE1	2.54	0.43
1:A:901:LEU:HD22	1:A:919:ILE:HG23	2.00	0.43
2:B:46:GLN:OE1	2:B:47:GLN:N	2.52	0.43
2:B:597:MET:O	2:B:600:LEU:HB2	2.19	0.43
2:B:992:ILE:HD11	9:K:67:PHE:HE2	1.83	0.43
3:C:258:ILE:HG22	3:C:259:LEU:N	2.33	0.43
1:A:31:SER:HB2	1:A:81:PHE:O	2.18	0.43
1:A:678:GLU:CA	1:A:681:GLU:HG2	2.34	0.43
1:A:765:VAL:HG22	1:A:800:VAL:HB	1.97	0.43
1:A:1015:VAL:HG12	1:A:1015:VAL:O	2.18	0.43
1:A:1377:THR:HB	4:E:176:PRO:CA	2.48	0.43
1:A:1392:SER:C	1:A:1394:THR:N	2.77	0.43
1:A:1402:PHE:CZ	1:A:1403:GLU:OE2	2.72	0.43
2:B:211:VAL:HG12	2:B:212:LEU:N	2.34	0.43
3:C:123:ASN:HD22	3:C:125:MET:HG2	1.83	0.43
3:C:143:LEU:HG	8:J:2:ILE:HD11	2.01	0.43
9:K:94:ILE:O	9:K:95:ILE:C	2.61	0.43
12:T:6:DG:H4'	12:T:7:DA:OP1	2.19	0.43
1:A:295:LEU:O	1:A:298:PHE:HB3	2.18	0.43
1:A:384:ASN:O	1:A:385:ILE:C	2.61	0.43
1:A:775:ILE:HB	1:A:797:LYS:O	2.19	0.43
1:A:820:GLY:O	1:A:823:GLY:N	2.51	0.43
1:A:855:THR:HG22	1:A:866:PHE:O	2.19	0.43
1:A:1319:VAL:HB	1:A:1322:ILE:HD12	2.01	0.43
2:B:33:VAL:HG21	2:B:638:PHE:HZ	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:294:ASP:C	2:B:296:GLU:H	2.27	0.43
2:B:1002:THR:CG2	2:B:1006:ILE:CG1	2.96	0.43
6:H:114:VAL:CG2	6:H:125:LEU:HB3	2.49	0.43
1:A:622:VAL:O	1:A:630:ILE:HD11	2.19	0.43
1:A:675:THR:HG22	1:A:679:ILE:HD11	2.01	0.43
2:B:237:VAL:HG13	2:B:256:VAL:O	2.18	0.43
2:B:1154:ALA:O	2:B:1155:SER:CB	2.66	0.43
6:H:77:ARG:O	6:H:78:SER:C	2.61	0.43
9:K:44:ASN:HB2	9:K:61:TYR:OH	2.18	0.43
10:L:26:THR:C	10:L:27:LEU:O	2.60	0.43
1:A:379:VAL:HG12	1:A:380:VAL:H	1.84	0.43
1:A:769:SER:O	1:A:770:VAL:HB	2.18	0.43
1:A:1447:GLU:C	1:A:1449:SER:H	2.27	0.43
2:B:99:LYS:O	2:B:101:MET:HG3	2.18	0.43
2:B:763:GLN:HG2	2:B:765:PRO:HD2	2.01	0.43
2:B:764:SER:O	2:B:767:ASN:N	2.51	0.43
2:B:798:TYR:N	2:B:799:PRO:HD3	2.34	0.43
2:B:879:ARG:HH12	2:B:883:LEU:HB2	1.84	0.43
2:B:938:SER:O	2:B:940:PRO:HD3	2.19	0.43
3:C:27:LEU:HD12	3:C:228:PHE:CE2	2.43	0.43
3:C:204:SER:O	3:C:205:LYS:C	2.62	0.43
3:C:238:ILE:CG2	3:C:242:GLN:CB	2.93	0.43
8:J:45:CYS:SG	8:J:46:CYS:N	2.92	0.43
9:K:56:VAL:HG13	9:K:77:THR:HG23	2.01	0.43
1:A:575:LYS:O	1:A:579:SER:OG	2.36	0.42
1:A:846:GLU:HG2	1:A:1424:VAL:HG21	2.01	0.42
1:A:1057:VAL:HG12	1:A:1058:VAL:N	2.33	0.42
2:B:113:TYR:HB3	2:B:114:PRO:CD	2.49	0.42
2:B:248:SER:HA	2:B:418:LYS:HD3	2.01	0.42
2:B:461:LEU:HD12	2:B:480:SER:HB2	2.01	0.42
2:B:821:GLN:HE22	2:B:851:PHE:HA	1.83	0.42
2:B:1111:MET:C	2:B:1119:VAL:HG13	2.44	0.42
3:C:52:GLU:OE2	3:C:154:LYS:HG2	2.19	0.42
4:E:99:HIS:CD2	4:E:103:LYS:HD2	2.53	0.42
1:A:253:ASN:CA	1:A:255:SER:H	2.19	0.42
1:A:619:LYS:O	1:A:623:GLY:N	2.52	0.42
1:A:853:ASP:O	1:A:854:ASN:HB2	2.19	0.42
1:A:1243:VAL:HG13	1:A:1244:ARG:CB	2.48	0.42
1:A:1278:ASN:HD22	1:A:1312:ASN:HB2	1.83	0.42
2:B:25:ILE:HG23	2:B:29:ASP:HB2	2.01	0.42
2:B:115:GLN:O	2:B:119:LEU:HG	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:603:LEU:HD12	2:B:609:ILE:HD11	2.01	0.42
2:B:973:ILE:HG22	2:B:974:PRO:N	2.34	0.42
2:B:979:LYS:O	2:B:980:PHE:CD1	2.71	0.42
5:F:97:ARG:HD3	5:F:100:GLN:OE1	2.18	0.42
8:J:64:ASN:HB3	8:J:65:PRO:HD3	2.01	0.42
1:A:37:PHE:HA	1:A:38:PRO:HD3	1.84	0.42
1:A:311:GLN:H	1:A:313:GLN:HG3	1.85	0.42
1:A:567:LYS:HZ2	6:H:46:LEU:HB2	1.84	0.42
1:A:775:ILE:HD13	1:A:775:ILE:HA	1.88	0.42
1:A:1173:HIS:O	1:A:1173:HIS:ND1	2.52	0.42
2:B:834:ASN:O	2:B:1013:ASN:HB2	2.19	0.42
2:B:973:ILE:O	2:B:974:PRO:C	2.56	0.42
3:C:3:GLU:HB3	9:K:104:ASN:ND2	2.11	0.42
7:I:100:PHE:CD2	7:I:111:THR:HG23	2.55	0.42
8:J:48:ARG:CZ	8:J:49:MET:HE1	2.49	0.42
11:R:9:G:C2	12:T:21:DC:N3	2.88	0.42
11:R:11:U:H3'	11:R:12:G:H5'	2.01	0.42
1:A:18:GLN:O	2:B:1215:ARG:HG2	2.20	0.42
1:A:19:PHE:O	1:A:1416:ALA:HA	2.18	0.42
1:A:33:ALA:HB3	1:A:82:GLY:CA	2.50	0.42
1:A:202:LEU:HB3	1:A:207:ILE:HD11	2.00	0.42
1:A:996:ASN:OD1	1:A:996:ASN:N	2.52	0.42
2:B:476:ARG:H	2:B:476:ARG:HD3	1.84	0.42
2:B:755:ILE:HD13	2:B:755:ILE:HA	1.76	0.42
2:B:872:GLU:O	2:B:914:LYS:HB2	2.17	0.42
2:B:879:ARG:HH12	2:B:883:LEU:CB	2.32	0.42
2:B:1182:CYS:HB3	2:B:1185:CYS:HB2	2.01	0.42
3:C:35:ARG:HB2	9:K:41:THR:HG23	2.02	0.42
6:H:4:THR:HA	6:H:60:ALA:CB	2.48	0.42
1:A:979:SER:OG	1:A:981:LEU:HD12	2.17	0.42
1:A:1394:THR:HB	1:A:1395:GLY:H	1.70	0.42
2:B:223:VAL:HG21	2:B:384:ARG:HG3	1.99	0.42
2:B:1020:ARG:H	2:B:1020:ARG:HG2	1.59	0.42
2:B:1119:VAL:O	2:B:1126:GLY:HA3	2.19	0.42
2:B:1133:MET:HG3	12:T:19:DT:H4'	2.02	0.42
3:C:98:VAL:HG22	3:C:158:VAL:HG13	2.01	0.42
3:C:108:GLU:OE1	3:C:108:GLU:HA	2.20	0.42
10:L:25:ALA:O	10:L:26:THR:C	2.63	0.42
1:A:497:THR:CG2	2:B:1146:PHE:CD1	2.90	0.42
2:B:174:LEU:CD1	2:B:204:ILE:CD1	2.98	0.42
2:B:436:VAL:O	2:B:436:VAL:HG13	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:863:GLU:CA	2:B:864:LYS:CB	2.71	0.42
2:B:1134:GLU:O	2:B:1135:ARG:C	2.63	0.42
10:L:48:CYS:SG	10:L:49:LYS:N	2.92	0.42
1:A:239:LEU:HD13	1:A:240:PRO:O	2.19	0.42
1:A:649:ILE:HG13	1:A:649:ILE:H	1.73	0.42
1:A:956:LEU:HD23	1:A:957:PRO:HD3	2.01	0.42
2:B:102:VAL:HG12	2:B:112:LEU:HB2	2.01	0.42
2:B:225:VAL:H	2:B:396:ASP:HB2	1.84	0.42
2:B:416:LEU:HD21	2:B:460:ALA:CB	2.50	0.42
2:B:729:ILE:O	2:B:729:ILE:HG22	2.19	0.42
2:B:941:LEU:HD13	2:B:942:ARG:N	2.27	0.42
2:B:1107:ALA:O	2:B:1108:ARG:CB	2.67	0.42
3:C:56:THR:HG22	3:C:147:LEU:HD21	2.02	0.42
4:E:64:PRO:HD3	4:E:76:GLY:O	2.20	0.42
7:I:65:ASP:HA	7:I:66:PRO:HD3	1.74	0.42
1:A:185:TRP:O	1:A:198:GLU:CD	2.63	0.42
1:A:446:ARG:NH1	1:A:479:ASN:HB3	2.35	0.42
1:A:587:HIS:NE2	1:A:969:GLN:HG2	2.35	0.42
1:A:1349:TYR:HA	1:A:1372:VAL:HG21	2.01	0.42
2:B:90:ILE:HG22	2:B:91:SER:H	1.84	0.42
2:B:436:VAL:HA	2:B:438:GLU:O	2.20	0.42
2:B:1168:LEU:HD22	2:B:1214:PRO:HD2	2.01	0.42
3:C:184:ASN:HD21	3:C:189:THR:H	1.68	0.42
3:C:212:PRO:HA	3:C:213:PRO:HD3	1.88	0.42
5:F:130:ILE:HA	5:F:131:PRO:HD3	1.90	0.42
1:A:17:VAL:HB	1:A:1419:ASP:HB3	2.01	0.42
1:A:310:GLY:HA2	1:A:311:GLN:CB	2.46	0.42
1:A:1072:ILE:HD11	1:A:1368:MET:CG	2.49	0.42
2:B:521:LEU:HD22	2:B:633:VAL:HB	2.00	0.42
2:B:622:LYS:HE2	7:I:59:VAL:HG13	2.02	0.42
2:B:842:ASN:HA	2:B:994:TYR:O	2.20	0.42
2:B:901:PRO:HB3	2:B:950:ASP:O	2.19	0.42
3:C:180:TYR:O	3:C:181:ASP:O	2.37	0.42
3:C:195:GLN:O	3:C:196:ASP:C	2.62	0.42
1:A:284:ALA:N	1:A:285:PRO:CD	2.82	0.42
1:A:737:LEU:HD23	1:A:737:LEU:HA	1.85	0.42
1:A:1027:ALA:O	1:A:1030:ARG:HB2	2.20	0.42
1:A:1148:ILE:HD13	1:A:1148:ILE:HA	1.98	0.42
2:B:778:MET:O	2:B:819:ALA:HA	2.20	0.42
3:C:15:LYS:H	3:C:15:LYS:HD2	1.85	0.42
8:J:44:TYR:HA	8:J:47:ARG:HD2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:K:32:VAL:O	9:K:32:VAL:HG13	2.20	0.42
1:A:91:PHE:HB3	1:A:96:ILE:HD11	2.02	0.41
1:A:356:ASP:HA	1:A:357:PRO:HD2	1.75	0.41
1:A:451:HIS:HB3	1:A:453:MET:HB2	2.02	0.41
1:A:527:THR:O	1:A:531:ILE:HG22	2.20	0.41
1:A:629:LEU:O	1:A:633:VAL:HG23	2.20	0.41
1:A:1352:VAL:O	1:A:1355:VAL:HG12	2.19	0.41
1:A:1377:THR:HB	4:E:176:PRO:HB3	2.01	0.41
2:B:273:LEU:HA	2:B:274:PRO:HD3	1.80	0.41
2:B:293:PRO:HB2	7:I:11:ASN:O	2.20	0.41
2:B:349:ILE:C	2:B:351:TYR:N	2.77	0.41
2:B:842:ASN:HD22	2:B:845:SER:HB3	1.85	0.41
2:B:1006:ILE:H	2:B:1006:ILE:HG12	1.60	0.41
2:B:1160:VAL:HG12	2:B:1161:HIS:N	2.35	0.41
6:H:100:THR:HG22	6:H:101:ALA:O	2.20	0.41
7:I:16:PRO:HB3	7:I:25:LEU:HD11	2.02	0.41
1:A:353:ILE:HD12	1:A:482:PHE:CE2	2.55	0.41
1:A:755:PHE:O	1:A:756:ILE:C	2.62	0.41
1:A:915:SER:CB	1:A:919:ILE:HG13	2.48	0.41
1:A:1063:MET:HB3	1:A:1063:MET:HE3	1.73	0.41
1:A:1142:THR:O	1:A:1145:SER:OG	2.35	0.41
2:B:45:SER:OG	2:B:46:GLN:N	2.53	0.41
2:B:515:HIS:CD2	2:B:516:ASN:N	2.88	0.41
2:B:522:VAL:HG11	2:B:537:LYS:HD2	2.03	0.41
2:B:634:TYR:CE1	2:B:692:TYR:HD1	2.36	0.41
2:B:798:TYR:CE2	8:J:4:PRO:HB3	2.55	0.41
2:B:844:SER:HB2	2:B:996:ARG:H	1.85	0.41
2:B:1162:ILE:O	2:B:1191:ILE:HG23	2.20	0.41
3:C:83:SER:OG	3:C:95:CYS:SG	2.77	0.41
3:C:217:ASP:HA	3:C:218:PRO:HD3	1.83	0.41
1:A:289:ILE:C	1:A:291:GLU:H	2.28	0.41
1:A:511:ILE:O	1:A:519:PRO:HA	2.20	0.41
1:A:815:PHE:O	1:A:818:MET:N	2.53	0.41
1:A:1364:ASN:OD1	1:A:1366:ARG:HD2	2.20	0.41
2:B:620:ARG:HD2	7:I:68:LEU:HD11	2.02	0.41
3:C:247:GLY:C	3:C:249:ASP:N	2.77	0.41
6:H:38:LEU:HD11	6:H:123:MET:HE2	2.03	0.41
9:K:21:ILE:CD1	9:K:33:ILE:HG12	2.50	0.41
1:A:57:ARG:HD3	1:A:57:ARG:HA	1.59	0.41
1:A:287:HIS:ND1	1:A:291:GLU:OE2	2.54	0.41
1:A:369:SER:HB3	9:K:2:ASN:HD21	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:414:ASP:O	1:A:418:SER:HB2	2.21	0.41
1:A:560:ILE:HA	1:A:561:PRO:HD3	1.92	0.41
1:A:1017:LEU:O	1:A:1018:PHE:C	2.63	0.41
2:B:486:TYR:CE2	2:B:777:ALA:O	2.74	0.41
2:B:658:ILE:HD12	2:B:658:ILE:HA	1.88	0.41
2:B:959:ASP:N	2:B:959:ASP:OD1	2.54	0.41
2:B:1207:LEU:HA	2:B:1210:MET:CE	2.50	0.41
4:E:198:ILE:HD11	4:E:212:ARG:CD	2.50	0.41
5:F:82:THR:HG22	5:F:84:TYR:HB2	2.03	0.41
1:A:99:ILE:O	1:A:103:CYS:SG	2.76	0.41
1:A:862:ASN:OD1	4:E:174:GLN:HA	2.21	0.41
1:A:992:ASP:O	1:A:995:GLU:HB2	2.21	0.41
2:B:35:SER:HB3	2:B:811:TYR:CE2	2.55	0.41
2:B:254:LEU:HD21	2:B:381:MET:SD	2.60	0.41
2:B:314:LEU:O	2:B:315:LYS:C	2.63	0.41
2:B:449:ASN:C	2:B:451:LYS:N	2.76	0.41
2:B:793:ALA:C	2:B:794:ASN:HD22	2.28	0.41
2:B:1084:GLN:NE2	3:C:192:TRP:HB2	2.36	0.41
3:C:133:ILE:HD11	3:C:237:SER:HA	2.02	0.41
1:A:18:GLN:CB	2:B:1215:ARG:HB2	2.50	0.41
1:A:35:ILE:HG13	1:A:241:VAL:HG21	2.03	0.41
1:A:658:LEU:HD13	2:B:831:SER:H	1.82	0.41
1:A:819:GLY:C	1:A:821:ARG:N	2.78	0.41
1:A:1059:HIS:ND1	5:F:86:THR:HA	2.35	0.41
1:A:1209:MET:HE3	1:A:1228:TRP:HB2	2.03	0.41
2:B:85:SER:H	2:B:86:ARG:HB3	1.85	0.41
2:B:816:GLU:O	8:J:56:LEU:HD21	2.19	0.41
2:B:831:SER:OG	2:B:832:GLY:N	2.50	0.41
2:B:910:VAL:CG1	2:B:911:ILE:N	2.83	0.41
2:B:1172:ILE:HG22	2:B:1174:LYS:HG3	2.01	0.41
4:E:40:GLU:O	4:E:41:ASP:HB2	2.21	0.41
6:H:81:PRO:HA	6:H:82:PRO:HD3	1.99	0.41
7:I:103:CYS:SG	7:I:106:CYS:N	2.93	0.41
3:C:10:ILE:HG23	3:C:20:PHE:HB3	2.01	0.41
3:C:255:VAL:O	3:C:258:ILE:HB	2.20	0.41
1:A:687:LYS:HG2	1:A:794:PRO:HG3	2.02	0.41
1:A:747:VAL:O	1:A:748:MET:C	2.63	0.41
1:A:1376:THR:HG23	4:E:212:ARG:HH22	1.84	0.41
2:B:174:LEU:HD11	2:B:204:ILE:CD1	2.50	0.41
2:B:214:ALA:O	2:B:499:ASN:N	2.53	0.41
2:B:256:VAL:HG12	2:B:385:LEU:HD22	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:301:ILE:HG12	2:B:382:ILE:HB	2.02	0.41
2:B:476:ARG:HG2	2:B:477:ALA:N	2.35	0.41
2:B:905:VAL:HG12	2:B:906:SER:H	1.85	0.41
2:B:1024:ALA:O	2:B:1028:GLU:N	2.45	0.41
3:C:215:GLU:CD	3:C:216:GLY:N	2.78	0.41
3:C:247:GLY:O	3:C:248:ILE:C	2.63	0.41
4:E:20:LYS:O	4:E:21:GLU:C	2.63	0.41
6:H:112:ILE:HG22	6:H:127:GLY:O	2.20	0.41
9:K:43:GLY:HA3	9:K:71:PHE:CD1	2.56	0.41
1:A:48:ALA:O	1:A:49:LYS:HD2	2.21	0.41
1:A:211:PHE:HA	1:A:214:ILE:HG12	2.02	0.41
1:A:335:ARG:HE	2:B:1202:LEU:HD11	1.85	0.41
1:A:393:ARG:C	1:A:395:GLY:H	2.29	0.41
1:A:463:ILE:HA	1:A:464:PRO:HD3	1.81	0.41
1:A:495:GLU:OE1	1:A:498:ARG:HD3	2.21	0.41
1:A:779:PHE:O	1:A:782:ARG:O	2.39	0.41
1:A:871:ASP:OD1	1:A:873:MET:HB2	2.21	0.41
1:A:977:LYS:HA	1:A:978:PRO:HD3	1.77	0.41
1:A:1006:ILE:HD13	1:A:1006:ILE:H	1.86	0.41
1:A:1301:GLU:HA	1:A:1302:PRO:HD3	1.95	0.41
1:A:1305:VAL:HG12	1:A:1306:LEU:N	2.36	0.41
1:A:1348:LEU:HD21	1:A:1375:MET:SD	2.60	0.41
2:B:90:ILE:CG2	2:B:91:SER:H	2.33	0.41
2:B:204:ILE:HD12	2:B:204:ILE:N	2.35	0.41
2:B:218:SER:HA	2:B:404:LYS:HB3	2.03	0.41
2:B:412:LEU:HB3	2:B:466:TRP:HE1	1.85	0.41
2:B:547:VAL:H	2:B:612:GLU:CD	2.25	0.41
2:B:850:LEU:HD12	8:J:8:PHE:CD1	2.56	0.41
2:B:852:ARG:HD3	2:B:973:ILE:HG23	2.03	0.41
2:B:1017:ILE:HD13	2:B:1017:ILE:HA	1.76	0.41
2:B:1080:LYS:HB2	3:C:180:TYR:OH	2.21	0.41
3:C:46:ILE:HG22	3:C:47:ASP:N	2.36	0.41
3:C:50:GLU:HG2	10:L:66:GLN:HG3	2.03	0.41
11:R:11:U:O4	11:R:12:G:C6	2.74	0.41
1:A:323:LYS:HG3	1:A:327:ALA:HB1	2.03	0.41
1:A:395:GLY:HA2	1:A:396:PRO:HD3	1.86	0.41
1:A:766:GLY:HA2	1:A:799:PHE:HE1	1.86	0.41
1:A:826:ASP:C	1:A:828:ALA:H	2.28	0.41
2:B:1132:GLU:HA	2:B:1135:ARG:HB3	2.03	0.41
3:C:43:THR:HG23	3:C:44:LEU:N	2.28	0.41
1:A:270:LEU:O	1:A:274:ILE:HG13	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:779:PHE:HD1	1:A:783:THR:O	2.05	0.40
1:A:939:ASP:O	1:A:942:PHE:N	2.54	0.40
1:A:1198:ASP:OD1	1:A:1198:ASP:N	2.54	0.40
2:B:494:HIS:HA	2:B:497:ARG:NH1	2.36	0.40
2:B:1022:THR:OG1	2:B:1025:HIS:HB3	2.21	0.40
2:B:1158:PHE:HB2	2:B:1198:TYR:HB2	2.03	0.40
3:C:27:LEU:O	3:C:29:MET:N	2.54	0.40
5:F:103:MET:O	5:F:105:ALA:N	2.54	0.40
8:J:9:SER:HG	8:J:45:CYS:HB2	1.81	0.40
1:A:444:PHE:CE2	1:A:470:LEU:CD2	3.04	0.40
1:A:562:THR:HA	1:A:563:PRO:HD3	1.91	0.40
1:A:707:GLY:HA2	1:A:1281:ARG:HB2	2.03	0.40
1:A:802:ASN:CG	2:B:729:ILE:H	2.28	0.40
1:A:866:PHE:CZ	4:E:211:TYR:HB2	2.57	0.40
1:A:1169:ILE:N	1:A:1170:ILE:HG22	2.32	0.40
2:B:855:PHE:CE2	2:B:857:ARG:HG3	2.56	0.40
4:E:35:VAL:C	4:E:37:LEU:H	2.28	0.40
5:F:137:TYR:CD2	5:F:143:PHE:HB3	2.56	0.40
9:K:63:VAL:O	9:K:64:GLU:C	2.63	0.40
11:R:2:U:H2'	11:R:3:C:C6	2.56	0.40
1:A:84:ILE:HG22	1:A:239:LEU:HB3	2.02	0.40
1:A:437:MET:O	1:A:438:ASP:C	2.63	0.40
1:A:517:ASN:OD1	1:A:517:ASN:O	2.39	0.40
1:A:912:LEU:HD22	1:A:1036:ARG:HH21	1.84	0.40
2:B:95:ILE:O	2:B:95:ILE:CG2	2.69	0.40
2:B:501:PRO:O	2:B:502:ILE:C	2.65	0.40
2:B:573:GLN:O	2:B:575:PRO:HD3	2.22	0.40
2:B:798:TYR:OH	3:C:66:ARG:NH1	2.48	0.40
2:B:843:GLN:HA	2:B:843:GLN:OE1	2.21	0.40
2:B:1008:PRO:HG3	2:B:1087:PHE:CD1	2.56	0.40
2:B:1082:MET:HA	3:C:189:THR:HA	2.04	0.40
2:B:1200:ALA:O	2:B:1201:LYS:C	2.63	0.40
1:A:31:SER:HB2	1:A:81:PHE:C	2.46	0.40
1:A:32:VAL:HB	1:A:57:ARG:CB	2.52	0.40
1:A:255:SER:CA	1:A:256:GLN:C	2.95	0.40
1:A:381:THR:C	1:A:383:TYR:N	2.80	0.40
1:A:840:ARG:HG2	1:A:1402:PHE:CZ	2.56	0.40
1:A:986:ILE:O	1:A:990:VAL:HG23	2.20	0.40
2:B:202:TYR:CE1	2:B:209:GLU:HG2	2.56	0.40
2:B:550:ASP:OD1	2:B:551:PRO:HD2	2.22	0.40
2:B:601:ARG:HA	2:B:615:MET:HE1	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:992:ILE:CD1	9:K:67:PHE:HE2	2.34	0.40
3:C:124:LEU:O	3:C:125:MET:C	2.64	0.40
5:F:109:VAL:HG23	5:F:124:GLU:HG2	2.02	0.40
6:H:15:VAL:HG12	6:H:51:ALA:HB2	2.03	0.40
1:A:320:ARG:CB	1:A:321:PRO:HD2	2.32	0.40
1:A:551:TYR:CE2	9:K:62:LYS:HD3	2.57	0.40
1:A:730:GLY:C	1:A:732:LEU:N	2.80	0.40
1:A:1248:LEU:HD23	1:A:1248:LEU:H	1.86	0.40
1:A:1353:TYR:C	1:A:1355:VAL:N	2.80	0.40
2:B:361:LEU:O	2:B:363:HIS:O	2.39	0.40
2:B:445:LYS:CA	2:B:447:ALA:H	2.27	0.40
2:B:898:LEU:CD1	2:B:952:VAL:HG11	2.46	0.40
3:C:80:LEU:O	3:C:161:LYS:HD2	2.21	0.40
4:E:3:GLN:HA	4:E:6:GLU:HB2	2.03	0.40
4:E:9:ILE:HG23	4:E:10:SER:N	2.36	0.40
7:I:84:VAL:HG22	7:I:85:PHE:N	2.36	0.40
7:I:85:PHE:CD1	7:I:85:PHE:C	2.99	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:418:SER:OG	3:C:87:PHE:O[2_555]	2.17	0.03

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	1438/1733 (83%)	1054 (73%)	303 (21%)	81 (6%)	1	15
2	B	1145/1224 (94%)	855 (75%)	231 (20%)	59 (5%)	1	16
3	C	269/318 (85%)	207 (77%)	48 (18%)	14 (5%)	1	16

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	E	213/215 (99%)	175 (82%)	33 (16%)	5 (2%)	5	29
5	F	83/155 (54%)	66 (80%)	14 (17%)	3 (4%)	2	21
6	H	132/146 (90%)	104 (79%)	22 (17%)	6 (4%)	2	18
7	I	117/122 (96%)	84 (72%)	29 (25%)	4 (3%)	3	23
8	J	63/70 (90%)	48 (76%)	12 (19%)	3 (5%)	2	17
9	K	112/120 (93%)	86 (77%)	24 (21%)	2 (2%)	6	32
10	L	44/70 (63%)	31 (70%)	9 (20%)	4 (9%)	0	8
All	All	3616/4173 (87%)	2710 (75%)	725 (20%)	181 (5%)	1	17

All (181) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	56	PRO
1	A	115	LEU
1	A	116	ASP
1	A	117	GLU
1	A	119	ASN
1	A	121	LEU
1	A	155	GLU
1	A	158	PRO
1	A	193	ASP
1	A	194	ALA
1	A	399	HIS
1	A	400	PRO
1	A	568	PRO
1	A	770	VAL
1	A	1089	VAL
1	A	1170	ILE
1	A	1394	THR
1	A	1435	PRO
2	B	58	THR
2	B	74	LEU
2	B	78	THR
2	B	439	ALA
2	B	475	SER
2	B	483	LEU
2	B	636	PRO
2	B	712	PRO
2	B	732	SER
2	B	793	ALA

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Mol	Chain	Res	Type
2	B	830	TYR
2	B	864	LYS
2	B	1046	PRO
2	B	1155	SER
3	C	125	MET
3	C	143	LEU
3	C	182	PRO
3	C	223	ALA
5	F	72	LYS
5	F	104	ASN
9	K	70	ARG
1	A	55	ASP
1	A	186	LYS
1	A	191	THR
1	A	255	SER
1	A	395	GLY
1	A	404	TYR
1	A	423	ASP
1	A	557	ASP
1	A	592	ASP
1	A	846	GLU
1	A	884	ASP
1	A	922	ASP
1	A	958	VAL
1	A	1085	HIS
1	A	1221	LYS
1	A	1391	ARG
1	A	1437	GLY
2	B	59	LEU
2	B	76	GLN
2	B	79	THR
2	B	365	THR
2	B	468	GLU
2	B	746	SER
2	B	782	LEU
2	B	1108	ARG
2	B	1133	MET
3	C	60	ASP
3	C	196	ASP
3	C	227	THR
4	E	206	GLY
6	H	75	ALA

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Mol	Chain	Res	Type
6	H	82	PRO
7	I	47	GLU
10	L	47	ARG
1	A	89	PRO
1	A	332	LYS
1	A	1172	LEU
1	A	1247	SER
1	A	1379	GLY
2	B	260	GLY
2	B	334	ILE
2	B	442	PHE
2	B	450	ALA
2	B	470	LYS
2	B	575	PRO
2	B	643	ASP
2	B	981	ALA
2	B	1017	ILE
3	C	142	VAL
3	C	205	LYS
4	E	76	GLY
4	E	187	TYR
6	H	34	ASP
7	I	3	THR
7	I	116	ASN
8	J	6	ARG
10	L	27	LEU
10	L	51	CYS
1	A	311	GLN
1	A	321	PRO
1	A	424	ILE
1	A	567	LYS
1	A	591	PHE
1	A	972	HIS
1	A	1091	SER
1	A	1156	PRO
1	A	1252	THR
2	B	77	HIS
2	B	441	ASP
2	B	489	SER
2	B	958	GLN
6	H	109	LYS
7	I	69	PRO

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Mol	Chain	Res	Type
8	J	16	ASP
10	L	59	ALA
1	A	120	GLU
1	A	149	GLU
1	A	252	PHE
1	A	364	VAL
1	A	377	PRO
1	A	599	SER
1	A	600	PRO
1	A	609	ASP
1	A	731	ARG
1	A	742	ASN
1	A	890	ASP
1	A	955	PRO
1	A	1087	ALA
1	A	1354	ASN
2	B	387	LEU
2	B	518	HIS
2	B	527	THR
2	B	592	ASN
2	B	676	VAL
2	B	717	GLU
2	B	784	ASN
2	B	907	GLY
2	B	1150	ARG
2	B	1214	PRO
3	C	28	ALA
3	C	90	ASP
3	C	181	ASP
3	C	214	ASN
6	H	32	THR
1	A	52	GLY
1	A	1255	GLU
1	A	1388	GLY
1	A	1390	ASN
1	A	1429	ILE
2	B	305	VAL
2	B	467	GLY
2	B	875	GLU
6	H	119	GLY
8	J	64	ASN
9	K	37	LYS

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Mol	Chain	Res	Type
1	A	79	GLY
1	A	250	ILE
1	A	385	ILE
1	A	719	VAL
1	A	1107	VAL
1	A	1190	PRO
1	A	1327	ILE
2	B	290	GLY
2	B	436	VAL
2	B	671	GLY
2	B	912	ILE
3	C	240	VAL
4	E	189	GLY
5	F	139	PRO
1	A	310	GLY
1	A	325	ILE
2	B	70	ILE
1	A	24	PRO
1	A	312	PRO
2	B	479	VAL
2	B	1103	ILE
1	A	514	PRO
2	B	25	ILE
2	B	976	ILE
4	E	86	PRO
1	A	244	PRO
2	B	251	ILE

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	1258/1520 (83%)	1004 (80%)	254 (20%)	1	8
2	B	1000/1061 (94%)	800 (80%)	200 (20%)	1	8
3	C	238/274 (87%)	184 (77%)	54 (23%)	1	5

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	E	196/197 (100%)	175 (89%)	21 (11%)	6	25
5	F	74/137 (54%)	61 (82%)	13 (18%)	2	12
6	H	119/128 (93%)	107 (90%)	12 (10%)	7	27
7	I	113/116 (97%)	98 (87%)	15 (13%)	4	19
8	J	60/65 (92%)	49 (82%)	11 (18%)	2	11
9	K	99/102 (97%)	78 (79%)	21 (21%)	1	7
10	L	40/57 (70%)	30 (75%)	10 (25%)	0	4
All	All	3197/3657 (87%)	2586 (81%)	611 (19%)	1	9

All (611) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	SER
1	A	8	SER
1	A	11	LEU
1	A	14	VAL
1	A	18	GLN
1	A	30	ILE
1	A	32	VAL
1	A	46	THR
1	A	49	LYS
1	A	57	ARG
1	A	58	LEU
1	A	61	ILE
1	A	63	ARG
1	A	65	LEU
1	A	74	MET
1	A	76	GLU
1	A	84	ILE
1	A	93	VAL
1	A	108	MET
1	A	113	LEU
1	A	120	GLU
1	A	121	LEU
1	A	123	ARG
1	A	131	SER
1	A	140	THR
1	A	155	GLU
1	A	156	ASP
1	A	157	ASP

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Mol	Chain	Res	Type
1	A	160	GLN
1	A	161	LEU
1	A	164	ARG
1	A	167	CYS
1	A	180	LYS
1	A	187	LYS
1	A	193	ASP
1	A	198	GLU
1	A	207	ILE
1	A	208	LEU
1	A	210	ILE
1	A	212	LYS
1	A	216	VAL
1	A	221	SER
1	A	222	LEU
1	A	226	GLU
1	A	227	VAL
1	A	230	ARG
1	A	239	LEU
1	A	241	VAL
1	A	252	PHE
1	A	256	GLN
1	A	257	ARG
1	A	260	ASP
1	A	262	LEU
1	A	263	THR
1	A	270	LEU
1	A	271	LYS
1	A	275	SER
1	A	289	ILE
1	A	295	LEU
1	A	296	LEU
1	A	306	ASN
1	A	308	ILE
1	A	311	GLN
1	A	313	GLN
1	A	322	VAL
1	A	323	LYS
1	A	332	LYS
1	A	333	GLU
1	A	336	ILE
1	A	340	LEU

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Mol	Chain	Res	Type
1	A	344	ARG
1	A	345	VAL
1	A	350	ARG
1	A	354	SER
1	A	359	LEU
1	A	370	ILE
1	A	373	THR
1	A	379	VAL
1	A	385	ILE
1	A	390	GLN
1	A	403	LYS
1	A	404	TYR
1	A	411	ASP
1	A	413	ILE
1	A	419	LYS
1	A	424	ILE
1	A	431	LYS
1	A	432	VAL
1	A	434	ARG
1	A	437	MET
1	A	442	VAL
1	A	443	LEU
1	A	449	SER
1	A	450	LEU
1	A	452	LYS
1	A	460	VAL
1	A	462	VAL
1	A	463	ILE
1	A	469	ARG
1	A	470	LEU
1	A	475	THR
1	A	481	ASP
1	A	504	LEU
1	A	518	LYS
1	A	521	MET
1	A	541	ILE
1	A	559	VAL
1	A	562	THR
1	A	565	ILE
1	A	571	LEU
1	A	572	TRP
1	A	576	GLN

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Mol	Chain	Res	Type
1	A	577	ILE
1	A	579	SER
1	A	580	VAL
1	A	595	THR
1	A	603	ASN
1	A	612	ILE
1	A	618	GLU
1	A	621	THR
1	A	630	ILE
1	A	634	THR
1	A	645	LEU
1	A	649	ILE
1	A	670	ILE
1	A	672	ASP
1	A	682	THR
1	A	687	LYS
1	A	688	LYS
1	A	693	VAL
1	A	694	THR
1	A	702	LEU
1	A	713	SER
1	A	735	VAL
1	A	739	ASP
1	A	740	LEU
1	A	743	VAL
1	A	760	GLN
1	A	767	GLN
1	A	771	GLU
1	A	775	ILE
1	A	783	THR
1	A	795	GLU
1	A	803	SER
1	A	805	LEU
1	A	808	LEU
1	A	809	THR
1	A	827	THR
1	A	839	ARG
1	A	857	ARG
1	A	858	ASN
1	A	859	SER
1	A	867	ILE
1	A	879	GLU

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Mol	Chain	Res	Type
1	A	883	LEU
1	A	884	ASP
1	A	885	THR
1	A	895	LYS
1	A	896	ARG
1	A	902	LEU
1	A	908	LEU
1	A	918	GLU
1	A	919	ILE
1	A	920	LEU
1	A	924	LYS
1	A	929	LEU
1	A	937	VAL
1	A	946	VAL
1	A	953	ASN
1	A	961	ARG
1	A	963	ILE
1	A	982	THR
1	A	987	VAL
1	A	996	ASN
1	A	1000	LEU
1	A	1001	ARG
1	A	1006	ILE
1	A	1017	LEU
1	A	1025	ARG
1	A	1029	ARG
1	A	1031	VAL
1	A	1033	GLN
1	A	1037	LEU
1	A	1039	LYS
1	A	1047	SER
1	A	1048	ASN
1	A	1052	GLN
1	A	1058	VAL
1	A	1062	GLU
1	A	1067	LEU
1	A	1078	GLN
1	A	1080	THR
1	A	1081	LEU
1	A	1083	THR
1	A	1084	PHE
1	A	1085	HIS

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Mol	Chain	Res	Type
1	A	1089	VAL
1	A	1098	VAL
1	A	1116	LEU
1	A	1118	VAL
1	A	1128	GLN
1	A	1141	THR
1	A	1142	THR
1	A	1146	VAL
1	A	1163	ILE
1	A	1168	GLU
1	A	1169	ILE
1	A	1170	ILE
1	A	1178	ASP
1	A	1222	ASN
1	A	1223	ASP
1	A	1226	VAL
1	A	1227	ILE
1	A	1229	SER
1	A	1235	LYS
1	A	1237	ILE
1	A	1240	CYS
1	A	1243	VAL
1	A	1248	LEU
1	A	1251	GLU
1	A	1257	ASP
1	A	1259	MET
1	A	1260	LEU
1	A	1264	GLU
1	A	1267	MET
1	A	1279	ILE
1	A	1280	GLU
1	A	1281	ARG
1	A	1283	VAL
1	A	1291	VAL
1	A	1314	SER
1	A	1322	ILE
1	A	1327	ILE
1	A	1333	ILE
1	A	1334	ASP
1	A	1335	ILE
1	A	1336	MET
1	A	1355	VAL

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Mol	Chain	Res	Type
1	A	1366	ARG
1	A	1372	VAL
1	A	1376	THR
1	A	1382	THR
1	A	1385	THR
1	A	1391	ARG
1	A	1392	SER
1	A	1394	THR
1	A	1401	SER
1	A	1403	GLU
1	A	1406	VAL
1	A	1420	ASP
1	A	1426	GLU
1	A	1448	GLU
1	A	1450	LEU
1	A	1451	VAL
2	B	35	SER
2	B	39	ARG
2	B	43	LEU
2	B	57	TYR
2	B	59	LEU
2	B	61	ASP
2	B	62	ILE
2	B	68	THR
2	B	69	LEU
2	B	71	LEU
2	B	72	GLU
2	B	74	LEU
2	B	79	THR
2	B	80	GLU
2	B	89	GLU
2	B	90	ILE
2	B	96	TYR
2	B	108	VAL
2	B	112	LEU
2	B	115	GLN
2	B	118	ARG
2	B	120	ARG
2	B	121	ASN
2	B	130	VAL
2	B	176	SER
2	B	213	ILE

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Mol	Chain	Res	Type
2	B	222	ILE
2	B	225	VAL
2	B	244	LEU
2	B	246	LYS
2	B	249	ARG
2	B	253	THR
2	B	254	LEU
2	B	264	SER
2	B	268	THR
2	B	276	ILE
2	B	282	ILE
2	B	283	VAL
2	B	284	ILE
2	B	287	ARG
2	B	302	CYS
2	B	305	VAL
2	B	310	MET
2	B	313	MET
2	B	315	LYS
2	B	317	CYS
2	B	323	VAL
2	B	327	ARG
2	B	337	ARG
2	B	353	LYS
2	B	355	ILE
2	B	364	ILE
2	B	371	GLU
2	B	372	SER
2	B	391	ASP
2	B	394	ASP
2	B	396	ASP
2	B	398	ARG
2	B	404	LYS
2	B	408	LEU
2	B	412	LEU
2	B	413	LEU
2	B	416	LEU
2	B	419	THR
2	B	420	LEU
2	B	425	THR
2	B	427	ASP
2	B	440	HIS

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Mol	Chain	Res	Type
2	B	445	LYS
2	B	457	LEU
2	B	463	THR
2	B	469	GLN
2	B	470	LYS
2	B	476	ARG
2	B	479	VAL
2	B	483	LEU
2	B	489	SER
2	B	490	SER
2	B	502	ILE
2	B	513	GLN
2	B	516	ASN
2	B	526	GLU
2	B	527	THR
2	B	529	GLU
2	B	531	GLN
2	B	533	CYS
2	B	539	LEU
2	B	542	MET
2	B	544	CYS
2	B	556	THR
2	B	563	MET
2	B	570	VAL
2	B	581	PHE
2	B	603	LEU
2	B	613	VAL
2	B	623	GLU
2	B	624	LEU
2	B	625	LYS
2	B	626	ILE
2	B	633	VAL
2	B	635	ARG
2	B	637	LEU
2	B	643	ASP
2	B	644	GLU
2	B	646	LEU
2	B	684	LEU
2	B	701	ILE
2	B	709	ASP
2	B	710	LEU
2	B	729	ILE

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Mol	Chain	Res	Type
2	B	730	ARG
2	B	736	THR
2	B	739	THR
2	B	748	ILE
2	B	763	GLN
2	B	764	SER
2	B	769	TYR
2	B	776	GLN
2	B	782	LEU
2	B	790	ASP
2	B	795	ILE
2	B	801	LYS
2	B	806	THR
2	B	824	ILE
2	B	827	ILE
2	B	840	ILE
2	B	843	GLN
2	B	844	SER
2	B	845	SER
2	B	852	ARG
2	B	854	LEU
2	B	856	PHE
2	B	857	ARG
2	B	864	LYS
2	B	871	THR
2	B	873	THR
2	B	878	GLN
2	B	879	ARG
2	B	883	LEU
2	B	886	LYS
2	B	899	ILE
2	B	911	ILE
2	B	919	SER
2	B	941	LEU
2	B	942	ARG
2	B	943	SER
2	B	948	ILE
2	B	951	GLN
2	B	953	LEU
2	B	963	PHE
2	B	970	THR
2	B	973	ILE

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Mol	Chain	Res	Type
2	B	975	GLN
2	B	983	ARG
2	B	987	LYS
2	B	992	ILE
2	B	997	GLU
2	B	999	MET
2	B	1006	ILE
2	B	1010	LEU
2	B	1011	ILE
2	B	1012	ILE
2	B	1019	SER
2	B	1022	THR
2	B	1025	HIS
2	B	1026	LEU
2	B	1028	GLU
2	B	1034	VAL
2	B	1037	LEU
2	B	1050	ILE
2	B	1051	THR
2	B	1060	ARG
2	B	1065	GLN
2	B	1071	VAL
2	B	1081	LEU
2	B	1082	MET
2	B	1087	PHE
2	B	1093	GLN
2	B	1096	ARG
2	B	1098	MET
2	B	1099	VAL
2	B	1102	LYS
2	B	1103	ILE
2	B	1113	VAL
2	B	1115	THR
2	B	1132	GLU
2	B	1133	MET
2	B	1138	MET
2	B	1139	ILE
2	B	1145	SER
2	B	1147	LEU
2	B	1150	ARG
2	B	1151	LEU
2	B	1155	SER

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Mol	Chain	Res	Type
2	B	1156	ASP
2	B	1159	ARG
2	B	1194	ILE
2	B	1196	ILE
2	B	1203	LEU
2	B	1206	GLU
3	C	4	GLU
3	C	10	ILE
3	C	18	VAL
3	C	22	LEU
3	C	25	VAL
3	C	32	SER
3	C	34	ARG
3	C	36	VAL
3	C	37	MET
3	C	43	THR
3	C	50	GLU
3	C	51	VAL
3	C	53	THR
3	C	57	VAL
3	C	58	LEU
3	C	61	GLU
3	C	77	ILE
3	C	80	LEU
3	C	81	GLU
3	C	83	SER
3	C	85	ASP
3	C	93	ASP
3	C	94	LYS
3	C	101	LEU
3	C	102	GLN
3	C	118	LEU
3	C	119	VAL
3	C	120	ILE
3	C	129	ILE
3	C	133	ILE
3	C	143	LEU
3	C	144	ILE
3	C	156	THR
3	C	157	CYS
3	C	158	VAL
3	C	163	ILE

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Mol	Chain	Res	Type
3	C	178	PHE
3	C	183	TRP
3	C	195	GLN
3	C	197	SER
3	C	199	LYS
3	C	215	GLU
3	C	222	LYS
3	C	226	ASP
3	C	228	PHE
3	C	229	TYR
3	C	232	VAL
3	C	237	SER
3	C	240	VAL
3	C	244	VAL
3	C	250	THR
3	C	254	LYS
3	C	258	ILE
3	C	259	LEU
4	E	3	GLN
4	E	4	GLU
4	E	31	THR
4	E	37	LEU
4	E	43	LYS
4	E	66	GLU
4	E	72	PHE
4	E	88	VAL
4	E	92	THR
4	E	134	THR
4	E	137	GLU
4	E	150	VAL
4	E	157	SER
4	E	165	LEU
4	E	169	ARG
4	E	182	ASP
4	E	196	VAL
4	E	198	ILE
4	E	202	SER
4	E	204	THR
4	E	210	SER
5	F	74	ILE
5	F	76	LYS
5	F	78	GLN

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Mol	Chain	Res	Type
5	F	79	ARG
5	F	93	ILE
5	F	97	ARG
5	F	99	LEU
5	F	107	VAL
5	F	111	LEU
5	F	120	ILE
5	F	123	LYS
5	F	148	VAL
5	F	149	GLU
6	H	11	GLN
6	H	16	ASP
6	H	24	CYS
6	H	39	THR
6	H	40	LEU
6	H	44	VAL
6	H	53	ASP
6	H	62	SER
6	H	89	LEU
6	H	95	TYR
6	H	121	LEU
6	H	137	GLN
7	I	3	THR
7	I	5	ARG
7	I	7	CYS
7	I	8	ARG
7	I	17	ARG
7	I	28	GLU
7	I	31	THR
7	I	50	THR
7	I	59	VAL
7	I	60	GLN
7	I	83	ASN
7	I	84	VAL
7	I	95	THR
7	I	111	THR
7	I	116	ASN
8	J	2	ILE
8	J	3	VAL
8	J	5	VAL
8	J	7	CYS
8	J	14	VAL

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Mol	Chain	Res	Type
8	J	16	ASP
8	J	23	ASN
8	J	31	ASP
8	J	34	THR
8	J	38	ARG
8	J	43	ARG
9	K	1	MET
9	K	5	ASP
9	K	12	LEU
9	K	18	LYS
9	K	31	VAL
9	K	33	ILE
9	K	34	THR
9	K	45	LEU
9	K	50	LEU
9	K	51	LEU
9	K	63	VAL
9	K	75	ILE
9	K	77	THR
9	K	85	ASP
9	K	94	ILE
9	K	95	ILE
9	K	101	LEU
9	K	102	LYS
9	K	107	THR
9	K	111	LEU
9	K	113	THR
10	L	26	THR
10	L	27	LEU
10	L	28	LYS
10	L	31	CYS
10	L	49	LYS
10	L	50	ASP
10	L	57	LEU
10	L	61	THR
10	L	66	GLN
10	L	68	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (103) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	64	ASN

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Mol	Chain	Res	Type
1	A	68	GLN
1	A	160	GLN
1	A	273	ASN
1	A	281	HIS
1	A	282	ASN
1	A	297	GLN
1	A	306	ASN
1	A	311	GLN
1	A	339	ASN
1	A	394	ASN
1	A	399	HIS
1	A	435	HIS
1	A	445	ASN
1	A	471	ASN
1	A	490	HIS
1	A	503	GLN
1	A	515	GLN
1	A	517	ASN
1	A	545	GLN
1	A	589	GLN
1	A	659	HIS
1	A	723	ASN
1	A	742	ASN
1	A	760	GLN
1	A	858	ASN
1	A	926	GLN
1	A	968	GLN
1	A	994	GLN
1	A	1048	ASN
1	A	1078	GLN
1	A	1082	ASN
1	A	1085	HIS
1	A	1211	GLN
1	A	1222	ASN
1	A	1278	ASN
1	A	1312	ASN
1	A	1354	ASN
1	A	1387	HIS
1	A	1393	ASN
1	A	1427	ASN
1	A	1432	GLN
2	B	103	ASN

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Mol	Chain	Res	Type
2	B	121	ASN
2	B	178	ASN
2	B	215	GLN
2	B	236	HIS
2	B	278	GLN
2	B	309	GLN
2	B	366	GLN
2	B	395	GLN
2	B	433	GLN
2	B	499	ASN
2	B	515	HIS
2	B	516	ASN
2	B	518	HIS
2	B	531	GLN
2	B	648	HIS
2	B	734	HIS
2	B	744	HIS
2	B	762	ASN
2	B	770	GLN
2	B	794	ASN
2	B	822	ASN
2	B	842	ASN
2	B	862	GLN
2	B	878	GLN
2	B	951	GLN
2	B	957	ASN
2	B	958	GLN
2	B	975	GLN
2	B	984	HIS
2	B	1040	ASN
2	B	1084	GLN
2	B	1141	HIS
2	B	1178	ASN
2	B	1179	GLN
2	B	1195	HIS
3	C	31	ASN
3	C	73	GLN
3	C	102	GLN
3	C	112	ASN
3	C	123	ASN
3	C	167	HIS
3	C	184	ASN

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Mol	Chain	Res	Type
3	C	188	HIS
3	C	195	GLN
3	C	203	GLN
4	E	8	ASN
4	E	101	GLN
4	E	104	ASN
4	E	113	GLN
4	E	179	GLN
6	H	11	GLN
6	H	128	ASN
6	H	137	GLN
7	I	46	HIS
7	I	60	GLN
7	I	90	GLN
9	K	44	ASN
9	K	65	HIS
9	K	104	ASN
9	K	112	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
11	R	11/12 (91%)	3 (27%)	0

All (3) RNA backbone outliers are listed below:

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

There are no RNA pucker outliers to report.

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

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	1442/1733 (83%)	-0.11	6 (0%) 88 73	72, 131, 247, 370	0
2	B	1153/1224 (94%)	-0.07	9 (0%) 82 62	71, 114, 240, 374	0
3	C	271/318 (85%)	-0.26	0 100 100	80, 106, 165, 306	0
4	E	215/215 (100%)	-0.13	0 100 100	106, 165, 276, 316	0
5	F	85/155 (54%)	-0.30	0 100 100	107, 137, 170, 200	0
6	H	136/146 (93%)	0.03	0 100 100	126, 169, 276, 299	0
7	I	119/122 (97%)	-0.14	0 100 100	109, 150, 180, 237	0
8	J	65/70 (92%)	-0.33	0 100 100	80, 94, 135, 153	0
9	K	114/120 (95%)	-0.33	0 100 100	83, 112, 136, 139	0
10	L	46/70 (65%)	0.17	1 (2%) 62 43	99, 175, 228, 246	0
11	R	12/12 (100%)	-0.15	0 100 100	104, 119, 182, 208	0
12	T	28/29 (96%)	0.31	0 100 100	102, 222, 413, 422	0
13	N	14/14 (100%)	0.55	0 100 100	270, 329, 352, 379	0
All	All	3700/4228 (87%)	-0.11	16 (0%) 88 73	71, 128, 251, 422	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	1211	ASN	3.2
2	B	441	ASP	2.8
2	B	262	GLU	2.6
1	A	266	LEU	2.6
2	B	529	GLU	2.4
2	B	531	GLN	2.4
1	A	323	LYS	2.3
1	A	1082	ASN	2.3
10	L	25	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
2	B	498	THR	2.2
2	B	882	THR	2.2
1	A	103	CYS	2.1
2	B	1206	GLU	2.1
2	B	1096	ARG	2.1
1	A	329	LEU	2.1
1	A	56	PRO	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
14	ZN	J	101	1/1	0.94	0.08	218,218,218,218	0
14	ZN	A	1734	1/1	0.96	0.04	232,232,232,232	0
14	ZN	A	1735	1/1	0.98	0.05	136,136,136,136	0
14	ZN	L	105	1/1	0.98	0.04	155,155,155,155	0
14	ZN	I	204	1/1	0.99	0.02	125,125,125,125	0
14	ZN	B	1307	1/1	0.99	0.03	163,163,163,163	0
14	ZN	I	203	1/1	0.99	0.02	103,103,103,103	0
14	ZN	C	319	1/1	1.00	0.03	118,118,118,118	0
15	MG	A	1736	1/1	1.00	0.02	113,113,113,113	0

6.5 Other polymers [i](#)

There are no such residues in this entry.