Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 09:01 AM GMT

PDB ID	:	3GTK
Title	:	Backtracked RNA polymerase II complex with 18mer RNA
Authors	:	Wang, D.; Bushnell, D.A.; Huang, X.; Westover, K.D.; Levitt, M.; Kornberg, R.D.
Deposited on	:	2009-03-27
Resolution	:	3.80 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

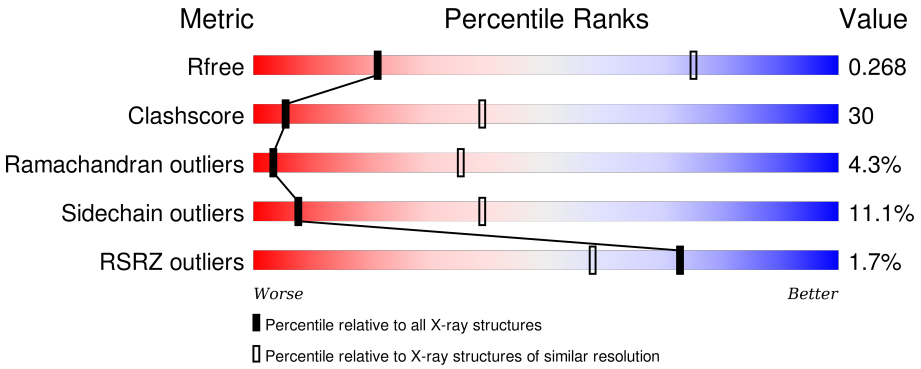
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 3.80 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}	91344	1317 (4.10-3.50)
Clashscore	102246	1458 (4.10-3.50)
Ramachandran outliers	100387	1397 (4.10-3.50)
Sidechain outliers	100360	1392 (4.10-3.50)
RSRZ outliers	91569	1325 (4.10-3.50)

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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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 <=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	2% 41% 34% 7% • 17%
2	B	1224	2% 44% 42% 7% • 6%
3	C	318	% 45% 36% 5% 15%
4	E	215	68% 30% •
5	F	155	33% 21% • 45%

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Mol	Chain	Length	Quality of chain
6	H	146	3% 51% 37% 5% 7%
7	I	122	% 43% 43% 11%
8	J	70	37% 43% 13% 7%
9	K	120	56% 33% 6% 5%
10	L	70	4% 40% 14% 11% 34%
11	R	18	11% 56% 11% 22%
12	T	29	10% 21% 45% 34%
13	N	14	7% 14% 79% 7%

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	C	319	-	-	X	-
14	ZN	J	101	-	-	X	-

2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 30111 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
			Total	C	N	O	S			
1	A	1442	11332	7133	1982	2156	61	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	1153	9168	5795	1604	1713	56	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	271	2135	1344	355	423	13	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	E	215	1757	1114	310	322	11	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	F	85	684	437	116	128	3	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
6	H	136	1087	684	183	215	5	0	0	0

- 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 DNA/RNA hybrid called DNA/RNA (5'-R(*AP*UP*CP*GP*AP*GP*AP*GP*GP*AP*UP*GP*C)-D(P*AP*GP*AP*CP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	R	14	Total	C	N	O	P	0	0	0
			284	126	55	90	13			

- Molecule 12 is a DNA chain called DNA (29-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	T	29	Total	C	N	O	P	0	0	0
			587	281	109	169	28			

- 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 (three-letter code: ZN) (formula: Zn).

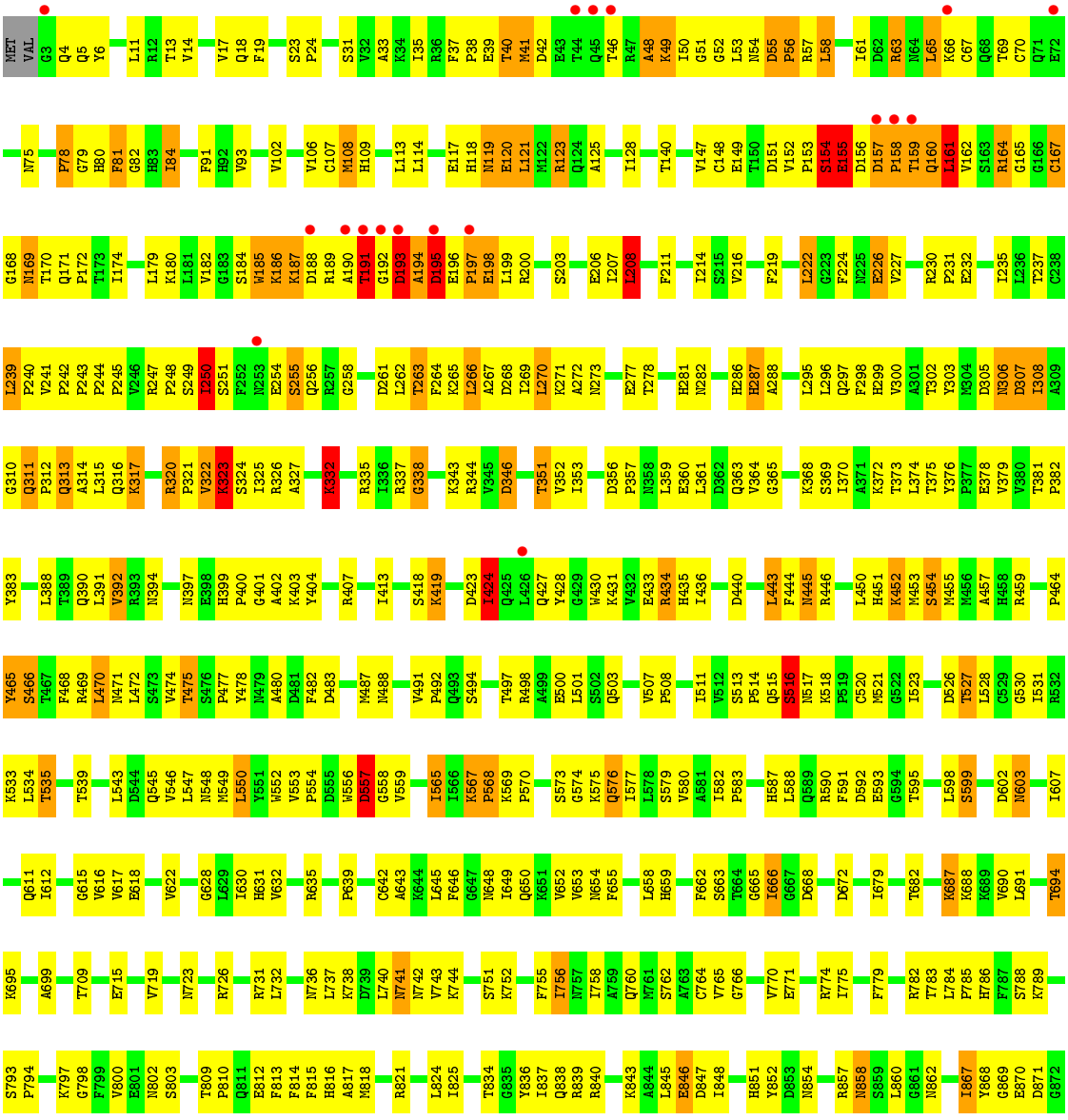
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	J	1	Total Zn 1 1	0	0
14	B	1	Total Zn 1 1	0	0
14	I	2	Total Zn 2 2	0	0
14	C	1	Total Zn 1 1	0	0
14	A	2	Total Zn 2 2	0	0
14	L	1	Total Zn 1 1	0	0

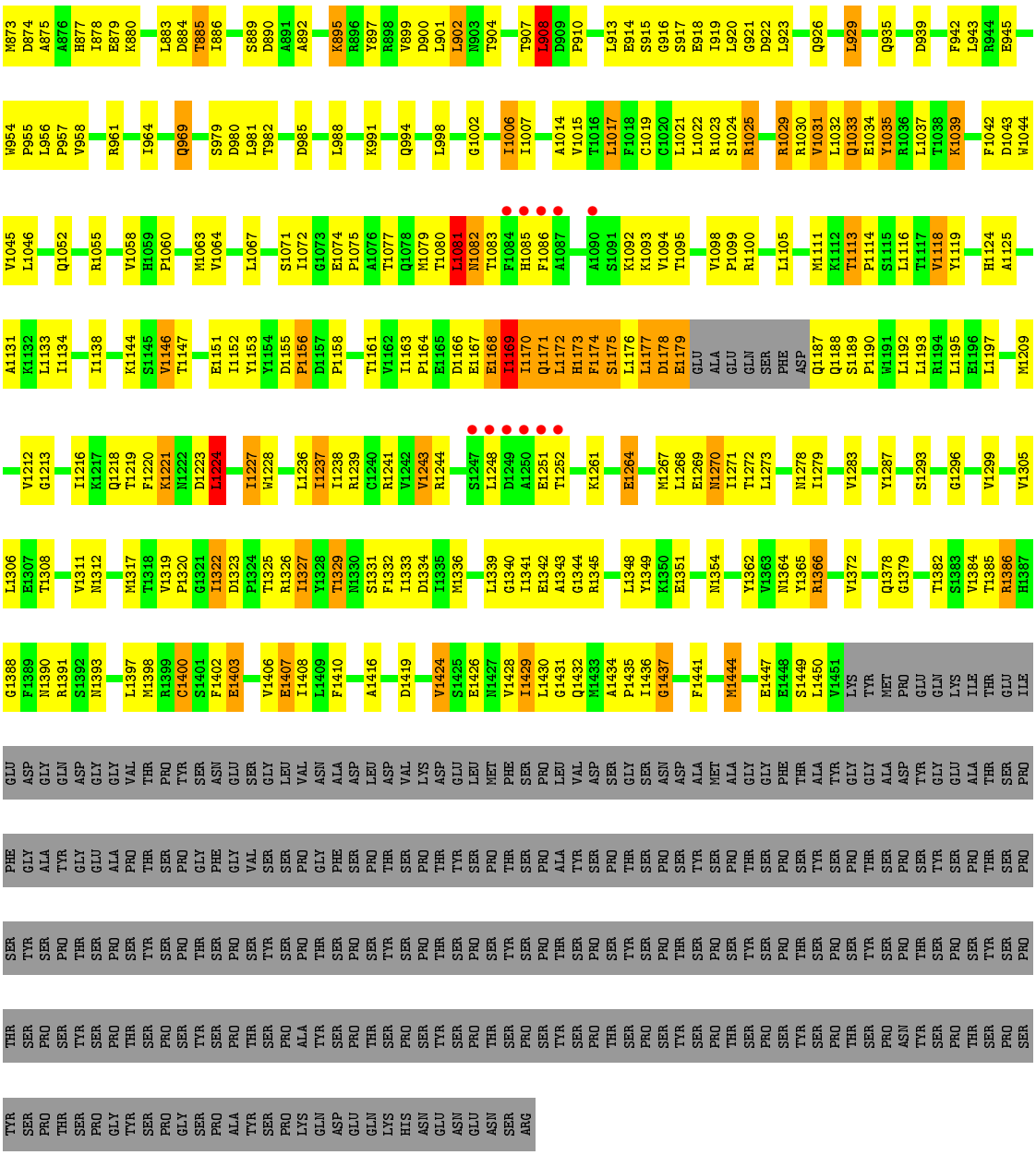
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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

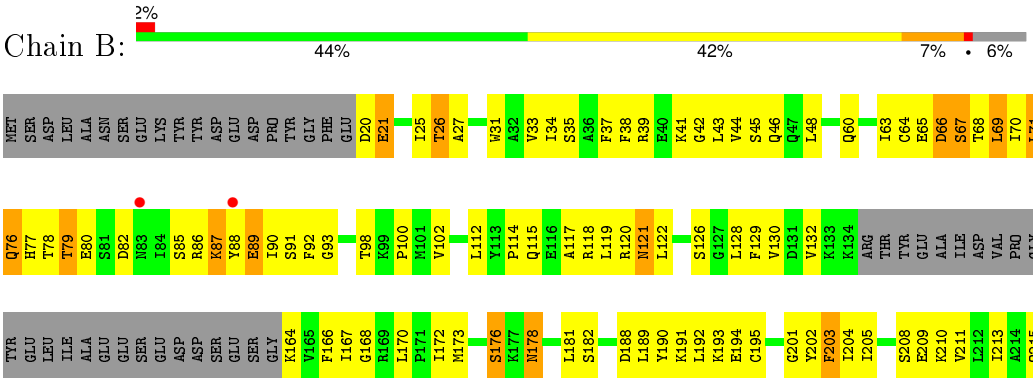
Chain A:

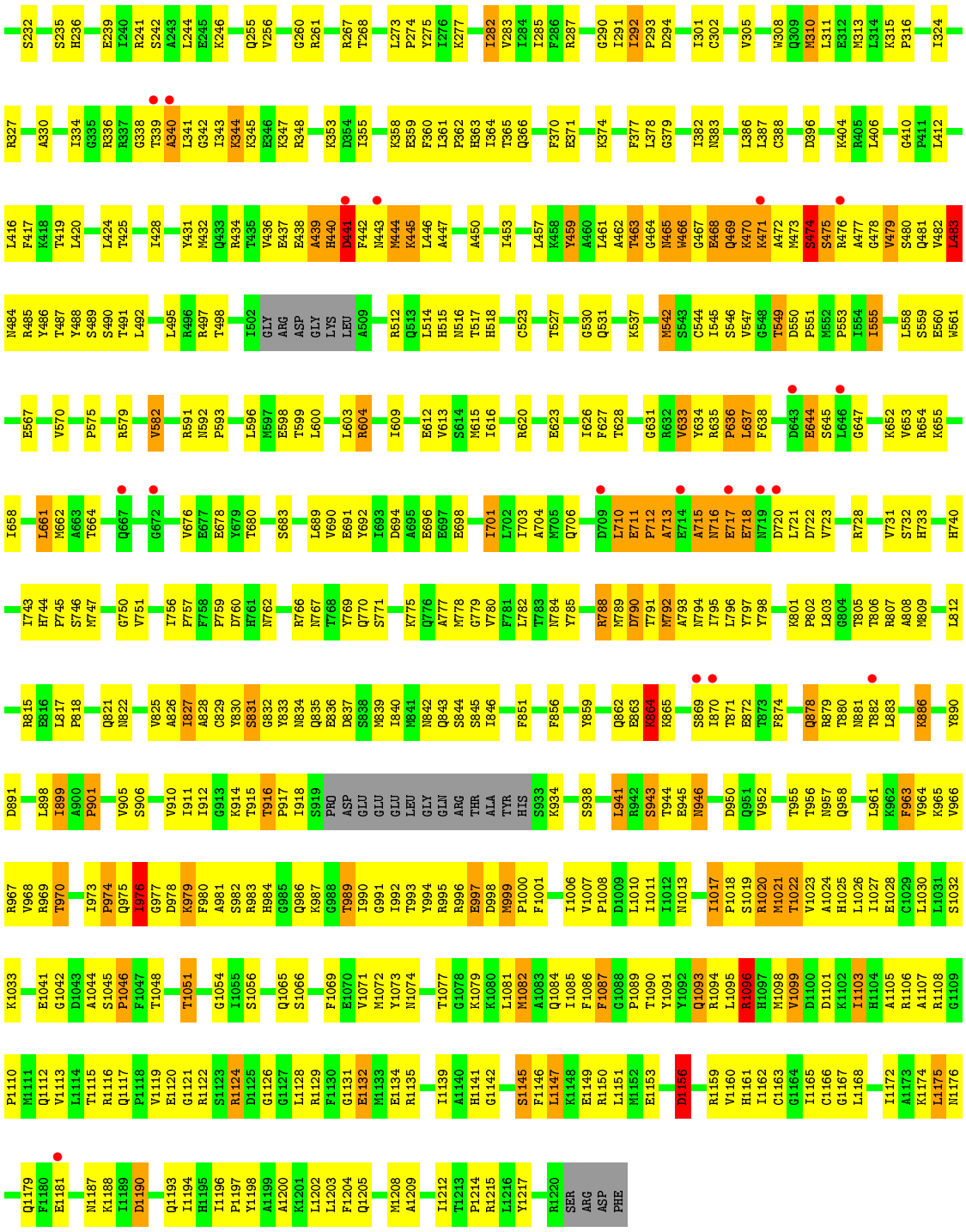




• Molecule 2: DNA-directed RNA polymerase II subunit RPB2

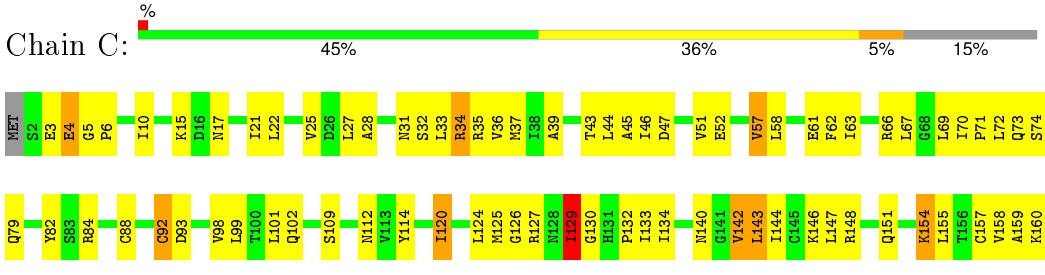
Chain B:

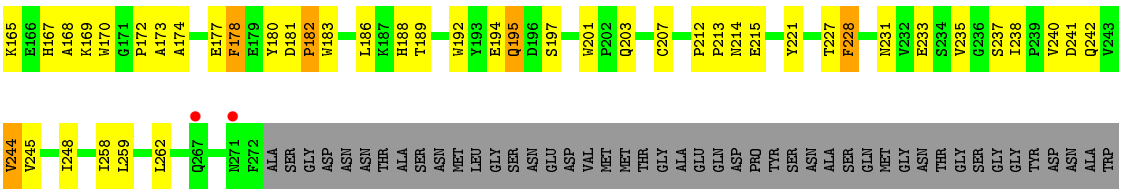




• Molecule 3: DNA-directed RNA polymerase II subunit RPB3

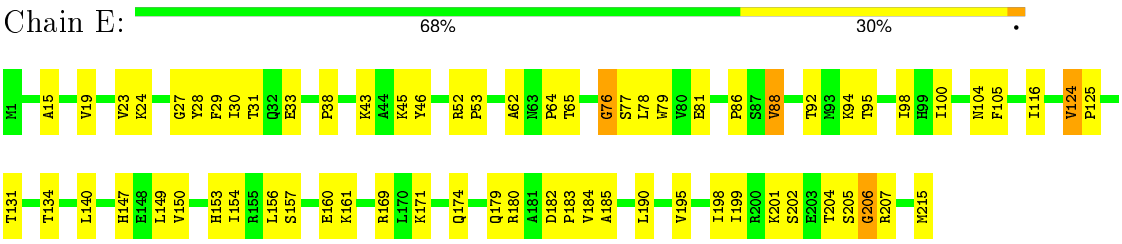
Chain C:





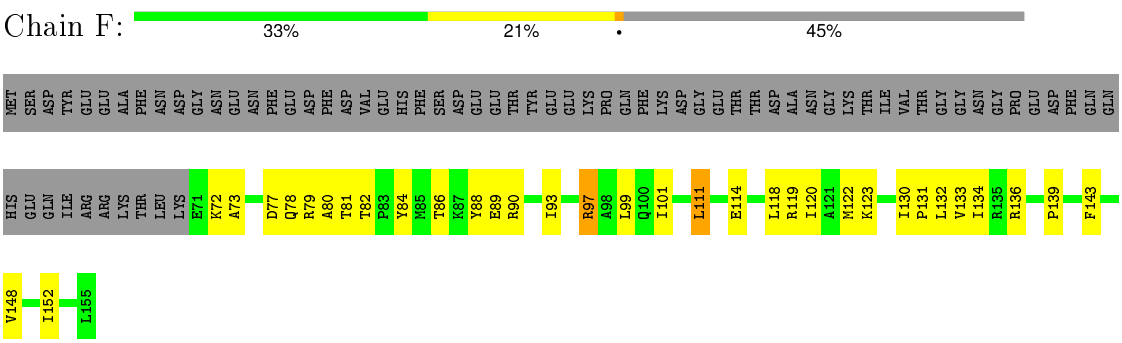
• Molecule 4: DNA-directed RNA polymerases I, II, and III subunit RPABC1

Chain E:



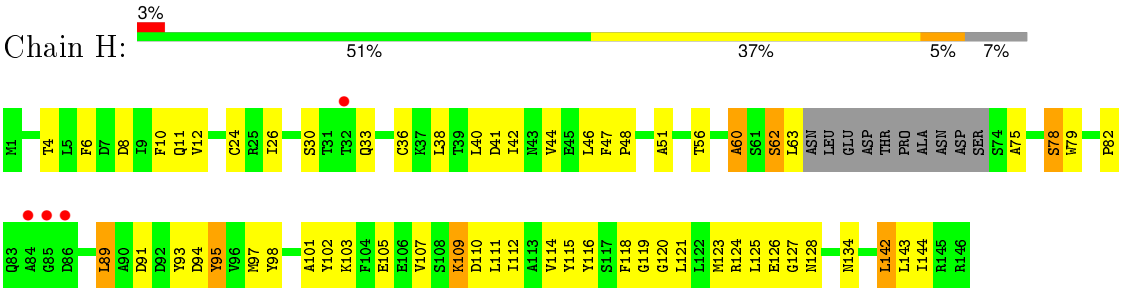
• Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC2

Chain F:



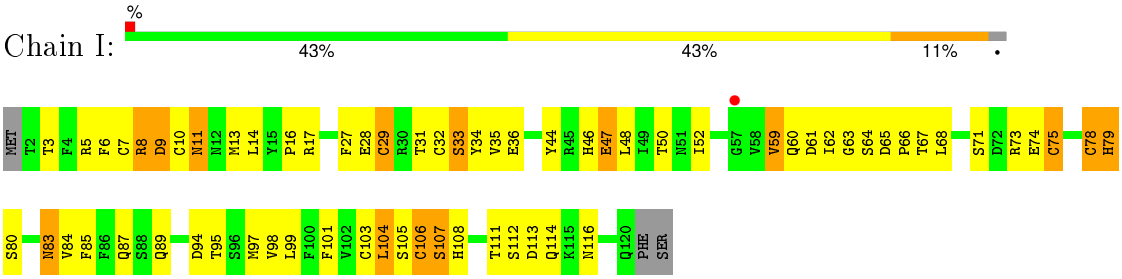
• Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC3

Chain H:



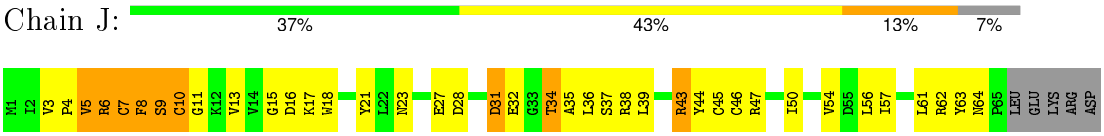
• Molecule 7: DNA-directed RNA polymerase II subunit RPB9

Chain I:



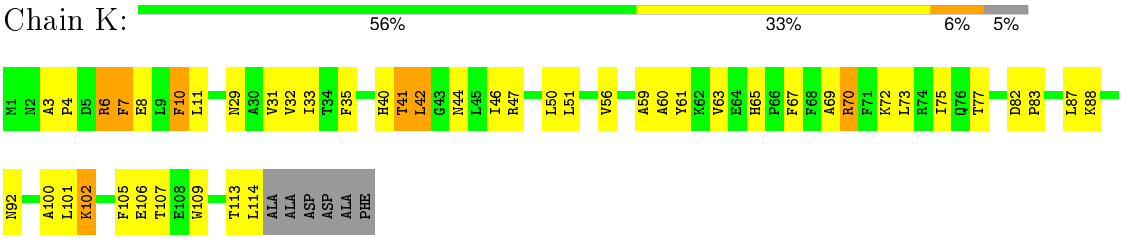
• Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC5

Chain J:



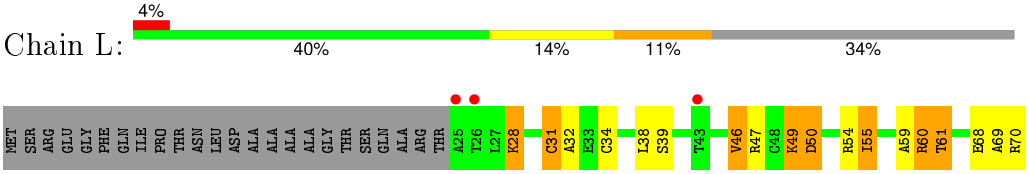
• Molecule 9: DNA-directed RNA polymerase II subunit RPB11

Chain K:



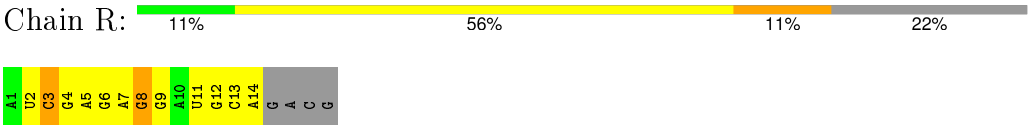
• Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC4

Chain L:



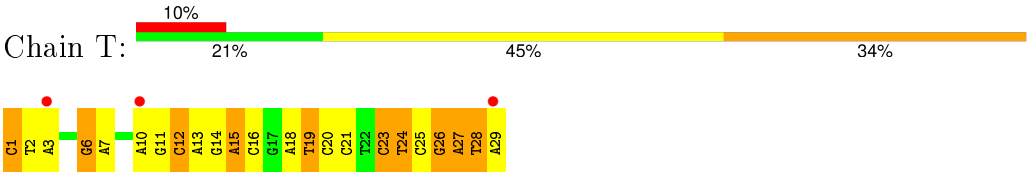
• Molecule 11: DNA/RNA (5'-R(*AP*UP*CP*GP*AP*GP*AP*GP*GP*AP*UP*GP*C)-D(P*AP*GP*AP*CP*G)-3')

Chain R:



• Molecule 12: DNA (29-MER)

Chain T:



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

Chain N:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	170.45Å 222.29Å 195.09Å 90.00° 101.72° 90.00°	Depositor
Resolution (Å)	50.00 – 3.80 39.90 – 3.80	Depositor EDS
% Data completeness (in resolution range)	97.4 (50.00-3.80) 97.5 (39.90-3.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.96 (at 3.76Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.247 , 0.278 0.240 , 0.268	Depositor DCC
R_{free} test set	3443 reflections (5.32%)	DCC
Wilson B-factor (Å^2)	116.7	Xtriage
Anisotropy	0.063	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.26 , 76.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Outliers	0 of 68227 reflections	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	30111	wwPDB-VP
Average B, all atoms (Å^2)	142.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.11% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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

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	0.58	1/11536 (0.0%)	0.72	14/15605 (0.1%)
2	B	0.64	1/9348 (0.0%)	0.76	12/12611 (0.1%)
3	C	0.65	0/2174	0.76	1/2946 (0.0%)
4	E	0.53	0/1793	0.60	0/2413
5	F	0.53	0/696	0.67	0/940
6	H	0.54	0/1105	0.68	0/1495
7	I	0.59	0/989	0.65	0/1331
8	J	0.66	0/541	0.75	0/727
9	K	0.63	0/937	0.71	1/1265 (0.1%)
10	L	0.68	0/365	0.84	1/485 (0.2%)
11	R	1.15	1/318 (0.3%)	1.79	5/496 (1.0%)
12	T	1.07	2/658 (0.3%)	1.88	27/1012 (2.7%)
13	N	1.54	0/317	2.03	19/488 (3.9%)
All	All	0.64	5/30777 (0.0%)	0.82	80/41814 (0.2%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	206	GLU	CD-OE2	5.85	1.32	1.25
12	T	28	DT	C1'-N1	5.59	1.56	1.49
2	B	544	CYS	CB-SG	-5.45	1.73	1.81
12	T	23	DC	C1'-N1	5.20	1.56	1.49
11	R	11	U	C1'-N1	5.17	1.56	1.48

All (80) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	T	25	DC	O4'-C1'-N1	10.24	115.17	108.00
12	T	28	DT	O4'-C4'-C3'	-10.00	100.00	106.00
12	T	27	DA	O4'-C4'-C3'	-9.05	100.57	106.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	715	ALA	CB-CA-C	8.60	122.99	110.10
12	T	28	DT	O4'-C1'-N1	8.54	113.98	108.00
12	T	19	DT	N3-C2-O2	-8.39	117.26	122.30
12	T	23	DC	O4'-C1'-N1	8.06	113.64	108.00
13	N	10	DG	P-O3'-C3'	7.76	129.01	119.70
1	A	41	MET	N-CA-CB	7.70	124.47	110.60
12	T	21	DC	O4'-C4'-C3'	-7.52	101.49	106.00
12	T	21	DC	C4'-C3'-C2'	-7.51	96.34	103.10
2	B	344	LYS	N-CA-CB	-7.41	97.26	110.60
1	A	516	SER	CB-CA-C	7.34	124.06	110.10
2	B	474	SER	CB-CA-C	-7.34	96.16	110.10
13	N	5	DT	C4-C5-C7	7.18	123.31	119.00
2	B	343	ILE	CB-CA-C	6.93	125.46	111.60
1	A	121	LEU	CA-CB-CG	6.92	131.23	115.30
12	T	28	DT	N3-C2-O2	-6.86	118.18	122.30
12	T	24	DT	O4'-C1'-N1	6.79	112.75	108.00
12	T	28	DT	C4-C5-C7	6.57	122.94	119.00
13	N	8	DT	O4'-C1'-N1	6.53	112.57	108.00
1	A	1125	ALA	N-CA-CB	-6.50	101.00	110.10
1	A	208	LEU	CA-CB-CG	6.48	130.21	115.30
13	N	9	DC	O4'-C1'-N1	6.47	112.53	108.00
12	T	19	DT	C6-C5-C7	-6.43	119.04	122.90
1	A	226	GLU	N-CA-CB	-6.23	99.38	110.60
2	B	74	LEU	CA-CB-CG	6.23	129.64	115.30
12	T	19	DT	C4-C5-C7	6.23	122.74	119.00
12	T	26	DG	O5'-P-OP2	-6.22	100.11	105.70
1	A	516	SER	N-CA-C	-6.21	94.24	111.00
1	A	1124	HIS	CB-CA-C	-6.21	97.99	110.40
13	N	9	DC	P-O3'-C3'	6.21	127.15	119.70
2	B	941	LEU	CA-CB-CG	6.18	129.52	115.30
12	T	15	DA	O4'-C1'-N9	6.17	112.32	108.00
13	N	11	DG	P-O3'-C3'	6.13	127.06	119.70
13	N	8	DT	P-O3'-C3'	6.11	127.04	119.70
11	R	8	G	N1-C6-O6	-6.02	116.29	119.90
11	R	2	U	O4'-C1'-N1	5.99	112.99	108.20
12	T	26	DG	N3-C4-C5	-5.99	125.61	128.60
1	A	397	ASN	N-CA-CB	-5.99	99.83	110.60
2	B	869	SER	CB-CA-C	5.97	121.44	110.10
10	L	50	ASP	N-CA-C	5.89	126.90	111.00
12	T	26	DG	N3-C4-N9	5.88	129.53	126.00
2	B	716	ASN	N-CA-C	5.82	126.71	111.00
11	R	11	U	P-O3'-C3'	5.72	126.56	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	T	6	DG	P-O3'-C3'	5.68	126.52	119.70
12	T	25	DC	N1-C2-O2	5.68	122.31	118.90
12	T	23	DC	C6-N1-C2	-5.67	118.03	120.30
3	C	195	GLN	N-CA-C	5.66	126.28	111.00
13	N	4	DC	N1-C2-O2	5.64	122.28	118.90
2	B	716	ASN	N-CA-CB	-5.62	100.48	110.60
2	B	976	ILE	N-CA-C	5.60	126.12	111.00
2	B	420	LEU	CA-CB-CG	-5.52	102.60	115.30
13	N	5	DT	C6-C5-C7	-5.52	119.59	122.90
1	A	40	THR	N-CA-C	5.50	125.85	111.00
11	R	2	U	C4'-C3'-C2'	-5.44	97.16	102.60
9	K	114	LEU	CA-CB-CG	5.43	127.80	115.30
12	T	27	DA	N7-C8-N9	5.43	116.52	113.80
12	T	1	DC	P-O3'-C3'	5.43	126.22	119.70
13	N	12	DT	C4-C5-C7	5.42	122.25	119.00
13	N	2	DT	C4-C5-C7	5.40	122.24	119.00
13	N	8	DT	C4-C5-C7	5.39	122.24	119.00
1	A	250	ILE	N-CA-CB	5.34	123.08	110.80
13	N	4	DC	O4'-C1'-N1	5.32	111.72	108.00
13	N	6	DT	N3-C2-O2	-5.32	119.11	122.30
12	T	28	DT	N1-C2-O2	5.32	127.35	123.10
12	T	12	DC	O4'-C1'-N1	5.31	111.72	108.00
11	R	3	C	O4'-C1'-N1	5.31	112.45	108.20
12	T	28	DT	C4'-C3'-C2'	-5.23	98.39	103.10
13	N	9	DC	N1-C2-O2	5.23	122.04	118.90
13	N	7	DA	P-O3'-C3'	5.22	125.97	119.70
12	T	27	DA	O4'-C1'-N9	5.22	111.65	108.00
12	T	25	DC	N3-C2-O2	-5.16	118.29	121.90
2	B	1156	ASP	N-CA-C	5.16	124.93	111.00
1	A	161	LEU	CA-CB-CG	5.16	127.16	115.30
13	N	6	DT	P-O3'-C3'	5.13	125.86	119.70
1	A	65	LEU	CA-CB-CG	5.12	127.07	115.30
13	N	6	DT	C4-C5-C7	5.10	122.06	119.00
13	N	5	DT	P-O3'-C3'	5.07	125.79	119.70
1	A	908	LEU	CA-CB-CG	5.04	126.89	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	11332	0	11391	806	0
2	B	9168	0	9179	616	0
3	C	2135	0	2091	139	0
4	E	1757	0	1781	48	0
5	F	684	0	703	30	0
6	H	1087	0	1062	59	0
7	I	971	0	930	63	0
8	J	532	0	544	49	0
9	K	919	0	929	55	0
10	L	363	0	389	13	0
11	R	284	0	142	19	0
12	T	587	0	327	24	0
13	N	284	0	161	3	0
14	A	2	0	0	2	0
14	B	1	0	0	0	0
14	C	1	0	0	2	0
14	I	2	0	0	0	0
14	J	1	0	0	2	0
14	L	1	0	0	0	0
All	All	30111	0	29629	1765	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 30.

All (1765) 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)
2:B:438:GLU:HB3	2:B:440:HIS:CD2	1.53	1.43
1:A:1168:GLU:CA	1:A:1171:GLN:HB2	1.51	1.41
1:A:1172:LEU:O	1:A:1174:PHE:N	1.56	1.34
2:B:439:ALA:CB	2:B:440:HIS:HA	1.56	1.29
1:A:1169:ILE:CB	1:A:1170:ILE:HB	1.60	1.29
1:A:1169:ILE:CG2	1:A:1170:ILE:HG13	1.64	1.26
1:A:1169:ILE:HB	1:A:1170:ILE:CB	1.67	1.23
1:A:1168:GLU:O	1:A:1169:ILE:HD12	1.38	1.21

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1169:ILE:CA	1:A:1170:ILE:HB	1.72	1.20
1:A:567:LYS:CG	1:A:568:PRO:HD2	1.70	1.20
2:B:439:ALA:HB3	2:B:440:HIS:CA	1.72	1.19
2:B:472:ALA:HB1	2:B:476:ARG:CG	1.72	1.18
1:A:157:ASP:CA	1:A:159:THR:HB	1.73	1.17
2:B:445:LYS:CA	2:B:446:LEU:HB3	1.74	1.17
1:A:1169:ILE:CG2	1:A:1170:ILE:CG1	2.23	1.15
2:B:438:GLU:CB	2:B:440:HIS:CD2	2.30	1.13
1:A:1169:ILE:N	1:A:1170:ILE:HB	1.60	1.13
1:A:1169:ILE:CB	1:A:1170:ILE:HD12	1.79	1.12
2:B:445:LYS:HA	2:B:446:LEU:CB	1.76	1.12
2:B:78:THR:H	2:B:79:THR:HB	1.02	1.12
2:B:444:MET:HG2	2:B:446:LEU:HD22	1.26	1.11
1:A:1168:GLU:HA	1:A:1171:GLN:CB	1.78	1.11
1:A:1168:GLU:HB2	1:A:1171:GLN:HG3	1.33	1.11
1:A:1178:ASP:CB	1:A:1179:GLU:HA	1.74	1.11
1:A:1169:ILE:HB	1:A:1170:ILE:HB	1.11	1.09
1:A:1168:GLU:CB	1:A:1171:GLN:CB	2.30	1.09
1:A:157:ASP:HA	1:A:159:THR:HB	1.13	1.09
1:A:419:LYS:NZ	1:A:419:LYS:HB3	1.66	1.08
1:A:1169:ILE:H	1:A:1170:ILE:C	1.55	1.07
1:A:1166:ASP:HB3	1:A:1170:ILE:CD1	1.84	1.07
1:A:156:ASP:C	1:A:158:PRO:HD3	1.74	1.07
3:C:32:SER:O	3:C:36:VAL:HG12	1.54	1.07
1:A:313:GLN:HG2	1:A:314:ALA:HB2	1.10	1.06
1:A:1169:ILE:HG22	1:A:1170:ILE:CG1	1.81	1.06
1:A:1169:ILE:HB	1:A:1170:ILE:CD1	1.85	1.06
1:A:1179:GLU:HG3	1:A:1179:GLU:O	1.52	1.06
1:A:1166:ASP:CB	1:A:1170:ILE:HD13	1.84	1.05
1:A:310:GLY:CA	1:A:311:GLN:HB3	1.86	1.05
1:A:567:LYS:CD	1:A:568:PRO:HD2	1.85	1.05
2:B:472:ALA:HB1	2:B:476:ARG:HG2	1.06	1.05
1:A:1168:GLU:HB2	1:A:1171:GLN:CB	1.87	1.05
1:A:1169:ILE:HB	1:A:1170:ILE:CG1	1.87	1.05
1:A:1173:HIS:NE2	1:A:1175:SER:HB3	1.72	1.04
1:A:1168:GLU:HB2	1:A:1171:GLN:CG	1.85	1.04
1:A:1178:ASP:CG	1:A:1179:GLU:HA	1.77	1.04
1:A:899:VAL:HB	1:A:929:LEU:HD11	1.38	1.04
1:A:1166:ASP:HB3	1:A:1170:ILE:HD13	1.09	1.03
1:A:313:GLN:HG2	1:A:314:ALA:CB	1.89	1.03
1:A:868:TYR:HE1	1:A:1064:VAL:HG11	1.24	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1187:ASN:HD21	2:B:1190:ASP:HB2	1.24	1.03
1:A:775:ILE:HB	1:A:797:LYS:O	1.59	1.02
1:A:1168:GLU:CA	1:A:1171:GLN:CB	2.35	1.02
1:A:154:SER:O	1:A:155:GLU:HB2	1.55	1.02
1:A:666:ILE:HD11	2:B:1026:LEU:HB3	1.42	1.01
1:A:1168:GLU:HG3	1:A:1171:GLN:HB3	1.43	1.01
3:C:142:VAL:HG22	3:C:143:LEU:H	1.24	1.00
1:A:1169:ILE:CB	1:A:1170:ILE:CB	2.30	1.00
1:A:1167:GLU:O	1:A:1170:ILE:HG22	1.62	1.00
1:A:187:LYS:HD3	1:A:188:ASP:N	1.76	0.99
1:A:567:LYS:HB2	1:A:568:PRO:CD	1.92	0.99
1:A:567:LYS:CB	1:A:568:PRO:CD	2.41	0.99
1:A:1169:ILE:CB	1:A:1170:ILE:CG1	2.40	0.99
2:B:955:THR:HG22	2:B:956:THR:H	1.28	0.98
1:A:1169:ILE:CG2	1:A:1170:ILE:CD1	2.40	0.97
1:A:118:HIS:CE1	1:A:155:GLU:HG2	1.98	0.97
1:A:192:GLY:O	1:A:193:ASP:HB3	1.63	0.97
1:A:172:PRO:HG3	1:A:185:TRP:NE1	1.79	0.96
1:A:1178:ASP:OD2	1:A:1179:GLU:HA	1.64	0.96
1:A:868:TYR:CE1	1:A:1064:VAL:HG11	2.01	0.95
2:B:1020:ARG:O	2:B:1021:MET:HB2	1.64	0.95
2:B:444:MET:C	2:B:445:LYS:HG3	1.86	0.95
1:A:249:SER:O	1:A:250:ILE:HG13	1.66	0.95
2:B:472:ALA:CB	2:B:476:ARG:CG	2.44	0.95
1:A:158:PRO:N	1:A:159:THR:CB	2.30	0.94
2:B:986:GLN:HE21	2:B:1022:THR:HG21	1.31	0.94
1:A:1169:ILE:HG22	1:A:1170:ILE:HG13	0.94	0.94
1:A:567:LYS:CB	1:A:568:PRO:HD2	1.97	0.94
1:A:187:LYS:O	1:A:189:ARG:HG3	1.67	0.94
1:A:1169:ILE:N	1:A:1170:ILE:CB	2.30	0.94
2:B:114:PRO:HG2	2:B:181:LEU:HD11	1.50	0.94
1:A:187:LYS:HZ2	1:A:188:ASP:H	1.01	0.93
1:A:1169:ILE:H	1:A:1171:GLN:N	1.64	0.93
1:A:157:ASP:HA	1:A:159:THR:CB	1.97	0.93
2:B:445:LYS:HA	2:B:446:LEU:HB3	0.96	0.93
1:A:310:GLY:N	1:A:311:GLN:HB3	1.82	0.93
2:B:444:MET:CE	2:B:446:LEU:HD13	1.99	0.93
1:A:157:ASP:C	1:A:159:THR:HB	1.88	0.93
2:B:1056:SER:HB3	2:B:1066:SER:O	1.68	0.93
2:B:472:ALA:CB	2:B:476:ARG:HG2	1.99	0.92
11:R:6:G:H2'	11:R:7:A:H8	1.32	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:167:HIS:HD2	3:C:169:LYS:H	1.08	0.92
2:B:843:GLN:HG2	2:B:993:THR:HB	1.50	0.92
1:A:1169:ILE:HG21	1:A:1170:ILE:CD1	1.98	0.92
6:H:109:LYS:HB3	6:H:111:LEU:H	1.33	0.91
1:A:310:GLY:HA2	1:A:311:GLN:HB3	1.50	0.91
1:A:1168:GLU:CG	1:A:1171:GLN:HB3	2.01	0.91
1:A:313:GLN:CG	1:A:314:ALA:HB2	2.00	0.91
1:A:49:LYS:HB3	1:A:55:ASP:OD2	1.71	0.91
1:A:419:LYS:HZ2	1:A:419:LYS:HB3	1.32	0.91
1:A:588:LEU:HB3	1:A:607:ILE:HB	1.53	0.90
1:A:1169:ILE:CB	1:A:1170:ILE:CD1	2.43	0.90
4:E:94:LYS:HE2	4:E:94:LYS:HA	1.51	0.90
2:B:78:THR:H	2:B:79:THR:CB	1.84	0.90
1:A:567:LYS:HB2	1:A:568:PRO:HD3	1.54	0.90
2:B:710:LEU:HD13	2:B:733:HIS:HB3	1.53	0.90
1:A:668:ASP:HB3	1:A:743:VAL:HG23	1.54	0.89
1:A:203:SER:O	1:A:207:ILE:CD1	2.20	0.89
1:A:1168:GLU:CB	1:A:1171:GLN:HB3	2.03	0.89
1:A:1168:GLU:CB	1:A:1171:GLN:HB2	1.98	0.89
1:A:158:PRO:N	1:A:159:THR:CA	2.33	0.89
2:B:438:GLU:HB3	2:B:440:HIS:CG	2.07	0.89
1:A:1169:ILE:HB	1:A:1170:ILE:HD12	1.44	0.88
2:B:273:LEU:HD21	2:B:360:PHE:HD1	1.39	0.88
2:B:444:MET:CG	2:B:446:LEU:HD22	2.02	0.88
2:B:85:SER:H	2:B:86:ARG:HB3	1.39	0.88
1:A:353:ILE:HD13	1:A:487:MET:HE2	1.54	0.88
2:B:77:HIS:HB3	2:B:78:THR:HB	1.56	0.88
1:A:148:CYS:HG	14:A:1734:ZN:ZN	0.88	0.88
1:A:158:PRO:N	1:A:159:THR:HB	1.89	0.87
1:A:310:GLY:H	1:A:311:GLN:HB3	1.37	0.87
2:B:759:PRO:HB3	2:B:767:ASN:HD21	1.39	0.87
1:A:378:GLU:OE1	1:A:434:ARG:HD3	1.73	0.87
2:B:636:PRO:CB	2:B:637:LEU:HA	2.03	0.87
1:A:161:LEU:HD22	1:A:162:VAL:N	1.90	0.87
2:B:78:THR:N	2:B:79:THR:HB	1.87	0.87
3:C:186:LEU:HB3	3:C:188:HIS:HD2	1.38	0.87
1:A:1178:ASP:CB	1:A:1179:GLU:CA	2.52	0.87
1:A:1169:ILE:CG2	1:A:1170:ILE:HD12	2.02	0.86
1:A:1178:ASP:HB2	1:A:1179:GLU:HA	1.57	0.86
2:B:863:GLU:HA	2:B:864:LYS:HB2	1.58	0.86
1:A:49:LYS:CB	1:A:55:ASP:OD2	2.24	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:157:ASP:N	1:A:158:PRO:HD3	1.85	0.85
1:A:1178:ASP:HB2	1:A:1179:GLU:CA	2.07	0.85
1:A:1172:LEU:HD23	1:A:1173:HIS:H	1.42	0.85
2:B:863:GLU:HA	2:B:864:LYS:CB	2.07	0.85
1:A:286:HIS:HB3	1:A:287:HIS:HB2	1.59	0.85
2:B:827:ILE:HD11	2:B:1086:PHE:CD2	2.12	0.85
1:A:157:ASP:C	1:A:159:THR:CG2	2.45	0.84
2:B:766:ARG:NH2	2:B:1020:ARG:NH1	2.25	0.84
1:A:158:PRO:N	1:A:159:THR:HA	1.93	0.84
2:B:1162:ILE:HG22	2:B:1163:CYS:H	1.41	0.84
1:A:752:LYS:HG3	2:B:1019:SER:HB2	1.60	0.84
1:A:575:LYS:HB3	1:A:612:ILE:HD11	1.58	0.84
3:C:167:HIS:CD2	3:C:169:LYS:H	1.95	0.83
6:H:109:LYS:HA	6:H:110:ASP:HB3	1.60	0.83
2:B:470:LYS:HE2	2:B:470:LYS:HA	1.59	0.83
1:A:567:LYS:CG	1:A:568:PRO:CD	2.55	0.83
1:A:40:THR:N	1:A:41:MET:HB2	1.93	0.83
1:A:310:GLY:H	1:A:311:GLN:CB	1.91	0.83
2:B:759:PRO:HB3	2:B:767:ASN:ND2	1.94	0.83
7:I:34:TYR:OH	7:I:36:GLU:HB3	1.77	0.83
1:A:326:ARG:HG2	1:A:1406:VAL:HG21	1.59	0.83
8:J:10:CYS:HG	14:J:101:ZN:ZN	0.51	0.82
2:B:715:ALA:HB3	2:B:716:ASN:HA	1.58	0.82
2:B:644:GLU:HG3	2:B:654:ARG:HH22	1.42	0.82
1:A:157:ASP:C	1:A:159:THR:CB	2.47	0.82
1:A:899:VAL:CG2	1:A:1029:ARG:HG2	2.09	0.82
1:A:1168:GLU:HA	1:A:1171:GLN:HB2	0.82	0.82
2:B:444:MET:O	2:B:445:LYS:HG3	1.80	0.82
2:B:308:TRP:HA	2:B:311:LEU:HD12	1.60	0.82
12:T:15:DA:H2"	12:T:16:DC:H5"	1.61	0.82
1:A:666:ILE:CD1	2:B:1026:LEU:HB3	2.09	0.82
1:A:335:ARG:HD2	2:B:1202:LEU:HD12	1.62	0.81
2:B:827:ILE:HD11	2:B:1086:PHE:HD2	1.44	0.81
2:B:944:THR:HG21	2:B:1122:ARG:NH2	1.96	0.81
2:B:634:TYR:CE1	2:B:692:TYR:HD1	1.98	0.81
2:B:1159:ARG:HD3	2:B:1193:GLN:HG3	1.62	0.81
1:A:899:VAL:HG23	1:A:1029:ARG:HG2	1.61	0.81
11:R:6:G:H2'	11:R:7:A:C8	2.15	0.81
1:A:573:SER:H	1:A:576:GLN:HG3	1.46	0.81
1:A:457:ALA:O	1:A:507:VAL:HG23	1.81	0.80
4:E:15:ALA:O	4:E:19:VAL:HG23	1.79	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:567:LYS:HG3	1:A:568:PRO:HD2	1.63	0.80
2:B:878:GLN:HG2	2:B:879:ARG:H	1.47	0.80
1:A:157:ASP:C	1:A:159:THR:HG22	2.01	0.80
2:B:999:MET:HG3	2:B:1000:PRO:HD2	1.62	0.80
1:A:156:ASP:C	1:A:158:PRO:CD	2.50	0.80
1:A:185:TRP:O	1:A:186:LYS:HB2	1.81	0.80
1:A:470:LEU:HD21	1:A:487:MET:HE3	1.64	0.80
3:C:57:VAL:HG21	8:J:57:ILE:HD11	1.64	0.80
11:R:4:G:H2'	11:R:5:A:H8	1.45	0.80
1:A:1402:PHE:CD2	1:A:1403:GLU:HB2	2.16	0.80
1:A:1169:ILE:H	1:A:1170:ILE:CA	1.95	0.80
1:A:14:VAL:H	1:A:1432:GLN:HE22	1.30	0.79
1:A:160:GLN:CD	1:A:160:GLN:N	2.36	0.79
7:I:98:VAL:HG11	7:I:113:ASP:HB2	1.64	0.79
1:A:118:HIS:HB2	1:A:123:ARG:HG2	1.64	0.79
2:B:716:ASN:O	2:B:717:GLU:CG	2.30	0.79
1:A:466:SER:O	2:B:1103:ILE:HD11	1.82	0.79
1:A:470:LEU:HD21	1:A:487:MET:CE	2.13	0.79
1:A:190:ALA:O	1:A:191:THR:HG23	1.83	0.79
1:A:886:ILE:HD11	1:A:943:LEU:HB3	1.63	0.79
2:B:472:ALA:CB	2:B:476:ARG:HD3	2.13	0.78
12:T:10:DA:H2"	12:T:11:DG:H5"	1.65	0.78
2:B:168:GLY:H	2:B:450:ALA:HB1	1.48	0.78
1:A:35:ILE:HG22	1:A:270:LEU:HD11	1.65	0.78
1:A:148:CYS:SG	14:A:1734:ZN:ZN	1.72	0.78
2:B:716:ASN:O	2:B:717:GLU:CB	2.32	0.78
1:A:58:LEU:HD21	1:A:244:PRO:HD2	1.66	0.78
1:A:40:THR:H	1:A:41:MET:HB2	1.49	0.78
3:C:47:ASP:HA	10:L:69:ALA:HB3	1.66	0.78
11:R:5:A:H2'	11:R:6:G:C8	2.18	0.78
7:I:78:CYS:O	7:I:79:HIS:HB2	1.83	0.78
2:B:803:LEU:N	2:B:822:ASN:HD21	1.81	0.78
2:B:863:GLU:CA	2:B:864:LYS:HB2	2.14	0.78
1:A:172:PRO:CG	1:A:185:TRP:NE1	2.46	0.77
2:B:65:GLU:CG	2:B:66:ASP:H	1.94	0.77
2:B:716:ASN:O	2:B:717:GLU:HG3	1.84	0.77
1:A:41:MET:HG3	1:A:42:ASP:H	1.48	0.77
3:C:148:ARG:HH22	8:J:64:ASN:HD22	1.30	0.77
2:B:176:SER:O	2:B:182:SER:HB3	1.85	0.77
2:B:444:MET:CE	2:B:446:LEU:CD1	2.63	0.77
6:H:44:VAL:HG13	6:H:48:PRO:HA	1.66	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:976:ILE:O	2:B:990:ILE:HB	1.85	0.76
2:B:906:SER:HA	2:B:946:ASN:HB2	1.65	0.76
2:B:65:GLU:HG2	2:B:66:ASP:N	1.98	0.76
3:C:57:VAL:CG2	8:J:57:ILE:HD11	2.15	0.76
1:A:320:ARG:HB3	1:A:321:PRO:CD	2.16	0.76
1:A:185:TRP:HH2	1:A:200:ARG:HD2	1.50	0.76
7:I:103:CYS:HB3	7:I:108:HIS:HB3	1.67	0.76
2:B:864:LYS:HG3	2:B:872:GLU:HB2	1.68	0.76
1:A:1082:ASN:HA	1:A:1083:THR:C	2.05	0.76
2:B:864:LYS:HA	2:B:864:LYS:HE2	1.67	0.76
1:A:472:LEU:O	1:A:475:THR:HB	1.86	0.76
6:H:109:LYS:HB3	6:H:111:LEU:N	2.01	0.76
9:K:65:HIS:HD2	9:K:67:PHE:HB2	1.51	0.76
1:A:158:PRO:CD	1:A:159:THR:HA	2.17	0.75
1:A:1178:ASP:OD2	1:A:1179:GLU:CA	2.34	0.75
1:A:161:LEU:HD22	1:A:162:VAL:H	1.50	0.75
2:B:445:LYS:CA	2:B:446:LEU:CB	2.49	0.75
2:B:827:ILE:CD1	2:B:1086:PHE:HD2	1.98	0.75
2:B:1065:GLN:HG2	2:B:1069:PHE:HB2	1.67	0.75
1:A:1167:GLU:C	1:A:1170:ILE:HG22	2.05	0.75
1:A:156:ASP:O	1:A:158:PRO:HD2	1.86	0.75
1:A:445:ASN:HB3	1:A:455:MET:HG2	1.67	0.75
2:B:438:GLU:HG2	2:B:440:HIS:NE2	2.01	0.75
1:A:419:LYS:HZ3	1:A:419:LYS:HB3	1.47	0.75
1:A:666:ILE:N	1:A:666:ILE:HD12	2.01	0.75
8:J:9:SER:OG	8:J:45:CYS:HB2	1.85	0.75
3:C:148:ARG:HH22	8:J:64:ASN:ND2	1.84	0.75
3:C:88:CYS:SG	3:C:92:CYS:HB3	2.27	0.75
5:F:101:ILE:HD13	5:F:120:ILE:HG22	1.69	0.74
5:F:111:LEU:H	5:F:111:LEU:HD22	1.51	0.74
1:A:508:PRO:O	1:A:511:ILE:HG13	1.86	0.74
1:A:193:ASP:O	1:A:194:ALA:CB	2.35	0.74
1:A:809:THR:HB	1:A:810:PRO:HD2	1.68	0.74
3:C:142:VAL:HG22	3:C:143:LEU:N	2.01	0.74
1:A:445:ASN:CB	1:A:455:MET:HG2	2.18	0.74
1:A:567:LYS:HD3	1:A:568:PRO:HD2	1.70	0.74
2:B:1162:ILE:HG22	2:B:1163:CYS:N	2.02	0.74
2:B:906:SER:HA	2:B:946:ASN:CB	2.17	0.74
2:B:862:GLN:HG2	2:B:963:PHE:HD1	1.53	0.73
6:H:38:LEU:HD13	6:H:125:LEU:HD13	1.69	0.73
1:A:156:ASP:O	1:A:158:PRO:CD	2.36	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:766:ARG:NH2	2:B:1020:ARG:HH12	1.85	0.73
2:B:515:HIS:HD2	2:B:517:THR:H	1.37	0.73
2:B:85:SER:N	2:B:86:ARG:HB3	2.03	0.73
1:A:482:PHE:O	2:B:989:THR:HG23	1.87	0.73
1:A:1179:GLU:CG	1:A:1179:GLU:O	2.31	0.73
1:A:1173:HIS:CD2	1:A:1175:SER:CB	2.72	0.73
2:B:899:ILE:HD11	2:B:911:ILE:HG23	1.70	0.73
1:A:1169:ILE:HG21	1:A:1170:ILE:HD12	1.65	0.73
2:B:981:ALA:HB2	2:B:987:LYS:HA	1.70	0.73
8:J:43:ARG:HH11	8:J:43:ARG:HB3	1.52	0.73
3:C:142:VAL:HG21	8:J:5:VAL:HG13	1.70	0.73
6:H:95:TYR:HE2	6:H:97:MET:HG3	1.54	0.73
1:A:310:GLY:CA	1:A:311:GLN:CB	2.67	0.73
2:B:956:THR:HA	2:B:961:LEU:O	1.88	0.72
1:A:192:GLY:O	1:A:193:ASP:CB	2.37	0.72
1:A:91:PHE:H	1:A:297:GLN:HE22	1.34	0.72
2:B:759:PRO:CB	2:B:767:ASN:HD21	2.02	0.72
1:A:193:ASP:O	1:A:194:ALA:HB3	1.88	0.72
2:B:472:ALA:HB2	2:B:476:ARG:HD3	1.69	0.72
2:B:515:HIS:H	2:B:518:HIS:CD2	2.07	0.72
2:B:64:CYS:SG	2:B:65:GLU:N	2.61	0.72
2:B:338:GLY:HA3	2:B:341:LEU:HG	1.71	0.72
2:B:1117:GLN:HG2	2:B:1156:ASP:OD2	1.89	0.72
6:H:112:ILE:HG22	6:H:127:GLY:O	1.89	0.72
1:A:567:LYS:NZ	6:H:46:LEU:HB2	2.05	0.72
2:B:445:LYS:HB3	2:B:447:ALA:H	1.55	0.72
1:A:187:LYS:NZ	1:A:187:LYS:HB2	2.03	0.71
4:E:24:LYS:HB3	4:E:30:ILE:HD12	1.70	0.71
1:A:731:ARG:HG3	1:A:755:PHE:CE1	2.25	0.71
2:B:636:PRO:HB2	2:B:637:LEU:HB3	1.70	0.71
1:A:630:ILE:HD12	1:A:630:ILE:H	1.55	0.71
1:A:1169:ILE:N	1:A:1170:ILE:CA	2.53	0.71
1:A:264:PHE:CE2	12:T:29:DA:H3'	2.26	0.71
3:C:124:LEU:O	3:C:127:ARG:HG2	1.89	0.71
1:A:1002:GLY:HA3	1:A:1007:ILE:HG21	1.70	0.71
1:A:1118:VAL:HG23	1:A:1306:LEU:HB2	1.72	0.71
1:A:39:GLU:HB3	1:A:41:MET:HB2	1.73	0.71
1:A:672:ASP:H	1:A:736:ASN:HD21	1.36	0.71
1:A:1169:ILE:N	1:A:1171:GLN:N	2.39	0.71
1:A:203:SER:O	1:A:207:ILE:HD12	1.89	0.71
2:B:770:GLN:HG2	2:B:983:ARG:O	1.90	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:463:THR:CG2	2:B:465:ASN:HD21	2.03	0.71
2:B:472:ALA:CB	2:B:476:ARG:CD	2.69	0.71
2:B:636:PRO:HB3	2:B:637:LEU:HA	1.71	0.71
1:A:1269:GLU:O	1:A:1270:ASN:HB2	1.90	0.71
2:B:1166:CYS:O	2:B:1215:ARG:HD2	1.91	0.71
1:A:1017:LEU:HB2	4:E:206:GLY:H	1.56	0.71
2:B:1106:ARG:NH1	2:B:1110:PRO:HD2	2.06	0.70
4:E:79:TRP:HE1	4:E:81:GLU:HG3	1.56	0.70
1:A:1168:GLU:O	1:A:1169:ILE:CD1	2.30	0.70
1:A:310:GLY:N	1:A:311:GLN:CB	2.50	0.70
1:A:185:TRP:O	1:A:186:LYS:CB	2.38	0.70
3:C:182:PRO:HB3	3:C:207:CYS:SG	2.31	0.70
2:B:636:PRO:CB	2:B:637:LEU:CA	2.69	0.70
1:A:1177:LEU:CD1	1:A:1177:LEU:O	2.39	0.70
2:B:439:ALA:HB3	2:B:440:HIS:HA	0.76	0.70
1:A:35:ILE:HG13	1:A:241:VAL:HG21	1.74	0.70
2:B:65:GLU:HG2	2:B:66:ASP:H	1.54	0.70
1:A:821:ARG:O	1:A:825:ILE:HG12	1.92	0.70
2:B:445:LYS:CA	2:B:447:ALA:H	2.05	0.70
2:B:444:MET:HE3	2:B:446:LEU:HD13	1.74	0.70
1:A:1155:ASP:HB3	1:A:1241:ARG:HH21	1.56	0.70
1:A:741:ASN:HD22	1:A:744:LYS:H	1.37	0.70
8:J:3:VAL:HG21	8:J:18:TRP:HB2	1.73	0.70
1:A:172:PRO:HG3	1:A:185:TRP:CE2	2.27	0.70
2:B:637:LEU:CD1	2:B:740:HIS:HB3	2.22	0.70
2:B:952:VAL:HG22	2:B:966:VAL:HG13	1.73	0.70
1:A:157:ASP:CA	1:A:159:THR:CB	2.59	0.69
1:A:1169:ILE:CG1	1:A:1170:ILE:HD12	2.21	0.69
1:A:187:LYS:CD	1:A:188:ASP:N	2.54	0.69
1:A:793:SER:HB2	1:A:794:PRO:HD2	1.73	0.69
2:B:438:GLU:CG	2:B:440:HIS:CD2	2.75	0.69
2:B:778:MET:CE	2:B:1094:ARG:HD3	2.22	0.69
8:J:7:CYS:SG	14:J:101:ZN:ZN	1.81	0.69
1:A:886:ILE:HD11	1:A:943:LEU:CB	2.23	0.69
1:A:187:LYS:NZ	1:A:188:ASP:H	1.85	0.69
1:A:1173:HIS:HD2	1:A:1175:SER:OG	1.75	0.69
1:A:154:SER:O	1:A:155:GLU:CB	2.37	0.69
5:F:101:ILE:HD13	5:F:120:ILE:CG2	2.23	0.69
2:B:515:HIS:H	2:B:518:HIS:HD2	1.38	0.69
2:B:464:GLY:HA2	2:B:480:SER:HB3	1.75	0.69
2:B:744:HIS:HD2	2:B:746:SER:OG	1.76	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:636:PRO:HB2	2:B:637:LEU:CA	2.22	0.69
2:B:717:GLU:O	2:B:720:ASP:N	2.26	0.69
1:A:731:ARG:HG3	1:A:755:PHE:CZ	2.27	0.69
1:A:858:ASN:HD22	1:A:858:ASN:C	1.95	0.69
9:K:46:ILE:O	9:K:50:LEU:HB2	1.91	0.69
1:A:14:VAL:H	1:A:1432:GLN:NE2	1.91	0.68
2:B:66:ASP:O	2:B:66:ASP:CG	2.30	0.68
2:B:944:THR:HG21	2:B:1122:ARG:HH22	1.57	0.68
2:B:213:ILE:HD11	2:B:481:GLN:OE1	1.93	0.68
3:C:133:ILE:HD11	3:C:237:SER:HA	1.74	0.68
2:B:239:GLU:HG2	2:B:255:GLN:HG2	1.75	0.68
2:B:1172:ILE:HG22	2:B:1174:LYS:HG3	1.74	0.68
2:B:65:GLU:CG	2:B:66:ASP:N	2.56	0.68
2:B:339:THR:O	2:B:340:ALA:HB3	1.93	0.68
2:B:334:ILE:HG22	2:B:334:ILE:O	1.94	0.68
2:B:872:GLU:HG2	2:B:916:THR:HB	1.75	0.68
7:I:14:LEU:HB3	7:I:27:PHE:HB3	1.75	0.68
3:C:88:CYS:SG	14:C:319:ZN:ZN	1.83	0.68
1:A:889:SER:HB2	1:A:892:ALA:H	1.59	0.68
2:B:634:TYR:CE1	2:B:692:TYR:CD1	2.82	0.68
1:A:55:ASP:H	1:A:56:PRO:HD2	1.60	0.67
3:C:88:CYS:HG	14:C:319:ZN:ZN	1.02	0.67
1:A:834:THR:HG21	1:A:1077:THR:HA	1.75	0.67
1:A:401:GLY:C	1:A:435:HIS:CD2	2.68	0.67
1:A:320:ARG:HA	1:A:320:ARG:HE	1.58	0.67
6:H:95:TYR:HB3	6:H:144:ILE:HB	1.77	0.67
1:A:382:PRO:HG3	1:A:428:TYR:CE2	2.29	0.67
5:F:93:ILE:HD11	5:F:134:ILE:HD11	1.76	0.67
1:A:264:PHE:HE2	12:T:29:DA:H3'	1.59	0.67
2:B:87:LYS:NZ	2:B:436:VAL:HG11	2.09	0.67
2:B:652:LYS:HB3	2:B:689:LEU:HD23	1.76	0.67
9:K:102:LYS:O	9:K:106:GLU:HG2	1.93	0.67
2:B:274:PRO:HB2	2:B:359:GLU:HB3	1.76	0.67
2:B:516:ASN:H	2:B:516:ASN:HD22	1.41	0.67
1:A:1173:HIS:CD2	1:A:1175:SER:HB3	2.29	0.67
5:F:132:LEU:O	5:F:148:VAL:HG23	1.95	0.67
2:B:784:ASN:OD1	2:B:788:ARG:HD2	1.95	0.67
9:K:63:VAL:O	9:K:63:VAL:HG23	1.95	0.67
2:B:195:CYS:HB3	2:B:782:LEU:HD22	1.77	0.67
2:B:530:GLY:H	11:R:12:G:H22	1.41	0.67
2:B:438:GLU:O	2:B:439:ALA:C	2.34	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:172:PRO:HG3	1:A:185:TRP:HE1	1.58	0.67
6:H:62:SER:O	6:H:63:LEU:O	2.12	0.67
3:C:102:GLN:HG2	3:C:154:LYS:HD2	1.77	0.67
2:B:827:ILE:CD1	2:B:1086:PHE:CD2	2.74	0.66
2:B:655:LYS:O	2:B:658:ILE:HG22	1.95	0.66
12:T:2:DT:H2"	12:T:3:DA:C8	2.31	0.66
2:B:440:HIS:C	2:B:442:PHE:H	1.98	0.66
1:A:1169:ILE:N	1:A:1170:ILE:C	2.40	0.66
2:B:438:GLU:CB	2:B:440:HIS:HD2	1.99	0.66
7:I:105:SER:O	7:I:106:CYS:HB3	1.95	0.66
2:B:976:ILE:HG23	2:B:977:GLY:H	1.61	0.66
2:B:911:ILE:HG22	2:B:912:ILE:HG13	1.77	0.66
1:A:599:SER:HB2	1:A:603:ASN:H	1.60	0.66
1:A:602:ASP:HB3	1:A:616:VAL:HG23	1.77	0.66
6:H:4:THR:HA	6:H:60:ALA:HB2	1.77	0.66
2:B:716:ASN:O	2:B:717:GLU:HB2	1.95	0.66
4:E:94:LYS:HE2	4:E:94:LYS:CA	2.26	0.66
2:B:715:ALA:N	2:B:716:ASN:HA	2.10	0.66
2:B:1077:THR:HG23	2:B:1079:LYS:H	1.60	0.66
1:A:1173:HIS:CD2	1:A:1175:SER:OG	2.49	0.66
6:H:12:VAL:HG13	6:H:26:ILE:HD11	1.77	0.66
7:I:63:GLY:HA3	7:I:104:LEU:HD11	1.78	0.66
2:B:778:MET:HE2	2:B:1094:ARG:HD3	1.77	0.66
1:A:809:THR:HB	1:A:810:PRO:CD	2.26	0.66
2:B:1001:PHE:CE2	2:B:1073:TYR:HB2	2.31	0.66
6:H:109:LYS:HA	6:H:110:ASP:CB	2.25	0.66
3:C:133:ILE:CD1	3:C:237:SER:HA	2.25	0.66
1:A:917:SER:O	1:A:918:GLU:HG3	1.96	0.66
2:B:445:LYS:CB	2:B:447:ALA:H	2.08	0.66
1:A:765:VAL:CG2	1:A:800:VAL:HB	2.25	0.66
1:A:1111:MET:HG3	1:A:1114:PRO:HG3	1.77	0.66
2:B:202:TYR:CD1	2:B:209:GLU:HB3	2.31	0.66
2:B:994:TYR:HB2	2:B:999:MET:HE1	1.77	0.65
1:A:1172:LEU:C	1:A:1174:PHE:N	2.43	0.65
2:B:706:GLN:O	2:B:710:LEU:HB2	1.96	0.65
2:B:463:THR:HG22	2:B:465:ASN:HD21	1.61	0.65
1:A:118:HIS:NE2	1:A:155:GLU:HG2	2.11	0.65
2:B:637:LEU:HD11	2:B:740:HIS:HB3	1.78	0.65
2:B:994:TYR:HB2	2:B:999:MET:CE	2.26	0.65
1:A:1161:THR:HG22	1:A:1163:ILE:H	1.62	0.65
11:R:5:A:H2'	11:R:6:G:H8	1.60	0.65

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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	0.65
5:F:114:GLU:OE2	5:F:119:ARG:HG3	1.97	0.65
2:B:715:ALA:HB3	2:B:716:ASN:CA	2.25	0.65
1:A:1386:ARG:NH2	12:T:15:DA:H8	1.94	0.65
3:C:43:THR:CG2	3:C:44:LEU:N	2.59	0.65
2:B:986:GLN:NE2	2:B:1022:THR:HG21	2.08	0.65
2:B:715:ALA:CB	2:B:716:ASN:HA	2.20	0.65
1:A:320:ARG:HB3	1:A:321:PRO:HD2	1.76	0.65
1:A:338:GLY:HA2	2:B:1129:ARG:HH22	1.62	0.65
1:A:1177:LEU:HD12	1:A:1177:LEU:O	1.94	0.65
1:A:118:HIS:NE2	1:A:155:GLU:CG	2.59	0.65
1:A:534:LEU:O	1:A:574:GLY:HA3	1.96	0.65
7:I:78:CYS:O	7:I:79:HIS:CB	2.45	0.65
1:A:779:PHE:CZ	2:B:517:THR:HA	2.32	0.65
2:B:463:THR:CG2	2:B:465:ASN:ND2	2.60	0.65
1:A:741:ASN:ND2	1:A:744:LYS:H	1.94	0.65
2:B:439:ALA:CB	2:B:440:HIS:CA	2.43	0.64
1:A:1269:GLU:O	1:A:1270:ASN:CB	2.44	0.64
1:A:535:THR:O	1:A:575:LYS:HE2	1.97	0.64
1:A:1173:HIS:NE2	1:A:1175:SER:CB	2.55	0.64
1:A:883:LEU:O	1:A:885:THR:N	2.30	0.64
6:H:93:TYR:CD1	6:H:143:LEU:HD23	2.32	0.64
2:B:291:ILE:N	2:B:291:ILE:HD12	2.12	0.64
2:B:986:GLN:HE21	2:B:1022:THR:CG2	2.07	0.64
2:B:715:ALA:HB3	2:B:716:ASN:C	2.17	0.64
1:A:503:GLN:HE22	5:F:90:ARG:HH21	1.45	0.64
8:J:43:ARG:NH1	8:J:43:ARG:HB3	2.12	0.64
1:A:109:HIS:HB2	1:A:167:CYS:SG	2.38	0.64
1:A:151:ASP:HB2	1:A:162:VAL:O	1.98	0.64
6:H:114:VAL:HG22	6:H:125:LEU:HB3	1.80	0.64
6:H:26:ILE:HG22	6:H:40:LEU:O	1.97	0.64
9:K:69:ALA:O	9:K:70:ARG:HB3	1.96	0.64
1:A:1441:PHE:CZ	5:F:89:GLU:HA	2.33	0.63
3:C:163:ILE:HD13	9:K:10:PHE:CE1	2.33	0.63
1:A:871:ASP:OD1	1:A:1366:ARG:NH2	2.32	0.63
1:A:658:LEU:HG	1:A:659:HIS:CD2	2.33	0.63
1:A:1021:LEU:HD11	1:A:1025:ARG:HE	1.64	0.63
1:A:875:ALA:HA	1:A:878:ILE:HD12	1.81	0.63
1:A:1172:LEU:HD23	1:A:1173:HIS:N	2.12	0.63
1:A:567:LYS:HB2	1:A:568:PRO:HD2	1.68	0.63
6:H:114:VAL:CG2	6:H:125:LEU:HB3	2.29	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:898:LEU:HD13	2:B:952:VAL:CG1	2.28	0.63
4:E:88:VAL:HG21	4:E:116:ILE:HD13	1.80	0.63
2:B:60:GLN:O	2:B:63:ILE:HG22	1.99	0.63
6:H:109:LYS:HG2	6:H:111:LEU:HD12	1.80	0.63
2:B:717:GLU:O	2:B:718:GLU:C	2.36	0.63
1:A:317:LYS:HD2	1:A:317:LYS:N	2.14	0.63
1:A:255:SER:HA	1:A:256:GLN:C	2.19	0.63
3:C:241:ASP:O	3:C:244:VAL:HG13	1.98	0.63
3:C:46:ILE:HD12	3:C:157:CYS:HB3	1.79	0.63
1:A:645:LEU:HG	1:A:649:ILE:HD11	1.81	0.63
3:C:114:TYR:CD2	3:C:140:ASN:HB3	2.34	0.63
11:R:4:G:H2'	11:R:5:A:C8	2.32	0.63
6:H:109:LYS:HD3	6:H:111:LEU:HB2	1.81	0.63
1:A:404:TYR:HA	1:A:413:ILE:O	1.99	0.63
1:A:630:ILE:HD12	1:A:630:ILE:N	2.14	0.62
2:B:464:GLY:CA	2:B:479:VAL:O	2.47	0.62
1:A:575:LYS:NZ	1:A:615:GLY:O	2.31	0.62
7:I:7:CYS:HB2	7:I:14:LEU:HD21	1.80	0.62
1:A:765:VAL:HG22	1:A:800:VAL:HB	1.80	0.62
1:A:587:HIS:HE2	1:A:969:GLN:HG2	1.62	0.62
1:A:587:HIS:NE2	1:A:969:GLN:HG2	2.13	0.62
1:A:523:ILE:HG23	1:A:527:THR:OG1	2.00	0.62
4:E:100:ILE:HG23	4:E:105:PHE:HB2	1.81	0.62
1:A:492:PRO:HB3	1:A:497:THR:HG22	1.81	0.62
1:A:158:PRO:HD2	1:A:160:GLN:OE1	1.99	0.62
2:B:803:LEU:H	2:B:822:ASN:HD21	1.45	0.62
1:A:511:ILE:HG12	1:A:521:MET:HE2	1.81	0.62
1:A:699:ALA:HB1	7:I:114:GLN:HG3	1.81	0.62
7:I:34:TYR:CZ	7:I:36:GLU:HB3	2.35	0.62
1:A:118:HIS:HE1	1:A:155:GLU:HG2	1.63	0.62
1:A:845:LEU:O	1:A:848:ILE:HG12	2.00	0.62
1:A:890:ASP:H	1:A:1296:GLY:HA3	1.65	0.62
1:A:483:ASP:HB3	2:B:837:ASP:HB3	1.81	0.62
12:T:6:DG:H2'	12:T:7:DA:C8	2.35	0.62
12:T:14:DG:H2'	12:T:15:DA:C4	2.33	0.62
2:B:996:ARG:HG3	2:B:1007:VAL:HG21	1.81	0.62
10:L:38:LEU:HD21	10:L:49:LYS:H	1.65	0.62
2:B:880:THR:HB	2:B:934:LYS:HB2	1.82	0.62
1:A:55:ASP:O	1:A:58:LEU:N	2.29	0.61
1:A:1085:HIS:HB2	1:A:1086:PHE:HA	1.80	0.61
8:J:3:VAL:HG21	8:J:18:TRP:CG	2.34	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:438:GLU:HG2	2:B:440:HIS:CD2	2.34	0.61
1:A:118:HIS:CE1	1:A:155:GLU:CG	2.80	0.61
1:A:535:THR:HG21	1:A:617:VAL:HG23	1.82	0.61
2:B:340:ALA:O	2:B:342:GLY:N	2.32	0.61
1:A:1030:ARG:HG2	1:A:1034:GLU:OE2	2.00	0.61
1:A:873:MET:C	1:A:1058:VAL:HG23	2.20	0.61
2:B:1072:MET:CE	2:B:1085:ILE:HD12	2.31	0.61
4:E:124:VAL:HB	4:E:125:PRO:HD3	1.82	0.61
1:A:158:PRO:HD2	1:A:159:THR:HA	1.82	0.61
1:A:196:GLU:N	1:A:197:PRO:HD3	2.15	0.61
4:E:79:TRP:NE1	4:E:81:GLU:HG3	2.14	0.61
2:B:1168:LEU:HD13	2:B:1208:MET:HE3	1.80	0.61
4:E:62:ALA:HB3	4:E:78:LEU:HB3	1.82	0.61
2:B:444:MET:HE3	2:B:446:LEU:CD1	2.27	0.61
2:B:636:PRO:HB2	2:B:637:LEU:HA	1.77	0.61
1:A:351:THR:OG1	2:B:1103:ILE:HG12	2.01	0.61
1:A:1189:SER:HB3	1:A:1241:ARG:HB3	1.82	0.61
1:A:31:SER:HB2	1:A:81:PHE:O	2.01	0.61
2:B:440:HIS:O	2:B:442:PHE:N	2.34	0.61
1:A:1080:THR:HG22	1:A:1081:LEU:N	2.15	0.61
3:C:70:ILE:HD11	3:C:144:ILE:HD12	1.83	0.61
1:A:779:PHE:CE1	1:A:785:PRO:HD3	2.36	0.61
2:B:807:ARG:HG2	2:B:1045:SER:OG	2.00	0.61
1:A:332:LYS:H	1:A:337:ARG:HB3	1.65	0.61
1:A:107:CYS:SG	1:A:108:MET:N	2.74	0.61
2:B:190:TYR:CE1	8:J:62:ARG:HG2	2.36	0.61
3:C:43:THR:HG23	3:C:74:SER:OG	2.01	0.60
1:A:185:TRP:HH2	1:A:200:ARG:CD	2.15	0.60
1:A:35:ILE:HG22	1:A:35:ILE:O	2.00	0.60
3:C:148:ARG:NH2	8:J:64:ASN:HD22	1.99	0.60
2:B:979:LYS:O	2:B:980:PHE:CD1	2.54	0.60
8:J:44:TYR:HA	8:J:47:ARG:HB2	1.82	0.60
1:A:452:LYS:HB2	2:B:1141:HIS:CE1	2.36	0.60
2:B:115:GLN:HG2	2:B:193:LYS:HB2	1.84	0.60
3:C:259:LEU:HD21	9:K:92:ASN:OD1	2.01	0.60
1:A:1119:TYR:CD1	1:A:1326:ARG:HB3	2.37	0.60
2:B:757:PRO:HG3	2:B:983:ARG:CZ	2.31	0.60
8:J:3:VAL:HG21	8:J:18:TRP:CB	2.30	0.60
2:B:898:LEU:HD13	2:B:952:VAL:HG11	1.83	0.60
1:A:302:THR:HG23	1:A:306:ASN:HB3	1.83	0.60
3:C:186:LEU:HB3	3:C:188:HIS:CD2	2.27	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1162:ILE:CG2	2:B:1163:CYS:H	2.14	0.60
1:A:265:LYS:HE2	1:A:303:TYR:HA	1.82	0.60
1:A:907:THR:HG22	1:A:908:LEU:H	1.67	0.60
1:A:1030:ARG:HG2	1:A:1034:GLU:CD	2.22	0.60
1:A:1119:TYR:HD1	1:A:1326:ARG:HB3	1.66	0.60
1:A:814:PHE:O	1:A:817:ALA:HB3	2.02	0.60
3:C:180:TYR:O	3:C:181:ASP:HB3	2.02	0.60
2:B:1020:ARG:HB3	2:B:1020:ARG:NH1	2.16	0.60
2:B:980:PHE:O	2:B:1095:LEU:HG	2.02	0.60
2:B:995:ARG:HB3	2:B:997:GLU:OE2	2.01	0.60
1:A:738:LYS:NZ	3:C:194:GLU:HA	2.17	0.60
1:A:1429:ILE:HG22	1:A:1429:ILE:O	2.02	0.60
2:B:982:SER:OG	2:B:983:ARG:N	2.35	0.60
5:F:97:ARG:HD2	5:F:101:ILE:HG13	1.83	0.60
1:A:1002:GLY:CA	1:A:1007:ILE:HG21	2.32	0.60
9:K:47:ARG:HD2	9:K:60:ALA:HA	1.84	0.60
1:A:1015:VAL:HG12	1:A:1019:CYS:SG	2.41	0.60
2:B:459:TYR:C	2:B:459:TYR:CD2	2.76	0.59
2:B:274:PRO:O	2:B:275:TYR:HB2	2.01	0.59
2:B:428:ILE:O	2:B:432:MET:HG3	2.03	0.59
1:A:775:ILE:HB	1:A:797:LYS:C	2.22	0.59
2:B:863:GLU:HA	2:B:864:LYS:CG	2.32	0.59
1:A:765:VAL:HG13	1:A:802:ASN:O	2.03	0.59
1:A:1193:LEU:HD21	1:A:1267:MET:HE2	1.82	0.59
2:B:444:MET:HE2	2:B:446:LEU:CD1	2.31	0.59
2:B:445:LYS:HB3	2:B:447:ALA:HB3	1.84	0.59
2:B:636:PRO:HB2	2:B:637:LEU:CB	2.32	0.59
2:B:1168:LEU:HD13	2:B:1208:MET:CE	2.32	0.59
2:B:1084:GLN:HG2	3:C:201:TRP:CH2	2.37	0.59
2:B:976:ILE:HG23	2:B:977:GLY:N	2.17	0.59
2:B:620:ARG:NE	7:I:89:GLN:HE22	2.00	0.59
1:A:751:SER:O	1:A:752:LYS:HD3	2.02	0.59
6:H:109:LYS:CB	6:H:111:LEU:H	2.10	0.59
3:C:102:GLN:HG2	3:C:154:LYS:CD	2.32	0.59
6:H:8:ASP:HB3	6:H:10:PHE:CE1	2.38	0.59
1:A:402:ALA:HB2	1:A:434:ARG:HA	1.84	0.59
2:B:221:ASN:OD1	2:B:242:SER:HA	2.02	0.59
1:A:836:TYR:CE2	1:A:840:ARG:HD2	2.38	0.59
1:A:39:GLU:HB3	1:A:41:MET:CB	2.32	0.59
4:E:179:GLN:O	4:E:182:ASP:HB2	2.03	0.59
1:A:648:ASN:O	1:A:652:VAL:HG23	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:I:83:ASN:C	7:I:83:ASN:HD22	2.06	0.59
8:J:7:CYS:SG	8:J:7:CYS:O	2.61	0.59
1:A:1323:ASP:OD1	1:A:1325:THR:HG22	2.03	0.59
1:A:313:GLN:HG2	1:A:314:ALA:CA	2.32	0.59
1:A:351:THR:CG2	1:A:352:VAL:N	2.65	0.59
2:B:530:GLY:N	11:R:12:G:H22	2.00	0.59
1:A:981:LEU:HD12	1:A:1032:LEU:HD21	1.85	0.59
1:A:719:VAL:HG12	1:A:723:ASN:HD21	1.66	0.59
2:B:843:GLN:HG2	2:B:993:THR:CB	2.28	0.58
1:A:482:PHE:CE1	2:B:836:GLU:HB2	2.37	0.58
2:B:793:ALA:C	2:B:794:ASN:HD22	2.06	0.58
1:A:752:LYS:NZ	11:R:14:DA:O5'	2.35	0.58
9:K:10:PHE:N	9:K:10:PHE:CD2	2.70	0.58
2:B:210:LYS:HZ2	2:B:482:VAL:HG22	1.68	0.58
1:A:1170:ILE:HD11	1:A:1239:ARG:HD2	1.85	0.58
2:B:444:MET:SD	2:B:446:LEU:HD13	2.42	0.58
1:A:302:THR:HG21	1:A:314:ALA:HB3	1.84	0.58
2:B:1056:SER:CB	2:B:1066:SER:O	2.45	0.58
1:A:317:LYS:HD2	1:A:317:LYS:H	1.68	0.58
2:B:806:THR:HG22	2:B:808:ALA:H	1.68	0.58
1:A:198:GLU:CD	1:A:198:GLU:N	2.57	0.58
6:H:36:CYS:HA	6:H:126:GLU:O	2.04	0.58
1:A:752:LYS:HG3	2:B:1019:SER:CB	2.33	0.58
1:A:56:PRO:O	1:A:57:ARG:HB2	2.03	0.58
1:A:913:LEU:HD11	1:A:981:LEU:O	2.03	0.58
2:B:901:PRO:HB3	2:B:950:ASP:O	2.03	0.58
1:A:756:ILE:O	1:A:760:GLN:HG2	2.03	0.58
2:B:955:THR:HG22	2:B:956:THR:N	2.09	0.58
1:A:464:PRO:HB2	1:A:465:TYR:HD1	1.68	0.58
9:K:65:HIS:CD2	9:K:67:PHE:HB2	2.37	0.58
1:A:1243:VAL:HG13	1:A:1244:ARG:HB2	1.85	0.58
1:A:106:VAL:HG11	1:A:214:ILE:HD11	1.83	0.58
2:B:716:ASN:N	2:B:716:ASN:OD1	2.36	0.58
1:A:351:THR:HG21	1:A:466:SER:O	2.03	0.58
1:A:573:SER:O	1:A:576:GLN:HB2	2.03	0.58
1:A:269:ILE:HD11	1:A:300:VAL:HA	1.85	0.58
1:A:662:PHE:HB3	2:B:829:CYS:SG	2.42	0.58
2:B:338:GLY:HA3	2:B:341:LEU:CG	2.33	0.58
5:F:93:ILE:HD11	5:F:134:ILE:CD1	2.33	0.58
2:B:287:ARG:NH2	2:B:294:ASP:OD2	2.37	0.58
2:B:445:LYS:HA	2:B:447:ALA:H	1.69	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:187:LYS:HZ2	1:A:187:LYS:HB2	1.68	0.58
1:A:1406:VAL:HG12	1:A:1410:PHE:CE1	2.39	0.58
3:C:101:LEU:HB3	3:C:155:LEU:HB2	1.86	0.58
2:B:485:ARG:HH11	2:B:485:ARG:HG2	1.69	0.58
1:A:298:PHE:CE1	1:A:313:GLN:HG3	2.39	0.58
7:I:103:CYS:CB	7:I:108:HIS:HB3	2.33	0.58
2:B:308:TRP:O	2:B:311:LEU:N	2.37	0.58
12:T:13:DA:H2"	12:T:14:DG:C8	2.39	0.58
2:B:797:TYR:HB3	2:B:798:TYR:CD1	2.39	0.58
5:F:99:LEU:HD13	5:F:99:LEU:O	2.04	0.58
1:A:58:LEU:HD21	1:A:244:PRO:CD	2.34	0.57
2:B:808:ALA:O	2:B:812:LEU:HG	2.04	0.57
1:A:994:GLN:HE22	1:A:1023:ARG:HE	1.50	0.57
1:A:1006:ILE:HD13	1:A:1006:ILE:H	1.69	0.57
1:A:666:ILE:CD1	1:A:666:ILE:N	2.67	0.57
2:B:273:LEU:HD21	2:B:360:PHE:CD1	2.30	0.57
2:B:1204:PHE:O	2:B:1208:MET:HG3	2.04	0.57
3:C:3:GLU:HG2	9:K:100:ALA:HB1	1.86	0.57
2:B:168:GLY:N	2:B:450:ALA:HB1	2.19	0.57
6:H:4:THR:HA	6:H:60:ALA:CB	2.34	0.57
8:J:10:CYS:SG	8:J:11:GLY:N	2.74	0.57
1:A:160:GLN:OE1	1:A:160:GLN:N	2.37	0.57
1:A:187:LYS:HE3	1:A:188:ASP:HB3	1.85	0.57
2:B:999:MET:HG2	2:B:1007:VAL:HG13	1.85	0.57
1:A:190:ALA:O	1:A:191:THR:CG2	2.52	0.57
2:B:464:GLY:HA3	2:B:479:VAL:O	2.04	0.57
1:A:102:VAL:HG11	1:A:211:PHE:HE1	1.69	0.57
2:B:89:GLU:O	2:B:89:GLU:HG2	2.03	0.57
1:A:423:ASP:O	1:A:424:ILE:HB	2.03	0.57
1:A:148:CYS:SG	1:A:167:CYS:HB2	2.45	0.57
2:B:87:LYS:HZ1	2:B:436:VAL:HG11	1.69	0.57
6:H:142:LEU:HD12	6:H:143:LEU:N	2.19	0.57
1:A:413:ILE:HD12	1:A:413:ILE:N	2.19	0.57
3:C:112:ASN:HD21	3:C:146:LYS:HD3	1.70	0.57
1:A:346:ASP:OD1	1:A:346:ASP:N	2.37	0.57
1:A:153:PRO:C	1:A:155:GLU:H	2.06	0.57
1:A:465:TYR:CD1	1:A:465:TYR:N	2.69	0.57
1:A:497:THR:HG23	2:B:1146:PHE:HD1	1.70	0.57
9:K:56:VAL:HG13	9:K:77:THR:HG22	1.87	0.57
8:J:7:CYS:O	8:J:8:PHE:C	2.43	0.57
2:B:784:ASN:CG	2:B:788:ARG:HD2	2.25	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1008:PRO:HG3	2:B:1087:PHE:CE1	2.40	0.57
2:B:555:ILE:HD11	2:B:582:VAL:HG11	1.87	0.57
2:B:1001:PHE:HE1	3:C:178:PHE:HB3	1.70	0.56
1:A:515:GLN:HG3	1:A:1071:SER:HB3	1.87	0.56
2:B:417:PHE:CE1	2:B:453:ILE:HD13	2.40	0.56
2:B:603:LEU:HB2	2:B:609:ILE:HG12	1.87	0.56
1:A:1187:GLN:HB3	1:A:1188:GLN:HA	1.87	0.56
9:K:11:LEU:HD12	9:K:11:LEU:N	2.20	0.56
3:C:228:PHE:CD1	3:C:228:PHE:N	2.69	0.56
1:A:277:GLU:O	1:A:281:HIS:HD2	1.88	0.56
3:C:162:GLY:HA3	3:C:170:TRP:CE2	2.40	0.56
1:A:1172:LEU:CG	1:A:1173:HIS:N	2.68	0.56
1:A:567:LYS:HZ1	6:H:46:LEU:HB2	1.70	0.56
1:A:157:ASP:N	1:A:158:PRO:CD	2.66	0.56
2:B:1187:ASN:ND2	2:B:1190:ASP:HB2	2.08	0.56
2:B:1020:ARG:NH2	11:R:14:DA:OP2	2.38	0.56
2:B:978:ASP:O	2:B:980:PHE:HD1	1.86	0.56
3:C:71:PRO:O	3:C:133:ILE:HG13	2.04	0.56
2:B:474:SER:O	2:B:475:SER:O	2.23	0.56
1:A:365:GLY:O	1:A:468:PHE:HA	2.04	0.56
1:A:187:LYS:HZ2	1:A:188:ASP:N	1.87	0.56
2:B:1142:GLY:HA3	5:F:88:TYR:HE2	1.71	0.56
2:B:208:SER:HB2	2:B:482:VAL:HG13	1.88	0.56
1:A:242:PRO:HG3	2:B:1209:ALA:HB1	1.87	0.56
1:A:343:LYS:HZ1	2:B:1197:PRO:HB3	1.70	0.56
2:B:467:GLY:O	2:B:468:GLU:C	2.42	0.56
1:A:187:LYS:C	1:A:187:LYS:HD3	2.26	0.56
6:H:107:VAL:O	6:H:109:LYS:HG3	2.06	0.56
1:A:981:LEU:HD21	1:A:1039:LYS:HA	1.88	0.56
1:A:789:LYS:HD3	2:B:620:ARG:HH12	1.70	0.56
3:C:15:LYS:H	3:C:15:LYS:HD2	1.68	0.56
1:A:351:THR:HG22	1:A:352:VAL:O	2.05	0.56
1:A:272:ALA:O	1:A:296:LEU:HD13	2.05	0.56
2:B:235:SER:OG	2:B:236:HIS:HD2	1.89	0.56
1:A:451:HIS:NE2	1:A:1074:GLU:HG3	2.20	0.56
2:B:48:LEU:HD23	2:B:173:MET:SD	2.46	0.56
1:A:858:ASN:ND2	1:A:860:LEU:H	2.02	0.56
2:B:1120:GLU:HG2	2:B:1121:GLY:H	1.69	0.56
8:J:10:CYS:SG	8:J:45:CYS:SG	3.04	0.56
7:I:75:CYS:HB2	7:I:78:CYS:SG	2.46	0.56
1:A:55:ASP:N	1:A:56:PRO:CD	2.69	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:645:LEU:O	1:A:649:ILE:HG13	2.06	0.56
1:A:35:ILE:CG2	1:A:270:LEU:HD11	2.33	0.56
1:A:18:GLN:O	2:B:1215:ARG:HG2	2.05	0.56
7:I:68:LEU:HB3	7:I:84:VAL:CG2	2.36	0.56
4:E:45:LYS:HD3	4:E:46:TYR:CE1	2.41	0.56
2:B:955:THR:HG23	10:L:54:ARG:O	2.06	0.55
1:A:203:SER:O	1:A:207:ILE:HD11	2.03	0.55
1:A:511:ILE:HG12	1:A:521:MET:CE	2.36	0.55
2:B:1082:MET:HA	3:C:189:THR:HA	1.88	0.55
1:A:443:LEU:HD23	1:A:444:PHE:H	1.70	0.55
2:B:287:ARG:HA	2:B:291:ILE:O	2.05	0.55
2:B:310:MET:O	2:B:313:MET:HB2	2.07	0.55
9:K:82:ASP:OD1	9:K:83:PRO:HD2	2.06	0.55
1:A:1167:GLU:O	1:A:1170:ILE:CG2	2.44	0.55
1:A:324:SER:OG	1:A:325:ILE:N	2.39	0.55
2:B:706:GLN:HB2	2:B:710:LEU:HD23	1.88	0.55
1:A:1410:PHE:HD2	2:B:1212:ILE:HD11	1.72	0.55
2:B:1084:GLN:NE2	3:C:192:TRP:HB2	2.22	0.55
3:C:27:LEU:HD12	3:C:228:PHE:CE2	2.42	0.55
1:A:114:LEU:HD11	1:A:171:GLN:HE22	1.71	0.55
1:A:691:LEU:O	1:A:695:LYS:HB2	2.05	0.55
1:A:187:LYS:HD3	1:A:188:ASP:CA	2.36	0.55
9:K:70:ARG:HG3	9:K:70:ARG:O	2.05	0.55
2:B:459:TYR:C	2:B:459:TYR:HD2	2.10	0.55
2:B:122:LEU:HD22	2:B:958:GLN:HG3	1.88	0.55
2:B:523:CYS:SG	2:B:750:GLY:N	2.80	0.55
1:A:157:ASP:O	1:A:157:ASP:CG	2.43	0.55
2:B:67:SER:HB2	2:B:92:PHE:HD1	1.71	0.55
1:A:423:ASP:CG	1:A:424:ILE:H	2.08	0.55
1:A:1287:TYR:CD2	1:A:1305:VAL:HG21	2.41	0.55
2:B:545:ILE:CD1	2:B:633:VAL:HG13	2.36	0.55
1:A:1219:THR:HG21	1:A:1271:ILE:HD11	1.89	0.55
1:A:1386:ARG:HH22	12:T:15:DA:H8	1.54	0.55
1:A:1444:MET:HB2	5:F:133:VAL:HG12	1.87	0.55
1:A:899:VAL:HB	1:A:929:LEU:CD1	2.25	0.55
2:B:1181:GLU:HA	2:B:1187:ASN:O	2.07	0.55
7:I:80:SER:HB3	7:I:105:SER:HB2	1.87	0.55
1:A:55:ASP:O	1:A:57:ARG:N	2.39	0.55
3:C:147:LEU:HD13	3:C:151:GLN:O	2.06	0.55
2:B:1110:PRO:HB2	2:B:1119:VAL:CG2	2.37	0.55
3:C:3:GLU:HG3	3:C:4:GLU:H	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:628:GLY:O	1:A:632:VAL:HG23	2.07	0.55
2:B:31:TRP:O	2:B:34:ILE:N	2.40	0.55
1:A:679:ILE:O	1:A:682:THR:HG22	2.07	0.55
9:K:35:PHE:HD1	9:K:35:PHE:H	1.55	0.55
12:T:15:DA:H2"	12:T:16:DC:C5'	2.35	0.55
1:A:814:PHE:CE1	2:B:514:LEU:HD21	2.42	0.55
2:B:434:ARG:HA	2:B:437:GLU:HG3	1.89	0.54
1:A:306:ASN:HB2	1:A:313:GLN:OE1	2.07	0.54
2:B:984:HIS:CE1	2:B:1025:HIS:HA	2.42	0.54
2:B:344:LYS:HG2	2:B:347:LYS:HD2	1.89	0.54
1:A:157:ASP:O	1:A:159:THR:HG22	2.06	0.54
1:A:302:THR:O	1:A:324:SER:HB2	2.07	0.54
2:B:979:LYS:HG2	2:B:1095:LEU:HD12	1.88	0.54
3:C:93:ASP:O	3:C:127:ARG:NH2	2.40	0.54
4:E:45:LYS:HD3	4:E:46:TYR:HE1	1.72	0.54
1:A:1339:LEU:HD13	4:E:147:HIS:CD2	2.43	0.54
1:A:1223:ASP:O	1:A:1224:LEU:HB3	2.06	0.54
2:B:440:HIS:C	2:B:442:PHE:N	2.61	0.54
8:J:7:CYS:SG	8:J:9:SER:OG	2.63	0.54
2:B:211:VAL:O	2:B:480:SER:HA	2.08	0.54
2:B:1072:MET:HE2	2:B:1085:ILE:HD12	1.89	0.54
1:A:1213:GLY:HA2	1:A:1216:ILE:HD12	1.88	0.54
2:B:42:GLY:O	2:B:43:LEU:HD23	2.07	0.54
3:C:262:LEU:HD22	9:K:88:LYS:HE2	1.88	0.54
4:E:157:SER:OG	4:E:160:GLU:HB2	2.07	0.54
2:B:863:GLU:HA	2:B:864:LYS:HG2	1.89	0.54
2:B:516:ASN:ND2	2:B:516:ASN:H	2.04	0.54
2:B:71:LEU:H	2:B:88:TYR:HA	1.72	0.54
1:A:1105:LEU:HD22	1:A:1384:VAL:HG21	1.90	0.54
2:B:788:ARG:NH1	2:B:790:ASP:OD1	2.41	0.54
1:A:900:ASP:HA	1:A:926:GLN:HE22	1.73	0.54
8:J:37:SER:OG	8:J:47:ARG:NH2	2.41	0.54
1:A:1261:LYS:O	1:A:1264:GLU:HG3	2.08	0.54
2:B:260:GLY:O	2:B:267:ARG:HD3	2.08	0.54
1:A:526:ASP:HB2	2:B:835:GLN:CD	2.28	0.54
2:B:831:SER:OG	2:B:832:GLY:N	2.40	0.54
1:A:825:ILE:HD12	2:B:512:ARG:HB3	1.89	0.54
2:B:1084:GLN:HG2	3:C:201:TRP:CZ2	2.42	0.54
1:A:6:TYR:O	2:B:1175:LEU:HD21	2.08	0.54
6:H:30:SER:OG	6:H:33:GLN:HB2	2.08	0.54
6:H:78:SER:O	6:H:79:TRP:C	2.46	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1168:GLU:HG2	1:A:1168:GLU:O	2.08	0.54
1:A:868:TYR:CE1	1:A:1064:VAL:HG21	2.43	0.54
7:I:80:SER:CB	7:I:105:SER:HB2	2.38	0.54
7:I:16:PRO:HG3	7:I:27:PHE:CE2	2.43	0.54
2:B:515:HIS:CD2	2:B:517:THR:H	2.23	0.54
4:E:27:GLY:O	4:E:65:THR:HG22	2.08	0.54
2:B:25:ILE:HG22	2:B:26:THR:N	2.23	0.54
5:F:82:THR:HG22	5:F:84:TYR:H	1.72	0.54
2:B:438:GLU:CG	2:B:440:HIS:NE2	2.71	0.54
1:A:567:LYS:HG3	1:A:568:PRO:CD	2.30	0.54
1:A:567:LYS:HZ2	6:H:46:LEU:HB2	1.73	0.54
1:A:295:LEU:HA	1:A:298:PHE:HB3	1.89	0.54
1:A:189:ARG:CZ	1:A:196:GLU:O	2.56	0.54
2:B:957:ASN:HB3	2:B:961:LEU:HG	1.90	0.54
1:A:444:PHE:CE2	1:A:470:LEU:HD23	2.43	0.54
1:A:286:HIS:HB3	1:A:287:HIS:CB	2.35	0.54
1:A:858:ASN:ND2	1:A:858:ASN:C	2.62	0.54
3:C:241:ASP:HB3	9:K:109:TRP:CE2	2.43	0.54
2:B:383:ASN:O	2:B:387:LEU:HB2	2.08	0.54
4:E:94:LYS:CE	4:E:94:LYS:HA	2.21	0.53
2:B:301:ILE:HG22	2:B:302:CYS:N	2.22	0.53
9:K:73:LEU:CD2	9:K:75:ILE:HD11	2.38	0.53
2:B:491:THR:O	2:B:495:LEU:HG	2.07	0.53
1:A:55:ASP:N	1:A:56:PRO:HD2	2.23	0.53
1:A:1085:HIS:CB	1:A:1086:PHE:HA	2.37	0.53
1:A:419:LYS:NZ	1:A:419:LYS:CB	2.50	0.53
2:B:652:LYS:HB3	2:B:689:LEU:CD2	2.39	0.53
1:A:901:LEU:HD12	1:A:926:GLN:HG2	1.90	0.53
1:A:1080:THR:HG22	1:A:1081:LEU:H	1.73	0.53
1:A:1209:MET:O	1:A:1212:VAL:HB	2.07	0.53
1:A:1378:GLN:OE1	1:A:1382:THR:HG21	2.08	0.53
7:I:17:ARG:HH11	7:I:17:ARG:HB2	1.73	0.53
2:B:471:LYS:NZ	11:R:4:G:H1'	2.23	0.53
1:A:470:LEU:HD21	1:A:487:MET:HE1	1.87	0.53
2:B:906:SER:HA	2:B:946:ASN:HB3	1.89	0.53
2:B:620:ARG:HE	7:I:89:GLN:HE22	1.57	0.53
1:A:390:GLN:O	1:A:394:ASN:HB2	2.08	0.53
3:C:31:ASN:ND2	3:C:35:ARG:HD2	2.24	0.53
2:B:790:ASP:N	2:B:790:ASP:OD2	2.42	0.53
1:A:902:LEU:HG	1:A:926:GLN:HG3	1.90	0.53
9:K:29:ASN:ND2	9:K:77:THR:O	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1027:ILE:O	2:B:1030:LEU:N	2.42	0.53
2:B:567:GLU:CD	2:B:567:GLU:H	2.12	0.53
2:B:827:ILE:HG13	2:B:1086:PHE:O	2.09	0.53
9:K:73:LEU:HD23	9:K:75:ILE:HD11	1.90	0.53
1:A:316:GLN:HB3	1:A:317:LYS:HD2	1.91	0.53
2:B:1072:MET:HE2	2:B:1085:ILE:CD1	2.39	0.53
3:C:228:PHE:HD1	3:C:228:PHE:N	2.06	0.53
2:B:964:VAL:HG12	2:B:965:LYS:N	2.23	0.53
1:A:153:PRO:C	1:A:155:GLU:N	2.62	0.53
6:H:112:ILE:HG22	6:H:128:ASN:HA	1.91	0.53
1:A:392:VAL:HG11	1:A:424:ILE:HG21	1.91	0.53
1:A:775:ILE:HG13	1:A:798:GLY:HA3	1.92	0.52
3:C:163:ILE:HD12	3:C:163:ILE:H	1.73	0.52
1:A:874:ASP:N	1:A:1058:VAL:HG23	2.24	0.52
1:A:265:LYS:HA	1:A:268:ASP:HB2	1.90	0.52
2:B:71:LEU:HG	2:B:72:GLU:N	2.21	0.52
1:A:53:LEU:HD23	1:A:53:LEU:C	2.29	0.52
2:B:445:LYS:HA	2:B:447:ALA:N	2.25	0.52
2:B:983:ARG:HD2	2:B:1091:TYR:HD2	1.74	0.52
1:A:106:VAL:HG11	1:A:214:ILE:CD1	2.39	0.52
1:A:500:GLU:OE1	2:B:1145:SER:N	2.42	0.52
6:H:105:GLU:HB2	6:H:115:TYR:HE1	1.74	0.52
2:B:189:LEU:HA	2:B:192:LEU:HD12	1.90	0.52
2:B:445:LYS:N	2:B:446:LEU:HB3	2.24	0.52
7:I:7:CYS:O	7:I:11:ASN:HA	2.09	0.52
2:B:126:SER:HB2	2:B:172:ILE:HD11	1.91	0.52
1:A:1220:PHE:O	1:A:1221:LYS:HB2	2.10	0.52
3:C:164:ALA:O	3:C:167:HIS:N	2.43	0.52
1:A:401:GLY:O	1:A:435:HIS:CD2	2.63	0.52
7:I:28:GLU:HB3	7:I:35:VAL:HG22	1.91	0.52
6:H:40:LEU:HD12	6:H:41:ASP:H	1.75	0.52
1:A:528:LEU:HA	1:A:531:ILE:HG22	1.92	0.52
2:B:76:GLN:HA	2:B:82:ASP:HA	1.91	0.52
1:A:249:SER:C	1:A:250:ILE:HG13	2.27	0.52
2:B:1110:PRO:HB2	2:B:1119:VAL:HG22	1.92	0.52
2:B:1112:GLN:HG3	2:B:1119:VAL:HG12	1.91	0.52
3:C:52:GLU:HB3	3:C:154:LYS:HB3	1.90	0.52
3:C:99:LEU:HB2	3:C:157:CYS:HB2	1.92	0.52
2:B:546:SER:OG	2:B:631:GLY:N	2.32	0.52
1:A:75:ASN:HA	2:B:1116:ARG:HH22	1.73	0.52
1:A:1134:ILE:O	1:A:1138:ILE:HG12	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:32:SER:O	3:C:36:VAL:CG1	2.44	0.52
1:A:37:PHE:HB2	1:A:52:GLY:HA3	1.92	0.52
2:B:486:TYR:CE2	2:B:777:ALA:O	2.62	0.52
2:B:976:ILE:O	2:B:990:ILE:O	2.26	0.52
2:B:115:GLN:OE1	2:B:115:GLN:HA	2.09	0.52
3:C:73:GLN:HE21	3:C:75:MET:N	2.07	0.52
1:A:1434:ALA:O	1:A:1436:ILE:N	2.43	0.52
1:A:867:ILE:HD13	1:A:1014:ALA:HB2	1.92	0.52
1:A:784:LEU:HB3	1:A:786:HIS:HD2	1.74	0.52
6:H:95:TYR:HD2	6:H:95:TYR:C	2.12	0.52
1:A:1082:ASN:HA	1:A:1083:THR:O	2.10	0.52
2:B:545:ILE:HD12	2:B:633:VAL:HG13	1.90	0.52
2:B:344:LYS:O	2:B:347:LYS:N	2.41	0.52
2:B:712:PRO:O	2:B:713:ALA:HB2	2.10	0.52
2:B:628:THR:O	2:B:628:THR:HG22	2.10	0.52
1:A:49:LYS:H	1:A:50:ILE:HA	1.75	0.52
2:B:620:ARG:NH1	7:I:68:LEU:HD21	2.25	0.52
1:A:247:ARG:NH1	1:A:263:THR:HG23	2.25	0.52
2:B:910:VAL:HG13	2:B:938:SER:OG	2.09	0.52
1:A:153:PRO:O	1:A:155:GLU:N	2.43	0.52
2:B:1101:ASP:HA	2:B:1122:ARG:HH22	1.75	0.52
2:B:64:CYS:O	2:B:65:GLU:HB3	2.10	0.52
1:A:1444:MET:HB2	5:F:133:VAL:CG1	2.40	0.52
1:A:1349:TYR:HA	1:A:1372:VAL:HG21	1.92	0.52
2:B:483:LEU:HD22	2:B:484:ASN:H	1.75	0.52
4:E:94:LYS:O	4:E:98:ILE:HG12	2.09	0.51
12:T:11:DG:H1	13:N:4:DC:H42	1.58	0.51
1:A:91:PHE:H	1:A:297:GLN:NE2	2.05	0.51
2:B:85:SER:CA	2:B:86:ARG:HB3	2.40	0.51
2:B:878:GLN:O	2:B:879:ARG:NH2	2.42	0.51
3:C:258:ILE:HD12	9:K:42:LEU:HD21	1.92	0.51
9:K:56:VAL:HA	9:K:77:THR:HG22	1.92	0.51
1:A:17:VAL:HB	1:A:1419:ASP:HB3	1.91	0.51
2:B:1051:THR:HB	2:B:1054:GLY:H	1.74	0.51
1:A:709:THR:HG23	7:I:94:ASP:HA	1.92	0.51
2:B:73:GLN:HG3	2:B:86:ARG:HG3	1.91	0.51
2:B:635:ARG:HB2	2:B:636:PRO:HD2	1.91	0.51
2:B:715:ALA:H	2:B:716:ASN:HA	1.74	0.51
1:A:356:ASP:HB3	1:A:359:LEU:HB2	1.92	0.51
1:A:834:THR:CG2	1:A:1077:THR:HA	2.41	0.51
6:H:12:VAL:CG1	6:H:51:ALA:HA	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:35:ARG:NH1	9:K:41:THR:OG1	2.42	0.51
1:A:37:PHE:HB3	1:A:39:GLU:OE1	2.09	0.51
1:A:190:ALA:O	1:A:191:THR:CB	2.58	0.51
4:E:199:ILE:O	4:E:199:ILE:HG22	2.10	0.51
7:I:16:PRO:HG3	7:I:27:PHE:HE2	1.75	0.51
7:I:32:CYS:O	7:I:33:SER:OG	2.18	0.51
1:A:1082:ASN:N	1:A:1082:ASN:HD22	2.08	0.51
2:B:339:THR:O	2:B:340:ALA:CB	2.58	0.51
1:A:1094:VAL:HA	1:A:1113:THR:HG21	1.91	0.51
1:A:569:LYS:HD2	3:C:221:TYR:HB2	1.93	0.51
1:A:172:PRO:CD	1:A:185:TRP:NE1	2.74	0.51
1:A:48:ALA:O	1:A:49:LYS:HD2	2.11	0.51
3:C:57:VAL:HG23	8:J:57:ILE:HD11	1.91	0.51
1:A:14:VAL:HB	1:A:1432:GLN:HE22	1.76	0.51
2:B:1095:LEU:C	2:B:1096:ARG:O	2.48	0.51
4:E:29:PHE:C	4:E:30:ILE:HG13	2.30	0.51
1:A:1177:LEU:HD13	1:A:1177:LEU:O	2.10	0.51
1:A:1131:ALA:HA	1:A:1134:ILE:HD12	1.93	0.51
4:E:185:ALA:HA	4:E:190:LEU:HD23	1.92	0.51
12:T:19:DT:H2'	12:T:20:DC:C6	2.46	0.51
1:A:446:ARG:HD2	1:A:480:ALA:HB2	1.92	0.51
2:B:905:VAL:CG1	2:B:941:LEU:HG	2.40	0.51
4:E:180:ARG:HB2	4:E:215:MET:OXT	2.10	0.51
7:I:73:ARG:HG3	7:I:101:PHE:CE2	2.46	0.51
10:L:31:CYS:SG	10:L:34:CYS:HB2	2.51	0.51
9:K:51:LEU:HD11	9:K:59:ALA:HB3	1.92	0.51
4:E:23:VAL:HG12	4:E:28:TYR:HB2	1.92	0.51
1:A:219:PHE:O	1:A:222:LEU:HD12	2.11	0.51
6:H:95:TYR:CD2	6:H:95:TYR:C	2.84	0.51
7:I:105:SER:O	7:I:106:CYS:CB	2.58	0.51
1:A:665:GLY:O	1:A:668:ASP:HB2	2.11	0.51
6:H:118:PHE:O	6:H:120:GLY:N	2.44	0.51
8:J:44:TYR:C	8:J:44:TYR:CD1	2.84	0.51
2:B:662:MET:C	2:B:664:THR:H	2.14	0.51
9:K:44:ASN:HA	9:K:61:TYR:CE2	2.46	0.51
2:B:69:LEU:H	2:B:90:ILE:HG22	1.75	0.51
8:J:35:ALA:O	8:J:39:LEU:HD13	2.10	0.51
2:B:132:VAL:HG21	2:B:445:LYS:HZ1	1.76	0.51
2:B:715:ALA:HB3	2:B:716:ASN:O	2.10	0.51
2:B:879:ARG:CZ	2:B:879:ARG:HA	2.40	0.51
1:A:33:ALA:HB3	1:A:82:GLY:CA	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:172:PRO:HD3	1:A:185:TRP:HE1	1.76	0.50
2:B:899:ILE:HD11	2:B:911:ILE:HG12	1.93	0.50
2:B:71:LEU:HG	2:B:72:GLU:HB2	1.93	0.50
5:F:84:TYR:CE1	5:F:152:ILE:HD12	2.47	0.50
2:B:628:THR:O	2:B:628:THR:CG2	2.59	0.50
3:C:43:THR:HG22	3:C:44:LEU:N	2.25	0.50
6:H:41:ASP:HB2	6:H:121:LEU:HB3	1.92	0.50
1:A:235:ILE:HD12	1:A:235:ILE:O	2.10	0.50
1:A:158:PRO:N	1:A:159:THR:HG22	2.25	0.50
2:B:955:THR:CG2	2:B:956:THR:H	2.07	0.50
6:H:109:LYS:CD	6:H:111:LEU:HB2	2.41	0.50
7:I:10:CYS:SG	7:I:29:CYS:SG	3.10	0.50
1:A:351:THR:HG23	1:A:352:VAL:N	2.25	0.50
2:B:365:THR:HG21	2:B:370:PHE:CG	2.47	0.50
2:B:599:THR:O	2:B:603:LEU:HG	2.12	0.50
7:I:106:CYS:O	7:I:107:SER:HB2	2.12	0.50
1:A:50:ILE:HG12	1:A:51:GLY:N	2.27	0.50
4:E:62:ALA:N	4:E:78:LEU:O	2.42	0.50
1:A:873:MET:HG2	1:A:957:PRO:HG3	1.93	0.50
1:A:310:GLY:H	1:A:311:GLN:HB2	1.73	0.50
3:C:148:ARG:N	3:C:151:GLN:OE1	2.43	0.50
2:B:558:LEU:C	2:B:560:GLU:H	2.15	0.50
1:A:843:LYS:HD3	1:A:846:GLU:OE2	2.12	0.50
1:A:356:ASP:OD2	9:K:65:HIS:HE1	1.94	0.50
3:C:241:ASP:HB3	9:K:109:TRP:CZ2	2.47	0.50
1:A:852:TYR:O	5:F:81:THR:HG22	2.12	0.50
2:B:291:ILE:CD1	2:B:291:ILE:N	2.75	0.50
1:A:815:PHE:O	1:A:818:MET:N	2.45	0.50
2:B:1008:PRO:HG3	2:B:1087:PHE:HE1	1.77	0.50
2:B:842:ASN:HD22	2:B:845:SER:HB3	1.77	0.50
3:C:165:LYS:O	9:K:6:ARG:NH1	2.44	0.50
1:A:1172:LEU:HG	1:A:1173:HIS:N	2.26	0.50
6:H:42:ILE:HG23	6:H:95:TYR:HE1	1.77	0.50
1:A:848:ILE:HD13	1:A:858:ASN:HB3	1.94	0.50
1:A:125:ALA:O	1:A:128:ILE:HG22	2.12	0.50
4:E:201:LYS:HE2	4:E:207:ARG:NH1	2.27	0.50
1:A:591:PHE:HA	1:A:595:THR:HG21	1.94	0.50
8:J:32:GLU:O	8:J:36:LEU:HG	2.11	0.50
1:A:1193:LEU:HD21	1:A:1267:MET:CE	2.42	0.49
3:C:235:VAL:HG11	8:J:6:ARG:HH21	1.77	0.49
1:A:187:LYS:CE	1:A:188:ASP:HB3	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:46:THR:C	1:A:48:ALA:H	2.14	0.49
2:B:830:TYR:O	2:B:831:SER:CB	2.59	0.49
7:I:111:THR:HG22	7:I:113:ASP:H	1.77	0.49
3:C:43:THR:HG23	3:C:44:LEU:H	1.75	0.49
1:A:273:ASN:HD22	1:A:296:LEU:HD21	1.77	0.49
1:A:579:SER:HB3	1:A:611:GLN:HA	1.94	0.49
5:F:118:LEU:O	5:F:122:MET:HG3	2.12	0.49
2:B:1181:GLU:HG2	2:B:1188:LYS:HG2	1.94	0.49
2:B:728:ARG:HH21	2:B:1048:THR:H	1.58	0.49
1:A:158:PRO:N	1:A:159:THR:CG2	2.71	0.49
1:A:1158:PRO:HG3	1:A:1188:GLN:HE21	1.76	0.49
1:A:1195:LEU:HB2	1:A:1238:ILE:HB	1.93	0.49
3:C:177:GLU:HB2	3:C:231:ASN:HB3	1.93	0.49
1:A:67:CYS:O	1:A:70:CYS:HB2	2.12	0.49
1:A:255:SER:HA	1:A:256:GLN:O	2.13	0.49
2:B:637:LEU:O	2:B:690:VAL:HA	2.11	0.49
2:B:213:ILE:HG23	2:B:497:ARG:O	2.12	0.49
1:A:531:ILE:O	1:A:531:ILE:HG12	2.13	0.49
3:C:258:ILE:HG22	3:C:259:LEU:N	2.27	0.49
1:A:908:LEU:CD2	1:A:908:LEU:H	2.25	0.49
2:B:467:GLY:O	2:B:468:GLU:O	2.30	0.49
9:K:44:ASN:HA	9:K:61:TYR:HE2	1.77	0.49
2:B:591:ARG:O	2:B:592:ASN:HB3	2.12	0.49
2:B:549:THR:HG22	2:B:550:ASP:H	1.77	0.49
1:A:577:ILE:O	1:A:580:VAL:HB	2.12	0.49
1:A:286:HIS:CB	1:A:287:HIS:HB2	2.37	0.49
2:B:87:LYS:HZ3	2:B:436:VAL:HG11	1.78	0.49
6:H:142:LEU:C	6:H:143:LEU:HD12	2.32	0.49
1:A:1039:LYS:HE2	1:A:1043:ASP:OD2	2.12	0.49
2:B:363:HIS:O	2:B:364:ILE:HB	2.11	0.49
1:A:679:ILE:HA	1:A:682:THR:HG22	1.95	0.49
1:A:862:ASN:OD1	4:E:174:GLN:HA	2.12	0.49
1:A:464:PRO:HB2	1:A:465:TYR:CD1	2.48	0.49
2:B:1074:ASN:HB3	2:B:1077:THR:HG22	1.94	0.49
1:A:907:THR:HG22	1:A:908:LEU:N	2.27	0.49
2:B:998:ASP:OD2	3:C:35:ARG:NH2	2.45	0.49
2:B:760:ASP:OD2	2:B:1046:PRO:O	2.31	0.49
1:A:84:ILE:HG22	1:A:239:LEU:O	2.11	0.49
1:A:556:TRP:O	1:A:558:GLY:N	2.46	0.49
2:B:112:LEU:HD11	2:B:117:ALA:HB2	1.94	0.49
1:A:1167:GLU:O	1:A:1170:ILE:O	2.30	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:T:27:DA:H2	12:T:28:DT:H1'	1.77	0.49
1:A:800:VAL:HG13	1:A:812:GLU:CD	2.33	0.49
2:B:794:ASN:HD22	2:B:794:ASN:N	2.10	0.49
3:C:112:ASN:ND2	3:C:146:LYS:HD3	2.26	0.49
5:F:82:THR:O	5:F:136:ARG:NH1	2.44	0.49
1:A:19:PHE:O	1:A:1416:ALA:HA	2.13	0.49
1:A:1251:GLU:HG2	1:A:1252:THR:H	1.78	0.49
2:B:817:LEU:N	2:B:818:PRO:HD3	2.27	0.49
1:A:785:PRO:HB2	2:B:703:ILE:HD12	1.95	0.49
2:B:620:ARG:HH11	7:I:68:LEU:HD21	1.78	0.49
3:C:84:ARG:HD2	9:K:11:LEU:HD21	1.94	0.49
8:J:17:LYS:HB3	8:J:39:LEU:HD23	1.94	0.49
2:B:846:ILE:HG23	2:B:974:PRO:HG2	1.95	0.49
3:C:92:CYS:SG	3:C:93:ASP:N	2.85	0.49
3:C:142:VAL:CG2	8:J:5:VAL:HG13	2.41	0.49
2:B:1020:ARG:CZ	2:B:1020:ARG:HB3	2.43	0.49
3:C:124:LEU:C	3:C:126:GLY:N	2.66	0.49
2:B:1084:GLN:CD	2:B:1084:GLN:H	2.16	0.49
2:B:344:LYS:CB	2:B:347:LYS:HB2	2.43	0.49
1:A:436:ILE:HD11	1:A:491:VAL:HG11	1.93	0.49
2:B:555:ILE:HA	2:B:558:LEU:HD12	1.95	0.48
2:B:1120:GLU:HG2	2:B:1121:GLY:N	2.27	0.48
2:B:31:TRP:CE3	2:B:34:ILE:HD12	2.48	0.48
1:A:1116:LEU:HB2	1:A:1308:THR:HB	1.95	0.48
1:A:635:ARG:HE	1:A:877:HIS:HA	1.77	0.48
2:B:798:TYR:CD2	8:J:4:PRO:HG3	2.48	0.48
3:C:238:ILE:CG2	3:C:242:GLN:HB2	2.43	0.48
2:B:345:LYS:HG2	2:B:348:ARG:HH21	1.78	0.48
1:A:1449:SER:HA	1:A:1450:LEU:C	2.34	0.48
1:A:360:GLU:HB2	1:A:363:GLN:OE1	2.13	0.48
1:A:1170:ILE:O	1:A:1170:ILE:HG22	2.12	0.48
1:A:465:TYR:HD1	1:A:465:TYR:N	2.09	0.48
1:A:901:LEU:N	1:A:926:GLN:HE21	2.11	0.48
2:B:1072:MET:HE3	2:B:1085:ILE:HD12	1.95	0.48
2:B:560:GLU:O	2:B:561:TRP:CD1	2.66	0.48
1:A:488:ASN:ND2	2:B:1128:LEU:HD12	2.27	0.48
1:A:254:GLU:HG3	2:B:918:ILE:HG21	1.95	0.48
2:B:488:TYR:C	2:B:490:SER:H	2.16	0.48
2:B:547:VAL:HG12	2:B:612:GLU:OE2	2.13	0.48
6:H:47:PHE:HB3	6:H:95:TYR:CD1	2.48	0.48
1:A:185:TRP:CH2	1:A:200:ARG:HD2	2.39	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:55:ASP:HA	1:A:58:LEU:O	2.13	0.48
2:B:1162:ILE:CG2	2:B:1163:CYS:N	2.72	0.48
2:B:20:ASP:N	2:B:655:LYS:HZ3	2.11	0.48
2:B:839:MET:CE	2:B:1010:LEU:HD12	2.43	0.48
1:A:419:LYS:HZ2	1:A:419:LYS:CB	2.13	0.48
2:B:1163:CYS:HB3	2:B:1167:GLY:H	1.78	0.48
2:B:1149:GLU:C	2:B:1151:LEU:H	2.17	0.48
1:A:374:LEU:O	1:A:436:ILE:HD13	2.13	0.48
2:B:865:LYS:HA	2:B:870:ILE:O	2.13	0.48
1:A:147:VAL:HG12	1:A:170:THR:HG22	1.95	0.48
1:A:24:PRO:HG3	1:A:237:THR:HB	1.95	0.48
1:A:666:ILE:CG1	2:B:1026:LEU:HB3	2.43	0.48
1:A:193:ASP:OD2	1:A:193:ASP:O	2.30	0.48
1:A:40:THR:HB	1:A:41:MET:HA	1.94	0.48
3:C:44:LEU:HD12	3:C:160:LYS:O	2.14	0.48
9:K:35:PHE:CD1	9:K:35:PHE:N	2.80	0.48
2:B:1017:ILE:HB	2:B:1018:PRO:HD3	1.95	0.48
1:A:1147:THR:HB	7:I:48:LEU:HD12	1.95	0.48
1:A:557:ASP:OD1	1:A:559:VAL:HB	2.13	0.48
2:B:445:LYS:HB3	2:B:447:ALA:CB	2.43	0.48
1:A:261:ASP:HB3	1:A:322:VAL:HG12	1.96	0.48
1:A:53:LEU:HD23	1:A:54:ASN:N	2.28	0.48
9:K:51:LEU:CD1	9:K:59:ALA:HB3	2.44	0.48
1:A:847:ASP:HB3	1:A:1424:VAL:HG23	1.95	0.48
1:A:370:ILE:HG23	2:B:1105:ALA:HB2	1.95	0.48
1:A:298:PHE:HE1	1:A:313:GLN:HG3	1.78	0.48
1:A:731:ARG:CG	1:A:755:PHE:CE1	2.95	0.48
1:A:741:ASN:ND2	1:A:741:ASN:C	2.67	0.48
1:A:814:PHE:CZ	2:B:514:LEU:HD21	2.49	0.48
1:A:423:ASP:O	1:A:424:ILE:CB	2.62	0.48
2:B:256:VAL:HG11	2:B:382:ILE:HD13	1.96	0.48
1:A:256:GLN:HA	12:T:29:DA:C2	2.49	0.48
7:I:33:SER:O	7:I:35:VAL:HG23	2.14	0.48
1:A:662:PHE:O	2:B:828:ALA:HA	2.14	0.48
4:E:171:LYS:HB2	4:E:174:GLN:HG3	1.96	0.48
4:E:77:SER:HB3	4:E:105:PHE:HD2	1.79	0.48
1:A:549:MET:O	1:A:552:TRP:HB2	2.14	0.48
1:A:899:VAL:HG23	1:A:1029:ARG:CG	2.39	0.47
3:C:143:LEU:C	3:C:143:LEU:HD12	2.34	0.47
9:K:7:PHE:HA	9:K:10:PHE:CE2	2.48	0.47
2:B:31:TRP:HA	2:B:34:ILE:HG13	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:381:THR:O	1:A:383:TYR:N	2.47	0.47
2:B:360:PHE:HE2	2:B:374:LYS:HB3	1.79	0.47
1:A:372:LYS:HA	1:A:435:HIS:ND1	2.29	0.47
1:A:464:PRO:HB3	9:K:4:PRO:HG3	1.95	0.47
1:A:738:LYS:HZ3	3:C:194:GLU:HA	1.78	0.47
9:K:56:VAL:HG13	9:K:77:THR:CG2	2.44	0.47
1:A:869:GLY:O	4:E:204:THR:HG21	2.15	0.47
1:A:322:VAL:C	1:A:324:SER:H	2.18	0.47
1:A:37:PHE:HA	1:A:38:PRO:HD3	1.74	0.47
1:A:981:LEU:CD2	1:A:1039:LYS:HA	2.44	0.47
2:B:26:THR:HB	2:B:27:ALA:H	1.49	0.47
2:B:441:ASP:O	2:B:443:ASN:N	2.42	0.47
1:A:567:LYS:HE2	6:H:95:TYR:CZ	2.49	0.47
2:B:1006:ILE:HD12	8:J:45:CYS:HB3	1.96	0.47
3:C:57:VAL:HG21	8:J:57:ILE:CD1	2.40	0.47
1:A:1082:ASN:H	1:A:1082:ASN:HD22	1.61	0.47
9:K:63:VAL:O	9:K:63:VAL:CG2	2.62	0.47
6:H:24:CYS:O	6:H:41:ASP:HA	2.14	0.47
2:B:1116:ARG:HD2	2:B:1198:TYR:CE2	2.50	0.47
2:B:842:ASN:ND2	2:B:845:SER:H	2.11	0.47
1:A:546:VAL:O	1:A:550:LEU:HD22	2.15	0.47
2:B:486:TYR:OH	2:B:1096:ARG:HB3	2.14	0.47
2:B:703:ILE:HG22	2:B:704:ALA:O	2.14	0.47
6:H:6:PHE:CZ	6:H:8:ASP:HB2	2.50	0.47
1:A:296:LEU:O	1:A:300:VAL:HG23	2.15	0.47
3:C:101:LEU:HD23	3:C:155:LEU:HD12	1.95	0.47
1:A:1060:PRO:HD2	5:F:86:THR:CG2	2.44	0.47
3:C:76:ASP:O	3:C:79:GLN:HG2	2.15	0.47
2:B:89:GLU:CG	2:B:89:GLU:O	2.62	0.47
1:A:1329:THR:HG23	1:A:1331:SER:H	1.79	0.47
2:B:121:ASN:HD22	2:B:121:ASN:N	2.12	0.47
1:A:1152:ILE:HB	7:I:44:TYR:HB3	1.95	0.47
1:A:1172:LEU:CD2	1:A:1173:HIS:N	2.76	0.47
1:A:323:LYS:O	1:A:324:SER:HB3	2.14	0.47
6:H:109:LYS:CG	6:H:111:LEU:HB2	2.44	0.47
1:A:91:PHE:CZ	1:A:207:ILE:HD12	2.50	0.47
6:H:118:PHE:CZ	6:H:142:LEU:HD23	2.50	0.47
3:C:244:VAL:O	3:C:248:ILE:HG13	2.14	0.47
1:A:1030:ARG:CG	1:A:1034:GLU:OE2	2.61	0.47
1:A:548:ASN:OD1	9:K:60:ALA:HB1	2.15	0.47
1:A:1341:ILE:HG22	4:E:182:ASP:OD2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:K:6:ARG:C	9:K:8:GLU:H	2.18	0.47
2:B:779:GLY:HA2	2:B:796:LEU:HB2	1.96	0.47
2:B:791:THR:O	2:B:792:MET:CB	2.63	0.47
1:A:598:LEU:HD21	6:H:124:ARG:HB2	1.96	0.47
2:B:644:GLU:HG3	2:B:654:ARG:NH2	2.22	0.47
2:B:358:LYS:O	2:B:362:PRO:HG3	2.15	0.47
1:A:453:MET:HB3	1:A:477:PRO:HB3	1.96	0.47
1:A:58:LEU:HD23	1:A:80:HIS:HB2	1.97	0.47
2:B:1084:GLN:NE2	3:C:192:TRP:CB	2.77	0.47
2:B:711:GLU:N	2:B:712:PRO:HD3	2.30	0.47
2:B:492:LEU:HB3	2:B:751:VAL:HG21	1.97	0.47
2:B:41:LYS:HB3	2:B:45:SER:HB3	1.97	0.47
1:A:119:ASN:O	1:A:120:GLU:O	2.33	0.47
1:A:964:ILE:HG21	1:A:1035:TYR:CD2	2.50	0.47
8:J:6:ARG:HG2	8:J:11:GLY:O	2.15	0.47
1:A:158:PRO:CD	1:A:159:THR:HB	2.45	0.47
1:A:161:LEU:HD22	1:A:162:VAL:O	2.14	0.47
1:A:575:LYS:HB3	1:A:612:ILE:CD1	2.36	0.47
2:B:1103:ILE:O	2:B:1122:ARG:NH1	2.48	0.47
1:A:469:ARG:NH2	2:B:991:GLY:O	2.48	0.47
1:A:1434:ALA:HB3	1:A:1436:ILE:HD12	1.97	0.47
5:F:101:ILE:CD1	5:F:120:ILE:HG22	2.41	0.47
2:B:1174:LYS:HB2	2:B:1179:GLN:O	2.15	0.47
11:R:8:G:O2'	11:R:9:G:H5'	2.15	0.47
1:A:278:THR:O	1:A:282:ASN:HB2	2.15	0.47
7:I:50:THR:HG22	7:I:52:ILE:H	1.80	0.47
1:A:899:VAL:HG22	1:A:1029:ARG:HG2	1.95	0.46
7:I:106:CYS:SG	7:I:107:SER:N	2.88	0.46
7:I:74:GLU:HG3	7:I:79:HIS:HA	1.98	0.46
1:A:91:PHE:HZ	1:A:207:ILE:HD12	1.79	0.46
1:A:444:PHE:HE2	1:A:470:LEU:HD23	1.80	0.46
1:A:892:ALA:HA	1:A:895:LYS:NZ	2.31	0.46
1:A:901:LEU:HB2	1:A:926:GLN:HG2	1.97	0.46
1:A:913:LEU:HG	1:A:915:SER:H	1.80	0.46
2:B:406:LEU:HD12	2:B:545:ILE:HD11	1.97	0.46
2:B:745:PRO:C	2:B:747:MET:N	2.68	0.46
3:C:45:ALA:HA	3:C:72:LEU:HD12	1.97	0.46
1:A:942:PHE:C	1:A:942:PHE:CD2	2.87	0.46
1:A:1172:LEU:O	1:A:1174:PHE:CA	2.56	0.46
2:B:715:ALA:H	2:B:716:ASN:CA	2.27	0.46
1:A:190:ALA:O	1:A:191:THR:OG1	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:301:ILE:HA	2:B:379:GLY:O	2.14	0.46
4:E:28:TYR:HA	4:E:64:PRO:HA	1.97	0.46
9:K:61:TYR:HA	9:K:72:LYS:O	2.15	0.46
1:A:527:THR:O	1:A:653:VAL:HG11	2.16	0.46
2:B:102:VAL:HG12	2:B:112:LEU:HB2	1.96	0.46
1:A:1447:GLU:C	1:A:1449:SER:H	2.18	0.46
1:A:1340:GLY:HA2	4:E:183:PRO:HD2	1.97	0.46
3:C:262:LEU:HD11	9:K:87:LEU:HD23	1.97	0.46
1:A:446:ARG:NH1	1:A:478:TYR:O	2.48	0.46
10:L:28:LYS:HG3	10:L:39:SER:OG	2.16	0.46
1:A:1151:GLU:HG3	1:A:1153:TYR:HE1	1.81	0.46
1:A:897:TYR:HE2	1:A:1024:SER:O	1.99	0.46
2:B:616:ILE:HG12	2:B:696:GLU:HG3	1.96	0.46
1:A:1167:GLU:C	1:A:1170:ILE:CG2	2.79	0.46
1:A:445:ASN:HB2	1:A:454:SER:O	2.16	0.46
2:B:1106:ARG:HH12	2:B:1110:PRO:HD2	1.79	0.46
2:B:1107:ALA:O	2:B:1108:ARG:HB3	2.16	0.46
12:T:12:DC:H42	13:N:3:DG:H1	1.62	0.46
1:A:78:PRO:HB3	2:B:1160:VAL:HG13	1.98	0.46
1:A:388:LEU:HA	1:A:391:LEU:HD12	1.97	0.46
1:A:160:GLN:O	1:A:161:LEU:HB2	2.16	0.46
3:C:262:LEU:CD1	9:K:87:LEU:HD23	2.46	0.46
3:C:82:TYR:CD1	3:C:161:LYS:HD3	2.51	0.46
2:B:805:THR:HG22	2:B:809:MET:SD	2.55	0.46
2:B:128:LEU:HB2	2:B:167:ILE:O	2.15	0.46
2:B:785:TYR:CD1	2:B:785:TYR:C	2.88	0.46
12:T:26:DG:N3	12:T:27:DA:C8	2.83	0.46
2:B:1019:SER:HG	11:R:14:DA:P	2.39	0.46
1:A:179:LEU:HB3	1:A:297:GLN:HG2	1.98	0.46
1:A:943:LEU:C	1:A:945:GLU:H	2.19	0.46
1:A:513:SER:HB2	1:A:520:CYS:HB3	1.98	0.46
2:B:638:PHE:CE1	2:B:743:ILE:HD13	2.51	0.46
7:I:5:ARG:HG3	7:I:6:PHE:H	1.81	0.46
1:A:203:SER:O	1:A:207:ILE:CG1	2.63	0.46
2:B:862:GLN:HG2	2:B:963:PHE:CD1	2.41	0.46
1:A:687:LYS:HD2	1:A:794:PRO:CG	2.46	0.46
1:A:913:LEU:HD12	1:A:914:GLU:H	1.81	0.46
2:B:475:SER:O	2:B:477:ALA:N	2.48	0.46
8:J:38:ARG:HB2	8:J:38:ARG:HH11	1.80	0.46
1:A:152:VAL:C	1:A:161:LEU:HD23	2.36	0.46
2:B:1084:GLN:HE22	3:C:192:TRP:HB2	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:25:ILE:HG22	2:B:26:THR:H	1.80	0.46
1:A:239:LEU:HD13	1:A:240:PRO:HD2	1.97	0.46
1:A:1116:LEU:CD2	1:A:1311:VAL:HA	2.46	0.46
3:C:173:ALA:O	3:C:174:ALA:HB3	2.16	0.46
1:A:61:ILE:O	1:A:63:ARG:NH2	2.49	0.46
2:B:1131:GLY:O	2:B:1134:GLU:N	2.39	0.46
1:A:630:ILE:HG23	1:A:642:CYS:SG	2.56	0.46
3:C:163:ILE:HD12	3:C:163:ILE:N	2.31	0.46
3:C:67:LEU:HD11	3:C:155:LEU:HD13	1.98	0.46
2:B:473:MET:HA	2:B:474:SER:HA	1.47	0.46
2:B:905:VAL:HG11	2:B:941:LEU:HG	1.98	0.46
1:A:168:GLY:O	1:A:169:ASN:O	2.34	0.46
2:B:636:PRO:O	2:B:691:GLU:O	2.33	0.45
1:A:575:LYS:HD3	1:A:612:ILE:HD11	1.97	0.45
1:A:741:ASN:HD22	1:A:741:ASN:C	2.19	0.45
1:A:901:LEU:HD22	1:A:919:ILE:HG22	1.98	0.45
11:R:3:C:N4	11:R:4:G:C6	2.84	0.45
11:R:5:A:C2	11:R:6:G:C5	3.04	0.45
1:A:172:PRO:CD	1:A:185:TRP:HE1	2.29	0.45
1:A:172:PRO:CG	1:A:185:TRP:HE1	2.23	0.45
1:A:455:MET:HE1	2:B:1134:GLU:HB3	1.98	0.45
1:A:1431:GLY:HA3	2:B:1197:PRO:HD3	1.98	0.45
2:B:1215:ARG:HB3	2:B:1217:TYR:HE1	1.81	0.45
1:A:900:ASP:HA	1:A:926:GLN:NE2	2.31	0.45
7:I:71:SER:OG	7:I:73:ARG:HG2	2.16	0.45
10:L:60:ARG:HG3	10:L:61:THR:H	1.81	0.45
2:B:205:ILE:HG21	2:B:462:ALA:HB2	1.98	0.45
2:B:978:ASP:HB2	2:B:980:PHE:HE1	1.81	0.45
2:B:20:ASP:O	2:B:21:GLU:HG2	2.16	0.45
2:B:361:LEU:O	2:B:363:HIS:O	2.34	0.45
1:A:269:ILE:HG13	1:A:299:HIS:HB3	1.98	0.45
2:B:835:GLN:HA	2:B:1013:ASN:HD22	1.81	0.45
3:C:75:MET:C	3:C:77:ILE:H	2.19	0.45
2:B:487:THR:HG22	2:B:488:TYR:N	2.31	0.45
3:C:33:LEU:HG	3:C:37:MET:HE3	1.99	0.45
1:A:407:ARG:HG2	1:A:430:TRP:CZ3	2.51	0.45
1:A:1178:ASP:HB2	1:A:1179:GLU:C	2.37	0.45
3:C:44:LEU:HD22	3:C:129:ILE:HD11	1.99	0.45
12:T:1:DC:H4'	12:T:2:DT:OP1	2.17	0.45
7:I:17:ARG:NH1	7:I:17:ARG:HB2	2.31	0.45
1:A:1192:LEU:HG	1:A:1193:LEU:N	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:55:ASP:H	1:A:56:PRO:CD	2.26	0.45
2:B:757:PRO:HB3	2:B:1044:ALA:CB	2.47	0.45
1:A:413:ILE:CD1	1:A:413:ILE:N	2.80	0.45
1:A:1279:ILE:HG13	1:A:1308:THR:HG21	1.97	0.45
1:A:375:THR:OG1	1:A:433:GLU:HB3	2.16	0.45
3:C:98:VAL:HG22	3:C:158:VAL:HG13	1.97	0.45
2:B:721:LEU:HA	2:B:722:ASP:HA	1.71	0.45
1:A:1166:ASP:C	1:A:1170:ILE:HG21	2.37	0.45
2:B:1019:SER:OG	11:R:14:DA:O5'	2.32	0.45
2:B:978:ASP:O	2:B:980:PHE:CD1	2.67	0.45
1:A:1144:LYS:HA	1:A:1268:LEU:HD22	1.99	0.45
1:A:658:LEU:HD12	1:A:658:LEU:O	2.17	0.45
1:A:266:LEU:HD21	1:A:303:TYR:CE1	2.52	0.45
2:B:361:LEU:N	2:B:362:PRO:HD3	2.31	0.45
2:B:1120:GLU:O	2:B:1124:ARG:HD3	2.17	0.45
6:H:102:TYR:O	6:H:103:LYS:HB2	2.17	0.45
1:A:737:LEU:HD23	1:A:737:LEU:HA	1.57	0.45
1:A:311:GLN:HA	1:A:312:PRO:HA	1.83	0.45
3:C:142:VAL:HG21	8:J:5:VAL:CG1	2.45	0.45
1:A:1319:VAL:HA	1:A:1320:PRO:HD3	1.80	0.45
1:A:1236:LEU:C	1:A:1237:ILE:HG13	2.36	0.45
3:C:58:LEU:HB3	3:C:62:PHE:HD2	1.81	0.45
2:B:232:SER:C	2:B:261:ARG:HH21	2.18	0.45
1:A:194:ALA:O	1:A:195:ASP:O	2.34	0.45
3:C:167:HIS:CE1	10:L:70:ARG:HA	2.51	0.45
2:B:1135:ARG:HG3	2:B:1147:LEU:HD11	1.98	0.45
5:F:120:ILE:O	5:F:123:LYS:N	2.45	0.45
1:A:848:ILE:CD1	1:A:858:ASN:HB3	2.47	0.45
3:C:34:ARG:HG2	3:C:35:ARG:N	2.31	0.45
4:E:64:PRO:HD3	4:E:76:GLY:O	2.16	0.45
3:C:130:GLY:O	3:C:132:PRO:HD3	2.17	0.45
2:B:386:LEU:C	2:B:388:CYS:H	2.19	0.45
2:B:766:ARG:HH22	2:B:1020:ARG:HH12	1.63	0.45
2:B:821:GLN:HE22	2:B:851:PHE:H	1.65	0.45
1:A:1189:SER:CB	1:A:1241:ARG:HB3	2.47	0.45
1:A:1030:ARG:C	1:A:1032:LEU:H	2.21	0.45
2:B:483:LEU:CD2	2:B:484:ASN:H	2.29	0.45
2:B:616:ILE:N	2:B:616:ILE:HD12	2.32	0.45
8:J:63:TYR:N	8:J:63:TYR:CD1	2.84	0.45
1:A:203:SER:O	1:A:207:ILE:HG13	2.17	0.45
2:B:273:LEU:HA	2:B:274:PRO:HD3	1.86	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:715:ALA:CB	2:B:716:ASN:CA	2.90	0.45
1:A:464:PRO:HD2	9:K:67:PHE:CD1	2.52	0.45
2:B:899:ILE:CD1	2:B:911:ILE:HG23	2.43	0.45
2:B:1072:MET:CE	2:B:1085:ILE:CD1	2.95	0.45
1:A:361:LEU:HD12	1:A:471:ASN:HD22	1.82	0.45
1:A:501:LEU:HA	1:A:501:LEU:HD23	1.62	0.45
3:C:143:LEU:HD12	3:C:144:ILE:N	2.33	0.44
1:A:13:THR:HG22	1:A:14:VAL:N	2.31	0.44
1:A:445:ASN:HB2	1:A:455:MET:HG2	1.95	0.44
12:T:2:DT:H3	13:N:13:DA:H61	1.65	0.44
1:A:545:GLN:O	1:A:549:MET:HG3	2.17	0.44
2:B:386:LEU:C	2:B:388:CYS:N	2.70	0.44
9:K:31:VAL:HG12	9:K:32:VAL:N	2.32	0.44
1:A:1293:SER:HB2	1:A:1299:VAL:HG23	1.99	0.44
1:A:172:PRO:N	1:A:185:TRP:CD1	2.85	0.44
3:C:39:ALA:CB	3:C:164:ALA:HB3	2.47	0.44
1:A:353:ILE:HG13	1:A:353:ILE:O	2.18	0.44
7:I:32:CYS:O	7:I:33:SER:CB	2.65	0.44
1:A:1436:ILE:O	1:A:1437:GLY:C	2.55	0.44
2:B:1149:GLU:HG3	2:B:1153:GLU:HB2	1.99	0.44
10:L:32:ALA:CB	10:L:55:ILE:HD11	2.47	0.44
6:H:101:ALA:HB2	6:H:116:TYR:CE2	2.52	0.44
3:C:172:PRO:C	3:C:235:VAL:HG23	2.37	0.44
3:C:142:VAL:HA	8:J:16:ASP:HB3	1.98	0.44
1:A:185:TRP:HE3	1:A:198:GLU:HG2	1.81	0.44
2:B:944:THR:CG2	2:B:1122:ARG:NH2	2.75	0.44
7:I:111:THR:HG22	7:I:112:SER:N	2.33	0.44
2:B:980:PHE:CE2	2:B:1094:ARG:HG3	2.52	0.44
1:A:815:PHE:O	1:A:816:HIS:C	2.56	0.44
2:B:31:TRP:CZ3	2:B:34:ILE:HD12	2.51	0.44
1:A:75:ASN:HA	2:B:1116:ARG:NH2	2.32	0.44
1:A:381:THR:C	1:A:383:TYR:N	2.70	0.44
2:B:780:VAL:HG21	8:J:56:LEU:HD13	1.98	0.44
1:A:379:VAL:HG22	1:A:431:LYS:HG2	2.00	0.44
1:A:41:MET:CG	1:A:42:ASP:H	2.21	0.44
2:B:1159:ARG:HD3	2:B:1193:GLN:CG	2.40	0.44
2:B:25:ILE:HD11	2:B:653:VAL:HB	1.98	0.44
2:B:874:PHE:CE1	2:B:964:VAL:HG23	2.52	0.44
1:A:590:ARG:O	1:A:591:PHE:HB2	2.17	0.44
1:A:391:LEU:HD23	1:A:400:PRO:C	2.37	0.44
1:A:530:GLY:HA2	1:A:533:LYS:HG3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:553:VAL:HA	1:A:554:PRO:HD3	1.91	0.44
2:B:955:THR:CG2	2:B:956:THR:N	2.77	0.44
1:A:11:LEU:HA	2:B:1193:GLN:O	2.18	0.44
6:H:12:VAL:HG13	6:H:26:ILE:CD1	2.46	0.44
1:A:344:ARG:NH1	2:B:1129:ARG:HB2	2.33	0.44
2:B:363:HIS:C	2:B:365:THR:H	2.19	0.44
2:B:38:PHE:HD2	2:B:42:GLY:O	2.00	0.44
2:B:315:LYS:N	2:B:316:PRO:CD	2.80	0.44
1:A:368:LYS:O	1:A:369:SER:C	2.55	0.44
1:A:910:PRO:HA	1:A:916:GLY:HA3	1.99	0.44
2:B:444:MET:HE2	2:B:446:LEU:CD2	2.47	0.44
3:C:167:HIS:C	3:C:167:HIS:CD2	2.90	0.44
1:A:402:ALA:N	1:A:435:HIS:CD2	2.84	0.44
9:K:3:ALA:HA	9:K:4:PRO:HD3	1.77	0.44
4:E:78:LEU:HD23	4:E:79:TRP:N	2.33	0.44
2:B:203:PHE:N	2:B:203:PHE:CD1	2.85	0.44
3:C:31:ASN:O	3:C:35:ARG:HG3	2.17	0.44
7:I:73:ARG:HG3	7:I:101:PHE:CD2	2.53	0.44
2:B:834:ASN:HB3	2:B:840:ILE:HG13	2.00	0.44
1:A:954:TRP:HA	1:A:955:PRO:HD3	1.86	0.44
2:B:1098:MET:O	2:B:1099:VAL:C	2.53	0.44
2:B:999:MET:HG3	2:B:1000:PRO:CD	2.41	0.44
6:H:12:VAL:HG11	6:H:51:ALA:HA	2.00	0.44
2:B:202:TYR:C	2:B:203:PHE:CD1	2.91	0.44
3:C:27:LEU:HD12	3:C:228:PHE:CZ	2.52	0.44
1:A:877:HIS:CD2	1:A:877:HIS:H	2.34	0.44
1:A:982:THR:HB	1:A:985:ASP:H	1.83	0.44
2:B:498:THR:HB	2:B:537:LYS:HB2	2.00	0.44
1:A:153:PRO:CA	1:A:161:LEU:HD23	2.48	0.44
3:C:167:HIS:CD2	3:C:168:ALA:N	2.86	0.44
1:A:668:ASP:OD2	1:A:742:ASN:HB2	2.18	0.44
1:A:91:PHE:HZ	1:A:207:ILE:CD1	2.30	0.44
2:B:770:GLN:NE2	2:B:770:GLN:O	2.51	0.44
1:A:337:ARG:NH2	1:A:839:ARG:NH2	2.66	0.44
1:A:709:THR:CG2	7:I:94:ASP:HA	2.48	0.44
7:I:62:ILE:C	7:I:64:SER:H	2.21	0.44
12:T:23:DC:C2'	12:T:24:DT:H5'	2.48	0.44
1:A:921:GLY:O	1:A:922:ASP:HB3	2.18	0.44
1:A:4:GLN:O	1:A:5:GLN:HG3	2.17	0.44
1:A:188:ASP:O	1:A:189:ARG:HG2	2.17	0.44
1:A:242:PRO:HA	1:A:243:PRO:HD3	1.89	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:353:ILE:HD13	1:A:487:MET:CE	2.37	0.44
2:B:879:ARG:HA	2:B:879:ARG:NE	2.33	0.44
5:F:111:LEU:H	5:F:111:LEU:CD2	2.28	0.44
3:C:244:VAL:HG21	9:K:105:PHE:CE1	2.53	0.44
2:B:613:VAL:HG22	2:B:628:THR:HA	2.00	0.44
2:B:859:TYR:OH	2:B:941:LEU:HD22	2.18	0.44
2:B:487:THR:O	2:B:490:SER:HB3	2.18	0.44
2:B:441:ASP:C	2:B:443:ASN:H	2.21	0.44
6:H:89:LEU:HB2	6:H:91:ASP:OD1	2.18	0.44
2:B:604:ARG:HD2	2:B:615:MET:CE	2.48	0.44
2:B:188:ASP:HA	2:B:191:LYS:HE3	2.00	0.44
2:B:1081:LEU:HA	2:B:1081:LEU:HD23	1.77	0.44
1:A:153:PRO:HA	1:A:161:LEU:HD23	2.00	0.43
4:E:15:ALA:HA	4:E:140:LEU:O	2.18	0.43
2:B:906:SER:CA	2:B:946:ASN:HB2	2.42	0.43
6:H:38:LEU:HD11	6:H:123:MET:HE2	1.99	0.43
1:A:871:ASP:HB3	4:E:205:SER:HB3	2.00	0.43
3:C:182:PRO:O	3:C:183:TRP:C	2.57	0.43
9:K:6:ARG:O	9:K:8:GLU:N	2.51	0.43
1:A:399:HIS:HB3	1:A:400:PRO:HD3	2.00	0.43
2:B:600:LEU:HB3	2:B:615:MET:SD	2.58	0.43
2:B:119:LEU:HD22	2:B:789:MET:HB2	1.99	0.43
3:C:142:VAL:CG2	3:C:143:LEU:N	2.75	0.43
7:I:78:CYS:SG	7:I:106:CYS:SG	3.08	0.43
1:A:244:PRO:HB2	1:A:245:PRO:HD3	1.99	0.43
1:A:809:THR:CB	1:A:810:PRO:CD	2.94	0.43
2:B:463:THR:HG21	2:B:465:ASN:HD21	1.81	0.43
4:E:205:SER:O	4:E:206:GLY:C	2.55	0.43
4:E:88:VAL:HG23	4:E:116:ILE:HA	2.00	0.43
1:A:451:HIS:CE1	1:A:1074:GLU:HG3	2.53	0.43
7:I:5:ARG:HG3	7:I:6:PHE:N	2.33	0.43
1:A:1332:PHE:CE1	1:A:1348:LEU:HD13	2.53	0.43
2:B:129:PHE:CE2	2:B:166:PHE:HB2	2.53	0.43
1:A:516:SER:HB3	1:A:1362:TYR:O	2.18	0.43
8:J:31:ASP:OD1	8:J:34:THR:OG1	2.36	0.43
2:B:550:ASP:HA	2:B:551:PRO:HD3	1.93	0.43
2:B:256:VAL:HG11	2:B:382:ILE:CD1	2.49	0.43
3:C:173:ALA:O	3:C:233:GLU:O	2.35	0.43
1:A:851:HIS:CD2	1:A:857:ARG:HG3	2.53	0.43
2:B:598:GLU:HA	2:B:598:GLU:OE2	2.18	0.43
1:A:782:ARG:HB3	1:A:788:SER:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:323:LYS:HG3	1:A:327:ALA:HB3	2.01	0.43
1:A:465:TYR:HD2	2:B:976:ILE:HB	1.82	0.43
2:B:980:PHE:CE1	2:B:990:ILE:HD11	2.53	0.43
3:C:43:THR:CG2	3:C:44:LEU:H	2.26	0.43
2:B:515:HIS:O	2:B:516:ASN:C	2.57	0.43
2:B:463:THR:HG22	2:B:465:ASN:ND2	2.29	0.43
1:A:1189:SER:HB3	1:A:1241:ARG:HD3	2.00	0.43
6:H:93:TYR:CG	6:H:143:LEU:HB3	2.54	0.43
1:A:492:PRO:HB3	1:A:497:THR:CG2	2.48	0.43
3:C:162:GLY:HA3	3:C:170:TRP:CD2	2.52	0.43
1:A:208:LEU:HB2	1:A:235:ILE:HD11	2.01	0.43
1:A:592:ASP:O	1:A:593:GLU:OE1	2.36	0.43
2:B:1200:ALA:O	2:B:1203:LEU:N	2.51	0.43
1:A:582:ILE:HA	1:A:583:PRO:HD3	1.91	0.43
1:A:565:ILE:HG23	1:A:567:LYS:HG2	2.00	0.43
2:B:471:LYS:HA	2:B:472:ALA:HA	1.63	0.43
7:I:11:ASN:O	7:I:11:ASN:CG	2.56	0.43
2:B:1131:GLY:O	2:B:1132:GLU:C	2.56	0.43
2:B:1117:GLN:CG	2:B:1156:ASP:OD2	2.65	0.43
1:A:738:LYS:HZ1	3:C:194:GLU:HA	1.83	0.43
2:B:34:ILE:HG23	2:B:542:MET:CE	2.48	0.43
12:T:18:DA:C2	12:T:19:DT:N3	2.87	0.43
1:A:224:PHE:CZ	1:A:231:PRO:HG3	2.53	0.43
2:B:1023:VAL:O	2:B:1024:ALA:C	2.57	0.43
1:A:1278:ASN:HD22	1:A:1312:ASN:HB2	1.84	0.43
6:H:42:ILE:HG23	6:H:95:TYR:CE1	2.52	0.43
6:H:114:VAL:HG11	6:H:134:ASN:HD22	1.83	0.43
2:B:465:ASN:O	2:B:466:TRP:C	2.57	0.43
1:A:1080:THR:CG2	1:A:1081:LEU:N	2.80	0.43
2:B:363:HIS:C	2:B:365:THR:N	2.71	0.43
1:A:346:ASP:HB3	2:B:1108:ARG:H	1.84	0.43
1:A:513:SER:HA	1:A:514:PRO:HD3	1.86	0.43
10:L:46:VAL:HG12	10:L:47:ARG:H	1.83	0.43
4:E:153:HIS:CE1	4:E:184:VAL:HG11	2.53	0.43
1:A:870:GLU:OE1	4:E:202:SER:HB2	2.19	0.43
1:A:1171:GLN:O	1:A:1171:GLN:CD	2.57	0.43
8:J:16:ASP:OD1	8:J:16:ASP:N	2.40	0.43
1:A:57:ARG:HA	1:A:57:ARG:HD3	1.85	0.43
2:B:864:LYS:HD2	2:B:872:GLU:CD	2.39	0.43
2:B:1095:LEU:O	2:B:1096:ARG:O	2.37	0.43
2:B:982:SER:O	2:B:1093:GLN:HG3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1155:ASP:HA	1:A:1156:PRO:HD3	1.81	0.43
2:B:698:GLU:HA	2:B:701:ILE:CD1	2.49	0.43
1:A:1227:ILE:HG22	1:A:1228:TRP:H	1.83	0.43
2:B:464:GLY:CA	2:B:480:SER:HB3	2.46	0.43
1:A:812:GLU:O	1:A:813:PHE:C	2.57	0.43
3:C:46:ILE:HA	3:C:159:ALA:HA	2.01	0.43
2:B:794:ASN:C	2:B:795:ILE:HD12	2.39	0.43
5:F:133:VAL:O	5:F:133:VAL:HG13	2.19	0.43
2:B:916:THR:HA	2:B:917:PRO:HD3	1.89	0.43
2:B:778:MET:HE1	2:B:1094:ARG:HD3	2.00	0.43
1:A:789:LYS:HE2	7:I:67:THR:HB	2.00	0.43
2:B:485:ARG:NH1	2:B:485:ARG:HG2	2.34	0.43
10:L:60:ARG:HG3	10:L:61:THR:N	2.34	0.43
1:A:184:SER:HB2	1:A:199:LEU:HD23	2.01	0.43
2:B:292:ILE:H	2:B:293:PRO:HD3	1.83	0.43
8:J:8:PHE:O	8:J:9:SER:O	2.37	0.43
1:A:302:THR:HG23	1:A:306:ASN:CB	2.49	0.43
1:A:775:ILE:O	1:A:797:LYS:HE2	2.19	0.43
1:A:402:ALA:CB	1:A:434:ARG:HA	2.47	0.43
7:I:27:PHE:O	7:I:28:GLU:HB3	2.19	0.43
1:A:1437:GLY:HA3	5:F:88:TYR:CD2	2.53	0.43
1:A:534:LEU:HA	1:A:539:THR:HG21	2.01	0.43
1:A:33:ALA:HB3	1:A:82:GLY:HA2	2.00	0.43
8:J:23:ASN:O	8:J:27:GLU:HB3	2.19	0.43
2:B:579:ARG:HG3	2:B:623:GLU:HG2	1.99	0.43
1:A:1133:LEU:HA	1:A:1133:LEU:HD23	1.89	0.43
12:T:26:DG:C4	12:T:27:DA:C8	3.07	0.42
3:C:167:HIS:CE1	10:L:70:ARG:HB3	2.54	0.42
1:A:464:PRO:HD2	9:K:67:PHE:HD1	1.84	0.42
2:B:464:GLY:HA2	2:B:480:SER:CB	2.45	0.42
1:A:1080:THR:CG2	1:A:1081:LEU:H	2.32	0.42
2:B:361:LEU:HD21	2:B:377:PHE:CD2	2.53	0.42
2:B:856:PHE:HB3	2:B:967:ARG:HD2	2.00	0.42
2:B:471:LYS:HZ2	11:R:4:G:H1'	1.84	0.42
1:A:305:ASP:OD1	1:A:306:ASN:N	2.52	0.42
2:B:803:LEU:HD13	2:B:1032:SER:O	2.20	0.42
1:A:1144:LYS:HD2	1:A:1269:GLU:HG2	2.00	0.42
7:I:104:LEU:HA	7:I:104:LEU:HD22	1.84	0.42
9:K:10:PHE:HD2	9:K:10:PHE:N	2.16	0.42
1:A:649:ILE:H	1:A:649:ILE:HG13	1.62	0.42
2:B:215:GLN:O	2:B:406:LEU:HA	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:550:ASP:O	2:B:553:PRO:HD2	2.20	0.42
2:B:204:ILE:O	2:B:205:ILE:HD13	2.18	0.42
1:A:1092:LYS:H	1:A:1093:LYS:HA	1.83	0.42
1:A:1033:GLN:HE21	1:A:1033:GLN:HB3	1.61	0.42
1:A:956:LEU:HA	1:A:956:LEU:HD23	1.87	0.42
1:A:444:PHE:HE2	1:A:470:LEU:CD2	2.32	0.42
1:A:402:ALA:HA	1:A:435:HIS:HD2	1.85	0.42
2:B:711:GLU:H	2:B:712:PRO:HD3	1.84	0.42
5:F:79:ARG:O	5:F:81:THR:N	2.52	0.42
1:A:391:LEU:HD23	1:A:400:PRO:O	2.19	0.42
1:A:1428:VAL:C	1:A:1430:LEU:H	2.22	0.42
1:A:979:SER:OG	1:A:980:ASP:N	2.51	0.42
1:A:715:GLU:OE1	1:A:774:ARG:HD3	2.19	0.42
1:A:267:ALA:O	1:A:271:LYS:HB2	2.20	0.42
1:A:650:GLN:HB3	1:A:654:ASN:HD21	1.84	0.42
1:A:315:LEU:H	1:A:315:LEU:HD22	1.83	0.42
2:B:444:MET:C	2:B:445:LYS:CG	2.68	0.42
2:B:952:VAL:HG13	2:B:966:VAL:HG22	2.01	0.42
9:K:7:PHE:CD1	9:K:7:PHE:C	2.92	0.42
4:E:88:VAL:CG2	4:E:116:ILE:HD13	2.48	0.42
3:C:46:ILE:HD12	3:C:157:CYS:CB	2.48	0.42
1:A:102:VAL:CG1	1:A:211:PHE:HE1	2.31	0.42
2:B:542:MET:SD	2:B:747:MET:HE2	2.59	0.42
1:A:1319:VAL:O	1:A:1322:ILE:HD12	2.19	0.42
1:A:1100:ARG:HH21	1:A:1351:GLU:CG	2.33	0.42
1:A:726:ARG:HD3	1:A:766:GLY:HA3	2.02	0.42
10:L:50:ASP:CG	10:L:50:ASP:O	2.57	0.42
1:A:302:THR:HA	1:A:305:ASP:O	2.19	0.42
12:T:28:DT:H2'	12:T:29:DA:O4'	2.20	0.42
1:A:179:LEU:HD13	1:A:297:GLN:HG3	2.02	0.42
2:B:64:CYS:O	2:B:67:SER:OG	2.30	0.42
1:A:356:ASP:HA	1:A:357:PRO:HD3	1.78	0.42
12:T:6:DG:H2"	12:T:7:DA:O5'	2.20	0.42
4:E:52:ARG:HA	4:E:53:PRO:HD3	1.72	0.42
1:A:140:THR:O	1:A:140:THR:HG22	2.20	0.42
1:A:1169:ILE:HG21	1:A:1170:ILE:HD11	1.96	0.42
2:B:445:LYS:CA	2:B:447:ALA:N	2.79	0.42
1:A:41:MET:HG3	1:A:42:ASP:N	2.26	0.42
1:A:919:ILE:HA	1:A:919:ILE:HD13	1.82	0.42
2:B:969:ARG:HD2	3:C:61:GLU:OE2	2.20	0.42
4:E:161:LYS:HD2	4:E:195:VAL:HG23	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:494:SER:O	1:A:498:ARG:HG3	2.20	0.42
2:B:457:LEU:HA	2:B:457:LEU:HD23	1.86	0.42
3:C:245:VAL:HG13	9:K:102:LYS:HD2	2.02	0.42
1:A:818:MET:HG2	2:B:514:LEU:O	2.19	0.42
9:K:82:ASP:HA	9:K:83:PRO:HD3	1.93	0.42
1:A:363:GLN:HG3	1:A:459:ARG:NH1	2.34	0.42
2:B:378:LEU:O	2:B:382:ILE:HG12	2.19	0.42
2:B:680:THR:O	2:B:683:SER:OG	2.37	0.42
2:B:324:ILE:HG21	2:B:330:ALA:HA	2.02	0.42
2:B:218:SER:HB3	2:B:241:ARG:NH1	2.35	0.42
2:B:444:MET:CE	2:B:446:LEU:HD11	2.48	0.42
1:A:306:ASN:HD22	1:A:306:ASN:N	2.18	0.42
2:B:469:GLN:O	2:B:470:LYS:HB2	2.19	0.42
2:B:757:PRO:HB3	2:B:1044:ALA:HB1	2.01	0.42
3:C:127:ARG:HG3	3:C:129:ILE:CG2	2.49	0.42
1:A:523:ILE:HG22	1:A:528:LEU:HB2	2.01	0.42
2:B:771:SER:O	2:B:775:LYS:HG3	2.20	0.42
2:B:1041:GLU:HG2	2:B:1042:GLY:N	2.35	0.42
1:A:1272:THR:C	1:A:1273:LEU:HD12	2.40	0.42
2:B:282:ILE:H	2:B:282:ILE:HG13	1.72	0.42
3:C:5:GLY:O	3:C:6:PRO:C	2.58	0.42
8:J:43:ARG:HG3	8:J:46:CYS:SG	2.59	0.42
7:I:7:CYS:SG	7:I:8:ARG:O	2.78	0.42
2:B:830:TYR:CE2	2:B:1000:PRO:HD3	2.55	0.42
2:B:213:ILE:CD1	2:B:481:GLN:OE1	2.65	0.42
1:A:1158:PRO:HG3	1:A:1188:GLN:NE2	2.35	0.42
7:I:17:ARG:HH11	7:I:17:ARG:CB	2.32	0.42
1:A:852:TYR:CE2	1:A:1060:PRO:HB2	2.55	0.42
2:B:550:ASP:OD1	2:B:551:PRO:HD2	2.20	0.42
3:C:62:PHE:O	3:C:66:ARG:HG3	2.20	0.42
2:B:780:VAL:HG21	8:J:56:LEU:CD1	2.50	0.42
4:E:153:HIS:O	4:E:154:ILE:HD13	2.19	0.42
1:A:1098:VAL:N	1:A:1099:PRO:CD	2.83	0.42
3:C:120:ILE:H	3:C:120:ILE:HG12	1.39	0.42
1:A:1172:LEU:CD2	1:A:1173:HIS:H	2.20	0.42
1:A:156:ASP:OD2	1:A:160:GLN:OE1	2.36	0.42
1:A:261:ASP:O	1:A:264:PHE:HB2	2.20	0.42
1:A:190:ALA:C	1:A:191:THR:OG1	2.57	0.42
1:A:359:LEU:HD23	1:A:359:LEU:HA	1.75	0.42
2:B:945:GLU:O	2:B:946:ASN:HB3	2.20	0.42
8:J:18:TRP:O	8:J:21:TYR:HB3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:93:ILE:HG23	5:F:132:LEU:HD12	2.02	0.42
1:A:917:SER:C	1:A:919:ILE:H	2.21	0.42
2:B:488:TYR:O	2:B:490:SER:N	2.53	0.42
1:A:1407:GLU:CD	1:A:1407:GLU:H	2.24	0.42
1:A:1193:LEU:HG	1:A:1193:LEU:O	2.19	0.41
1:A:567:LYS:O	1:A:569:LYS:N	2.53	0.41
1:A:482:PHE:CD1	2:B:836:GLU:HB2	2.54	0.41
2:B:658:ILE:O	2:B:661:LEU:HB2	2.20	0.41
1:A:902:LEU:CD2	1:A:923:LEU:HD23	2.50	0.41
1:A:1021:LEU:CD1	1:A:1025:ARG:HE	2.30	0.41
1:A:1039:LYS:C	1:A:1039:LYS:HD3	2.40	0.41
3:C:77:ILE:HD11	3:C:161:LYS:HG3	2.02	0.41
1:A:1072:ILE:O	1:A:1075:PRO:HD2	2.19	0.41
1:A:1146:VAL:O	1:A:1197:LEU:HD23	2.20	0.41
2:B:118:ARG:NH2	2:B:194:GLU:OE1	2.53	0.41
1:A:1397:LEU:HB2	1:A:1426:GLU:HG2	2.02	0.41
7:I:75:CYS:CB	7:I:78:CYS:SG	3.07	0.41
6:H:109:LYS:HB3	6:H:111:LEU:CA	2.50	0.41
2:B:273:LEU:CD1	2:B:285:ILE:HD12	2.50	0.41
1:A:148:CYS:SG	1:A:167:CYS:CB	3.08	0.41
1:A:1364:ASN:OD1	1:A:1366:ARG:HD2	2.19	0.41
2:B:1119:VAL:O	2:B:1126:GLY:HA3	2.20	0.41
2:B:567:GLU:OE1	2:B:567:GLU:N	2.39	0.41
1:A:857:ARG:HD2	5:F:139:PRO:HG3	2.02	0.41
1:A:376:TYR:CE1	1:A:498:ARG:HD2	2.55	0.41
7:I:87:GLN:NE2	7:I:97:MET:HG2	2.34	0.41
3:C:46:ILE:H	3:C:46:ILE:HG12	1.63	0.41
1:A:265:LYS:HZ3	1:A:265:LYS:HB2	1.84	0.41
2:B:582:VAL:HA	2:B:626:ILE:O	2.19	0.41
2:B:745:PRO:C	2:B:747:MET:H	2.23	0.41
7:I:65:ASP:HA	7:I:66:PRO:HD3	1.76	0.41
1:A:1343:ALA:HA	4:E:149:LEU:O	2.21	0.41
1:A:79:GLY:HA3	2:B:1205:GLN:HE21	1.86	0.41
1:A:991:LYS:HD2	1:A:991:LYS:HA	1.88	0.41
2:B:85:SER:N	2:B:86:ARG:CB	2.79	0.41
1:A:1436:ILE:HD13	2:B:1139:ILE:HG23	2.03	0.41
2:B:463:THR:HG21	2:B:465:ASN:ND2	2.33	0.41
1:A:1081:LEU:HG	11:R:13:C:H41	1.86	0.41
1:A:1344:GLY:O	1:A:1345:ARG:C	2.57	0.41
1:A:164:ARG:HB3	1:A:165:GLY:H	1.78	0.41
1:A:1192:LEU:HD11	1:A:1239:ARG:CZ	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:241:VAL:HA	1:A:242:PRO:HD3	1.92	0.41
2:B:994:TYR:HB2	2:B:999:MET:HE3	2.01	0.41
1:A:356:ASP:OD2	9:K:65:HIS:CE1	2.71	0.41
2:B:777:ALA:HB2	2:B:1093:GLN:NE2	2.35	0.41
2:B:1132:GLU:O	2:B:1135:ARG:HB3	2.21	0.41
2:B:340:ALA:C	2:B:342:GLY:N	2.74	0.41
3:C:73:GLN:NE2	3:C:75:MET:HB2	2.34	0.41
1:A:1319:VAL:O	1:A:1322:ILE:CD1	2.69	0.41
5:F:73:ALA:HB2	5:F:143:PHE:CZ	2.56	0.41
6:H:12:VAL:HG12	6:H:51:ALA:HA	2.02	0.41
1:A:1163:ILE:HA	1:A:1164:PRO:HD3	1.82	0.41
3:C:180:TYR:CD1	3:C:180:TYR:O	2.74	0.41
2:B:874:PHE:CE2	2:B:914:LYS:HD3	2.55	0.41
2:B:33:VAL:HG21	2:B:638:PHE:CZ	2.56	0.41
2:B:815:ARG:O	8:J:54:VAL:HG21	2.20	0.41
1:A:631:HIS:HE1	1:A:879:GLU:HB3	1.86	0.41
2:B:825:VAL:HG11	2:B:1090:THR:HB	2.02	0.41
1:A:935:GLN:NE2	1:A:939:ASP:OD1	2.53	0.41
1:A:1037:LEU:HD12	1:A:1042:PHE:HD1	1.86	0.41
1:A:55:ASP:O	1:A:56:PRO:C	2.58	0.41
1:A:91:PHE:CZ	1:A:207:ILE:CD1	3.04	0.41
2:B:128:LEU:HD21	2:B:170:LEU:HB2	2.03	0.41
7:I:59:VAL:HG12	7:I:60:GLN:H	1.86	0.41
1:A:306:ASN:O	1:A:307:ASP:HB2	2.21	0.41
1:A:470:LEU:CD2	1:A:487:MET:HE1	2.51	0.41
2:B:851:PHE:HB3	2:B:1094:ARG:HD2	2.03	0.41
6:H:98:TYR:C	6:H:118:PHE:HD2	2.24	0.41
2:B:880:THR:O	2:B:882:THR:N	2.51	0.41
2:B:915:THR:HB	2:B:934:LYS:HB3	2.02	0.41
3:C:51:VAL:HG22	3:C:155:LEU:CD2	2.51	0.41
2:B:791:THR:O	2:B:792:MET:HB2	2.21	0.41
2:B:969:ARG:HG2	2:B:970:THR:N	2.35	0.41
1:A:1052:GLN:O	1:A:1055:ARG:HB2	2.21	0.41
1:A:174:ILE:HA	1:A:182:VAL:O	2.21	0.41
2:B:431:TYR:CE2	2:B:447:ALA:HB2	2.56	0.41
1:A:262:LEU:HD11	1:A:325:ILE:HG12	2.02	0.41
1:A:188:ASP:C	1:A:189:ARG:CG	2.89	0.41
1:A:80:HIS:O	1:A:243:PRO:HG3	2.21	0.41
1:A:55:ASP:HB3	1:A:56:PRO:HD3	2.02	0.41
3:C:57:VAL:HG21	8:J:61:LEU:HD23	2.03	0.41
2:B:66:ASP:O	2:B:66:ASP:OD1	2.39	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:976:ILE:HD11	2:B:991:GLY:O	2.21	0.41
1:A:320:ARG:NE	1:A:320:ARG:HA	2.30	0.41
3:C:44:LEU:HD12	3:C:160:LYS:C	2.41	0.41
8:J:3:VAL:CG2	8:J:18:TRP:CG	3.04	0.41
2:B:361:LEU:HD21	2:B:377:PHE:HD2	1.85	0.41
1:A:273:ASN:ND2	1:A:296:LEU:HD21	2.36	0.41
1:A:662:PHE:HD2	2:B:829:CYS:SG	2.44	0.41
2:B:173:MET:HG3	2:B:201:GLY:HA2	2.02	0.41
1:A:239:LEU:HA	1:A:240:PRO:HD3	1.91	0.41
2:B:1160:VAL:HG12	2:B:1161:HIS:N	2.36	0.41
3:C:33:LEU:O	3:C:37:MET:HB2	2.20	0.41
1:A:230:ARG:HD3	1:A:232:GLU:OE2	2.21	0.41
1:A:230:ARG:HA	1:A:231:PRO:HD3	1.84	0.41
2:B:244:LEU:HD21	2:B:366:GLN:NE2	2.35	0.41
2:B:1033:LYS:HA	2:B:1089:PRO:HG2	2.02	0.41
1:A:1044:TRP:O	1:A:1045:VAL:C	2.60	0.41
1:A:690:VAL:O	1:A:694:THR:OG1	2.35	0.41
2:B:593:PRO:HA	2:B:596:LEU:HB3	2.03	0.41
2:B:886:LYS:HB2	2:B:890:TYR:OH	2.20	0.41
1:A:543:LEU:O	1:A:547:LEU:HG	2.21	0.41
1:A:880:LYS:HG3	1:A:880:LYS:O	2.21	0.41
1:A:1170:ILE:CG2	1:A:1170:ILE:O	2.69	0.41
1:A:752:LYS:HD2	1:A:752:LYS:HA	1.81	0.41
2:B:833:TYR:OH	9:K:65:HIS:CE1	2.74	0.41
1:A:1063:MET:SD	1:A:1436:ILE:HG12	2.61	0.41
1:A:343:LYS:HZ1	2:B:1156:ASP:CB	2.34	0.41
2:B:769:TYR:OH	11:R:12:G:H2'	2.21	0.41
1:A:645:LEU:O	1:A:646:PHE:C	2.59	0.41
1:A:360:GLU:HA	1:A:360:GLU:OE2	2.21	0.41
2:B:826:ALA:O	2:B:1011:ILE:HA	2.21	0.41
3:C:142:VAL:HG23	8:J:15:GLY:HA3	2.02	0.40
1:A:250:ILE:HD12	1:A:251:SER:H	1.85	0.40
3:C:167:HIS:HD2	3:C:169:LYS:N	1.93	0.40
1:A:109:HIS:C	1:A:167:CYS:SG	3.00	0.40
2:B:756:ILE:HA	2:B:757:PRO:HD3	1.88	0.40
2:B:1135:ARG:HG2	2:B:1139:ILE:HD11	2.01	0.40
1:A:343:LYS:HE2	2:B:1151:LEU:HD23	2.04	0.40
9:K:40:HIS:CE1	9:K:63:VAL:HG11	2.56	0.40
7:I:83:ASN:ND2	7:I:83:ASN:C	2.73	0.40
2:B:1107:ALA:O	2:B:1108:ARG:CB	2.68	0.40
2:B:344:LYS:HB3	2:B:347:LYS:HB2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:388:LEU:HA	1:A:388:LEU:HD23	1.90	0.40
3:C:63:ILE:O	3:C:66:ARG:HB2	2.21	0.40
7:I:46:HIS:O	7:I:47:GLU:O	2.40	0.40
2:B:100:PRO:HD3	2:B:178:ASN:O	2.21	0.40
1:A:1064:VAL:HG12	1:A:1064:VAL:O	2.22	0.40
1:A:508:PRO:HB3	1:A:643:ALA:HB2	2.02	0.40
1:A:33:ALA:HB3	1:A:82:GLY:HA3	2.02	0.40
2:B:834:ASN:HB2	2:B:839:MET:HA	2.02	0.40
2:B:292:ILE:H	2:B:293:PRO:CD	2.34	0.40
7:I:85:PHE:CD1	7:I:99:LEU:HD22	2.56	0.40
2:B:801:LYS:HA	2:B:802:PRO:HD2	1.91	0.40
1:A:287:HIS:HA	1:A:288:ALA:HA	1.47	0.40
2:B:899:ILE:HD11	2:B:911:ILE:CG2	2.46	0.40
1:A:622:VAL:O	1:A:630:ILE:HD11	2.22	0.40
1:A:655:PHE:O	1:A:658:LEU:HB3	2.21	0.40
1:A:1019:CYS:HA	1:A:1022:LEU:HB3	2.04	0.40
2:B:34:ILE:O	2:B:37:PHE:N	2.53	0.40
2:B:1175:LEU:HD23	2:B:1176:ASN:N	2.36	0.40
2:B:825:VAL:CG1	2:B:1090:THR:HB	2.52	0.40
1:A:1192:LEU:HG	1:A:1193:LEU:H	1.87	0.40
7:I:34:TYR:HH	7:I:36:GLU:HB3	1.82	0.40
1:A:1364:ASN:O	1:A:1365:TYR:C	2.60	0.40
2:B:20:ASP:CG	2:B:20:ASP:O	2.60	0.40
4:E:77:SER:HB3	4:E:105:PHE:CD2	2.55	0.40
1:A:1134:ILE:H	1:A:1134:ILE:HG13	1.66	0.40
2:B:487:THR:CG2	2:B:488:TYR:N	2.84	0.40
1:A:1398:MET:C	1:A:1400:CYS:N	2.72	0.40
5:F:130:ILE:HA	5:F:131:PRO:HD3	1.76	0.40
2:B:461:LEU:HD12	2:B:461:LEU:HA	1.99	0.40
1:A:535:THR:HG22	1:A:575:LYS:HG2	2.03	0.40
2:B:242:SER:HB2	2:B:362:PRO:HD2	2.03	0.40
2:B:441:ASP:C	2:B:443:ASN:N	2.75	0.40
10:L:32:ALA:HB3	10:L:55:ILE:HD11	2.03	0.40
1:A:1317:MET:HB3	1:A:1327:ILE:HD13	2.03	0.40
3:C:212:PRO:HA	3:C:213:PRO:HD3	1.98	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	1438/1733 (83%)	1083 (75%)	289 (20%)	66 (5%)	3 34
2	B	1145/1224 (94%)	877 (77%)	219 (19%)	49 (4%)	3 35
3	C	269/318 (85%)	205 (76%)	57 (21%)	7 (3%)	7 48
4	E	213/215 (99%)	180 (84%)	28 (13%)	5 (2%)	8 51
5	F	83/155 (54%)	66 (80%)	13 (16%)	4 (5%)	3 32
6	H	132/146 (90%)	100 (76%)	26 (20%)	6 (4%)	3 34
7	I	117/122 (96%)	82 (70%)	26 (22%)	9 (8%)	1 20
8	J	63/70 (90%)	53 (84%)	6 (10%)	4 (6%)	2 26
9	K	112/120 (93%)	97 (87%)	13 (12%)	2 (2%)	11 55
10	L	44/70 (63%)	29 (66%)	13 (30%)	2 (4%)	3 34
All	All	3616/4173 (87%)	2772 (77%)	690 (19%)	154 (4%)	3 35

All (154) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	55	ASP
1	A	117	GLU
1	A	120	GLU
1	A	169	ASN
1	A	186	LYS
1	A	191	THR
1	A	193	ASP
1	A	194	ALA
1	A	195	ASP
1	A	320	ARG
1	A	567	LYS
1	A	1170	ILE
1	A	1173	HIS
1	A	1270	ASN

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Mol	Chain	Res	Type
2	B	439	ALA
2	B	468	GLU
2	B	475	SER
2	B	483	LEU
2	B	636	PRO
2	B	713	ALA
2	B	717	GLU
2	B	718	GLU
2	B	864	LYS
2	B	1021	MET
2	B	1096	ARG
3	C	142	VAL
3	C	182	PRO
4	E	206	GLY
7	I	33	SER
7	I	47	GLU
7	I	79	HIS
7	I	106	CYS
7	I	116	ASN
8	J	9	SER
8	J	10	CYS
1	A	56	PRO
1	A	155	GLU
1	A	250	ILE
1	A	258	GLY
1	A	307	ASP
1	A	424	ILE
1	A	846	GLU
1	A	958	VAL
1	A	1169	ILE
1	A	1221	LYS
1	A	1390	ASN
1	A	1437	GLY
2	B	91	SER
2	B	176	SER
2	B	340	ALA
2	B	441	ASP
2	B	478	GLY
2	B	531	GLN
2	B	575	PRO
2	B	831	SER
2	B	881	ASN

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Mol	Chain	Res	Type
5	F	72	LYS
6	H	78	SER
6	H	119	GLY
7	I	107	SER
9	K	70	ARG
1	A	154	SER
1	A	185	TRP
1	A	255	SER
1	A	311	GLN
1	A	418	SER
1	A	557	ASP
1	A	1031	VAL
1	A	1081	LEU
1	A	1156	PRO
1	A	1218	GLN
1	A	1407	GLU
2	B	21	GLU
2	B	489	SER
2	B	712	PRO
2	B	732	SER
2	B	943	SER
4	E	76	GLY
5	F	77	ASP
5	F	78	GLN
5	F	80	ALA
6	H	82	PRO
6	H	109	LYS
7	I	3	THR
7	I	9	ASP
8	J	6	ARG
9	K	7	PHE
1	A	48	ALA
1	A	66	LYS
1	A	149	GLU
1	A	323	LYS
1	A	1190	PRO
1	A	1224	LEU
1	A	1388	GLY
1	A	1435	PRO
2	B	74	LEU
2	B	76	GLN
2	B	79	THR

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Mol	Chain	Res	Type
2	B	290	GLY
2	B	559	SER
2	B	946	ASN
2	B	1017	ILE
2	B	1150	ARG
3	C	28	ALA
3	C	214	ASN
4	E	86	PRO
6	H	60	ALA
6	H	75	ALA
8	J	8	PHE
10	L	59	ALA
1	A	248	PRO
1	A	287	HIS
1	A	332	LYS
1	A	599	SER
1	A	1171	GLN
2	B	277	LYS
2	B	647	GLY
2	B	676	VAL
2	B	711	GLU
2	B	792	MET
2	B	974	PRO
3	C	125	MET
3	C	227	THR
4	E	124	VAL
7	I	11	ASN
10	L	46	VAL
1	A	78	PRO
1	A	119	ASN
1	A	157	ASP
1	A	308	ILE
1	A	364	VAL
1	A	392	VAL
1	A	568	PRO
2	B	555	ILE
2	B	1214	PRO
3	C	129	ILE
1	A	158	PRO
1	A	338	GLY
1	A	639	PRO
1	A	756	ILE

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Mol	Chain	Res	Type
1	A	1424	VAL
1	A	1429	ILE
2	B	292	ILE
2	B	731	VAL
1	A	197	PRO
2	B	70	ILE
2	B	93	GLY
2	B	901	PRO
4	E	38	PRO
1	A	570	PRO
1	A	1379	GLY
2	B	410	GLY
2	B	976	ILE
2	B	1046	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	1258/1520 (83%)	1103 (88%)	155 (12%)	6 34
2	B	1000/1061 (94%)	882 (88%)	118 (12%)	6 35
3	C	238/274 (87%)	212 (89%)	26 (11%)	8 40
4	E	196/197 (100%)	184 (94%)	12 (6%)	23 65
5	F	74/137 (54%)	72 (97%)	2 (3%)	52 82
6	H	119/128 (93%)	112 (94%)	7 (6%)	24 66
7	I	113/116 (97%)	101 (89%)	12 (11%)	8 41
8	J	60/65 (92%)	52 (87%)	8 (13%)	5 31
9	K	99/102 (97%)	90 (91%)	9 (9%)	12 48
10	L	40/57 (70%)	33 (82%)	7 (18%)	2 17
All	All	3197/3657 (87%)	2841 (89%)	356 (11%)	8 39

All (356) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	SER
1	A	49	LYS
1	A	58	LEU
1	A	63	ARG
1	A	65	LEU
1	A	69	THR
1	A	81	PHE
1	A	84	ILE
1	A	93	VAL
1	A	108	MET
1	A	113	LEU
1	A	121	LEU
1	A	123	ARG
1	A	154	SER
1	A	155	GLU
1	A	159	THR
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	191	THR
1	A	193	ASP
1	A	195	ASP
1	A	198	GLU
1	A	208	LEU
1	A	216	VAL
1	A	222	LEU
1	A	226	GLU
1	A	227	VAL
1	A	239	LEU
1	A	250	ILE
1	A	263	THR
1	A	266	LEU
1	A	270	LEU
1	A	306	ASN
1	A	308	ILE
1	A	313	GLN
1	A	317	LYS
1	A	322	VAL
1	A	323	LYS
1	A	332	LYS

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Mol	Chain	Res	Type
1	A	346	ASP
1	A	351	THR
1	A	373	THR
1	A	403	LYS
1	A	419	LYS
1	A	424	ILE
1	A	427	GLN
1	A	434	ARG
1	A	440	ASP
1	A	443	LEU
1	A	445	ASN
1	A	450	LEU
1	A	452	LYS
1	A	454	SER
1	A	465	TYR
1	A	466	SER
1	A	470	LEU
1	A	474	VAL
1	A	475	THR
1	A	516	SER
1	A	517	ASN
1	A	518	LYS
1	A	527	THR
1	A	535	THR
1	A	550	LEU
1	A	557	ASP
1	A	565	ILE
1	A	576	GLN
1	A	603	ASN
1	A	618	GLU
1	A	663	SER
1	A	666	ILE
1	A	687	LYS
1	A	688	LYS
1	A	694	THR
1	A	732	LEU
1	A	740	LEU
1	A	741	ASN
1	A	758	ILE
1	A	762	SER
1	A	764	CYS
1	A	770	VAL

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Mol	Chain	Res	Type
1	A	771	GLU
1	A	783	THR
1	A	803	SER
1	A	824	LEU
1	A	837	ILE
1	A	838	GLN
1	A	854	ASN
1	A	858	ASN
1	A	867	ILE
1	A	884	ASP
1	A	885	THR
1	A	895	LYS
1	A	902	LEU
1	A	904	THR
1	A	908	LEU
1	A	920	LEU
1	A	929	LEU
1	A	961	ARG
1	A	969	GLN
1	A	988	LEU
1	A	998	LEU
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	1035	TYR
1	A	1039	LYS
1	A	1046	LEU
1	A	1067	LEU
1	A	1079	MET
1	A	1081	LEU
1	A	1082	ASN
1	A	1095	THR
1	A	1113	THR
1	A	1118	VAL
1	A	1146	VAL
1	A	1168	GLU
1	A	1169	ILE
1	A	1172	LEU
1	A	1174	PHE

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Mol	Chain	Res	Type
1	A	1175	SER
1	A	1176	LEU
1	A	1177	LEU
1	A	1178	ASP
1	A	1179	GLU
1	A	1224	LEU
1	A	1227	ILE
1	A	1237	ILE
1	A	1243	VAL
1	A	1248	LEU
1	A	1264	GLU
1	A	1283	VAL
1	A	1322	ILE
1	A	1327	ILE
1	A	1329	THR
1	A	1333	ILE
1	A	1334	ASP
1	A	1336	MET
1	A	1354	ASN
1	A	1366	ARG
1	A	1385	THR
1	A	1386	ARG
1	A	1391	ARG
1	A	1393	ASN
1	A	1400	CYS
1	A	1403	GLU
1	A	1408	ILE
1	A	1444	MET
2	B	26	THR
2	B	35	SER
2	B	39	ARG
2	B	44	VAL
2	B	46	GLN
2	B	66	ASP
2	B	67	SER
2	B	68	THR
2	B	69	LEU
2	B	71	LEU
2	B	72	GLU
2	B	74	LEU
2	B	80	GLU
2	B	87	LYS

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Mol	Chain	Res	Type
2	B	89	GLU
2	B	98	THR
2	B	120	ARG
2	B	121	ASN
2	B	130	VAL
2	B	164	LYS
2	B	178	ASN
2	B	203	PHE
2	B	246	LYS
2	B	268	THR
2	B	282	ILE
2	B	283	VAL
2	B	305	VAL
2	B	310	MET
2	B	327	ARG
2	B	336	ARG
2	B	353	LYS
2	B	355	ILE
2	B	371	GLU
2	B	396	ASP
2	B	404	LYS
2	B	412	LEU
2	B	416	LEU
2	B	419	THR
2	B	424	LEU
2	B	425	THR
2	B	440	HIS
2	B	441	ASP
2	B	444	MET
2	B	445	LYS
2	B	459	TYR
2	B	463	THR
2	B	465	ASN
2	B	466	TRP
2	B	469	GLN
2	B	470	LYS
2	B	471	LYS
2	B	474	SER
2	B	479	VAL
2	B	483	LEU
2	B	527	THR
2	B	542	MET

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Mol	Chain	Res	Type
2	B	549	THR
2	B	570	VAL
2	B	582	VAL
2	B	604	ARG
2	B	627	PHE
2	B	633	VAL
2	B	637	LEU
2	B	644	GLU
2	B	645	SER
2	B	661	LEU
2	B	678	GLU
2	B	694	ASP
2	B	701	ILE
2	B	710	LEU
2	B	723	VAL
2	B	762	ASN
2	B	788	ARG
2	B	790	ASP
2	B	827	ILE
2	B	844	SER
2	B	864	LYS
2	B	871	THR
2	B	878	GLN
2	B	883	LEU
2	B	886	LYS
2	B	891	ASP
2	B	899	ILE
2	B	916	THR
2	B	943	SER
2	B	963	PHE
2	B	968	VAL
2	B	970	THR
2	B	973	ILE
2	B	975	GLN
2	B	979	LYS
2	B	989	THR
2	B	992	ILE
2	B	997	GLU
2	B	999	MET
2	B	1020	ARG
2	B	1022	THR
2	B	1028	GLU

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Mol	Chain	Res	Type
2	B	1051	THR
2	B	1071	VAL
2	B	1082	MET
2	B	1087	PHE
2	B	1093	GLN
2	B	1096	ARG
2	B	1099	VAL
2	B	1103	ILE
2	B	1113	VAL
2	B	1115	THR
2	B	1124	ARG
2	B	1132	GLU
2	B	1145	SER
2	B	1147	LEU
2	B	1156	ASP
2	B	1165	ILE
2	B	1175	LEU
2	B	1190	ASP
2	B	1194	ILE
2	B	1196	ILE
3	C	4	GLU
3	C	10	ILE
3	C	17	ASN
3	C	21	ILE
3	C	22	LEU
3	C	25	VAL
3	C	34	ARG
3	C	57	VAL
3	C	69	LEU
3	C	77	ILE
3	C	92	CYS
3	C	109	SER
3	C	120	ILE
3	C	129	ILE
3	C	134	ILE
3	C	143	LEU
3	C	154	LYS
3	C	163	ILE
3	C	178	PHE
3	C	195	GLN
3	C	197	SER
3	C	203	GLN

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Mol	Chain	Res	Type
3	C	215	GLU
3	C	228	PHE
3	C	240	VAL
3	C	244	VAL
4	E	31	THR
4	E	33	GLU
4	E	43	LYS
4	E	88	VAL
4	E	92	THR
4	E	95	THR
4	E	104	ASN
4	E	131	THR
4	E	134	THR
4	E	150	VAL
4	E	156	LEU
4	E	169	ARG
5	F	97	ARG
5	F	111	LEU
6	H	11	GLN
6	H	56	THR
6	H	62	SER
6	H	89	LEU
6	H	94	ASP
6	H	95	TYR
6	H	142	LEU
7	I	8	ARG
7	I	9	ASP
7	I	13	MET
7	I	29	CYS
7	I	31	THR
7	I	59	VAL
7	I	61	ASP
7	I	75	CYS
7	I	78	CYS
7	I	83	ASN
7	I	95	THR
7	I	104	LEU
8	J	5	VAL
8	J	7	CYS
8	J	13	VAL
8	J	28	ASP
8	J	31	ASP

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Mol	Chain	Res	Type
8	J	34	THR
8	J	43	ARG
8	J	50	ILE
9	K	6	ARG
9	K	10	PHE
9	K	33	ILE
9	K	41	THR
9	K	42	LEU
9	K	101	LEU
9	K	102	LYS
9	K	107	THR
9	K	113	THR
10	L	28	LYS
10	L	31	CYS
10	L	49	LYS
10	L	55	ILE
10	L	60	ARG
10	L	61	THR
10	L	68	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (91) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	64	ASN
1	A	68	GLN
1	A	83	HIS
1	A	92	HIS
1	A	119	ASN
1	A	171	GLN
1	A	253	ASN
1	A	273	ASN
1	A	281	HIS
1	A	306	ASN
1	A	311	GLN
1	A	399	HIS
1	A	435	HIS
1	A	445	ASN
1	A	471	ASN
1	A	493	GLN
1	A	503	GLN
1	A	545	GLN
1	A	631	HIS

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Mol	Chain	Res	Type
1	A	640	GLN
1	A	659	HIS
1	A	660	ASN
1	A	723	ASN
1	A	736	ASN
1	A	741	ASN
1	A	742	ASN
1	A	760	GLN
1	A	786	HIS
1	A	858	ASN
1	A	877	HIS
1	A	926	GLN
1	A	968	GLN
1	A	994	GLN
1	A	1033	GLN
1	A	1082	ASN
1	A	1173	HIS
1	A	1188	GLN
1	A	1222	ASN
1	A	1387	HIS
1	A	1427	ASN
1	A	1432	GLN
2	B	121	ASN
2	B	215	GLN
2	B	236	HIS
2	B	366	GLN
2	B	395	GLN
2	B	440	HIS
2	B	465	ASN
2	B	494	HIS
2	B	515	HIS
2	B	516	ASN
2	B	518	HIS
2	B	531	GLN
2	B	538	ASN
2	B	648	HIS
2	B	744	HIS
2	B	761	HIS
2	B	762	ASN
2	B	767	ASN
2	B	794	ASN
2	B	821	GLN

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Mol	Chain	Res	Type
2	B	822	ASN
2	B	842	ASN
2	B	862	GLN
2	B	958	GLN
2	B	984	HIS
2	B	986	GLN
2	B	1015	HIS
2	B	1084	GLN
2	B	1141	HIS
2	B	1178	ASN
3	C	31	ASN
3	C	73	GLN
3	C	91	HIS
3	C	102	GLN
3	C	112	ASN
3	C	167	HIS
3	C	188	HIS
3	C	195	GLN
4	E	8	ASN
4	E	104	ASN
4	E	147	HIS
6	H	11	GLN
6	H	35	GLN
6	H	137	GLN
7	I	60	GLN
7	I	83	ASN
7	I	87	GLN
7	I	89	GLN
8	J	64	ASN
9	K	65	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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 carbohydrates in this entry.

5.6 Ligand geometry

Of 8 ligands modelled in this entry, 8 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, 95^{th} 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%)	-0.25	29 (2%) 68 53	77, 132, 243, 401	0
2	B	1153/1224 (94%)	-0.20	21 (1%) 71 56	77, 116, 250, 399	0
3	C	271/318 (85%)	-0.34	2 (0%) 89 80	86, 111, 177, 330	0
4	E	215/215 (100%)	-0.30	0 100 100	107, 153, 272, 354	0
5	F	85/155 (54%)	-0.30	0 100 100	107, 129, 169, 217	0
6	H	136/146 (93%)	-0.15	4 (2%) 55 38	120, 167, 307, 372	0
7	I	119/122 (97%)	-0.25	1 (0%) 87 77	107, 148, 191, 275	0
8	J	65/70 (92%)	-0.42	0 100 100	83, 101, 151, 176	0
9	K	114/120 (95%)	-0.32	0 100 100	83, 115, 150, 171	0
10	L	46/70 (65%)	0.13	3 (6%) 22 13	102, 161, 254, 269	0
11	R	14/18 (77%)	-0.24	0 100 100	106, 130, 215, 216	0
12	T	29/29 (100%)	0.23	3 (10%) 9 6	105, 216, 417, 435	0
13	N	14/14 (100%)	0.15	1 (7%) 19 11	263, 310, 353, 397	0
All	All	3703/4234 (87%)	-0.24	64 (1%) 73 58	77, 128, 255, 435	0

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	882	THR	6.7
1	A	44	THR	5.6
10	L	25	ALA	4.9
1	A	1250	ALA	4.8
1	A	45	GLN	4.7
6	H	85	GLY	4.7
6	H	84	ALA	4.3
1	A	1252	THR	4.3
2	B	339	THR	4.2

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Mol	Chain	Res	Type	RSRZ
1	A	1087	ALA	4.2
2	B	83	ASN	4.1
2	B	869	SER	4.1
2	B	476	ARG	3.7
1	A	1086	PHE	3.6
1	A	66	LYS	3.6
6	H	86	ASP	3.3
1	A	46	THR	3.3
2	B	471	LYS	3.3
1	A	1247	SER	3.3
2	B	88	TYR	3.2
2	B	719	ASN	3.1
1	A	1249	ASP	3.1
1	A	72	GLU	3.1
1	A	1251	GLU	3.1
1	A	1085	HIS	3.1
2	B	441	ASP	3.0
1	A	253	ASN	3.0
6	H	32	THR	2.9
2	B	870	ILE	2.9
10	L	26	THR	2.8
2	B	714	GLU	2.8
2	B	709	ASP	2.8
2	B	717	GLU	2.7
1	A	191	THR	2.6
3	C	271	ASN	2.6
2	B	720	ASP	2.6
12	T	29	DA	2.6
12	T	10	DA	2.6
2	B	1181	GLU	2.6
1	A	1084	PHE	2.5
2	B	672	GLY	2.5
2	B	643	ASP	2.5
1	A	426	LEU	2.5
2	B	340	ALA	2.5
1	A	1248	LEU	2.4
1	A	157	ASP	2.3
3	C	267	GLN	2.3
10	L	43	THR	2.3
13	N	1	DC	2.2
1	A	192	GLY	2.1
1	A	188	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	159	THR	2.1
7	I	57	GLY	2.1
2	B	443	ASN	2.1
2	B	667	GLN	2.1
1	A	195	ASP	2.1
1	A	190	ALA	2.1
1	A	193	ASP	2.1
1	A	3	GLY	2.1
1	A	1090	ALA	2.1
2	B	646	LEU	2.0
1	A	197	PRO	2.0
1	A	158	PRO	2.0
12	T	3	DA	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} 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	LLDF	B-factors(Å^2)	Q<0.9
14	ZN	A	1735	1/1	0.97	0.12	-0.85	149,149,149,149	0
14	ZN	I	204	1/1	0.96	0.13	-0.96	310,310,310,310	0
14	ZN	I	203	1/1	0.99	0.11	-0.98	132,132,132,132	0
14	ZN	C	319	1/1	0.99	0.06	-1.13	136,136,136,136	0
14	ZN	A	1734	1/1	0.69	0.06	-1.46	228,228,228,228	0
14	ZN	L	105	1/1	0.98	0.02	-2.61	131,131,131,131	0
14	ZN	J	101	1/1	0.99	0.17	-3.91	193,193,193,193	0
14	ZN	B	1307	1/1	0.99	0.08	-	157,157,157,157	0

6.5 Other polymers (i)

There are no such residues in this entry.