



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 06:45 PM UTC

PDB ID : 3GTJ / pdb_00003gtj
Title : Backtracked RNA polymerase II complex with 13mer RNA
Authors : Wang, D.; Bushnell, D.A.; Huang, X.; Westover, K.D.; Levitt, M.; Kornberg, R.D.
Deposited on : 2009-03-27
Resolution : 3.42 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

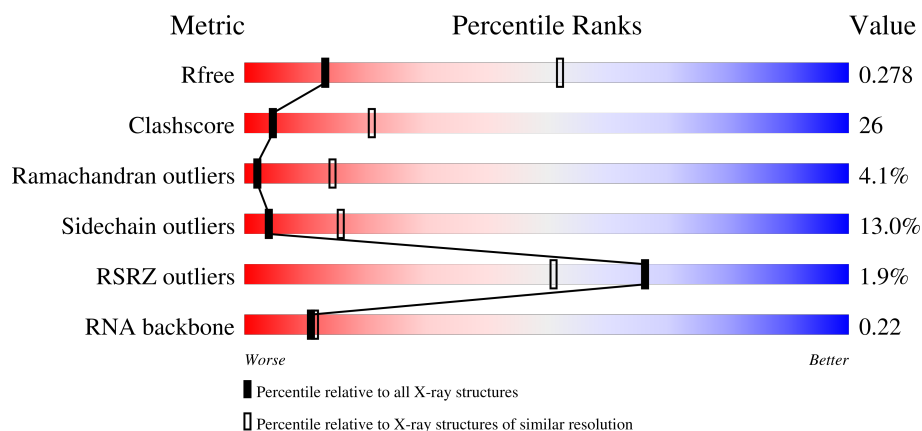
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.42 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1210 (3.48-3.36)
Clashscore	190562	1234 (3.48-3.36)
Ramachandran outliers	187476	1222 (3.48-3.36)
Sidechain outliers	187428	1222 (3.48-3.36)
RSRZ outliers	180081	1210 (3.48-3.36)
RNA backbone	3983	1162 (3.84-3.00)

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

Mol	Chain	Length	Quality of chain
1	A	1733	42% 31% 8% 18%
2	B	1224	49% 36% 9% 6%
3	C	318	45% 33% 8% 15%
4	E	215	67% 29%

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

2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 29974 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1429	Total	C	N	O	S	0	0	0
			11239	7077	1969	2132	61			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

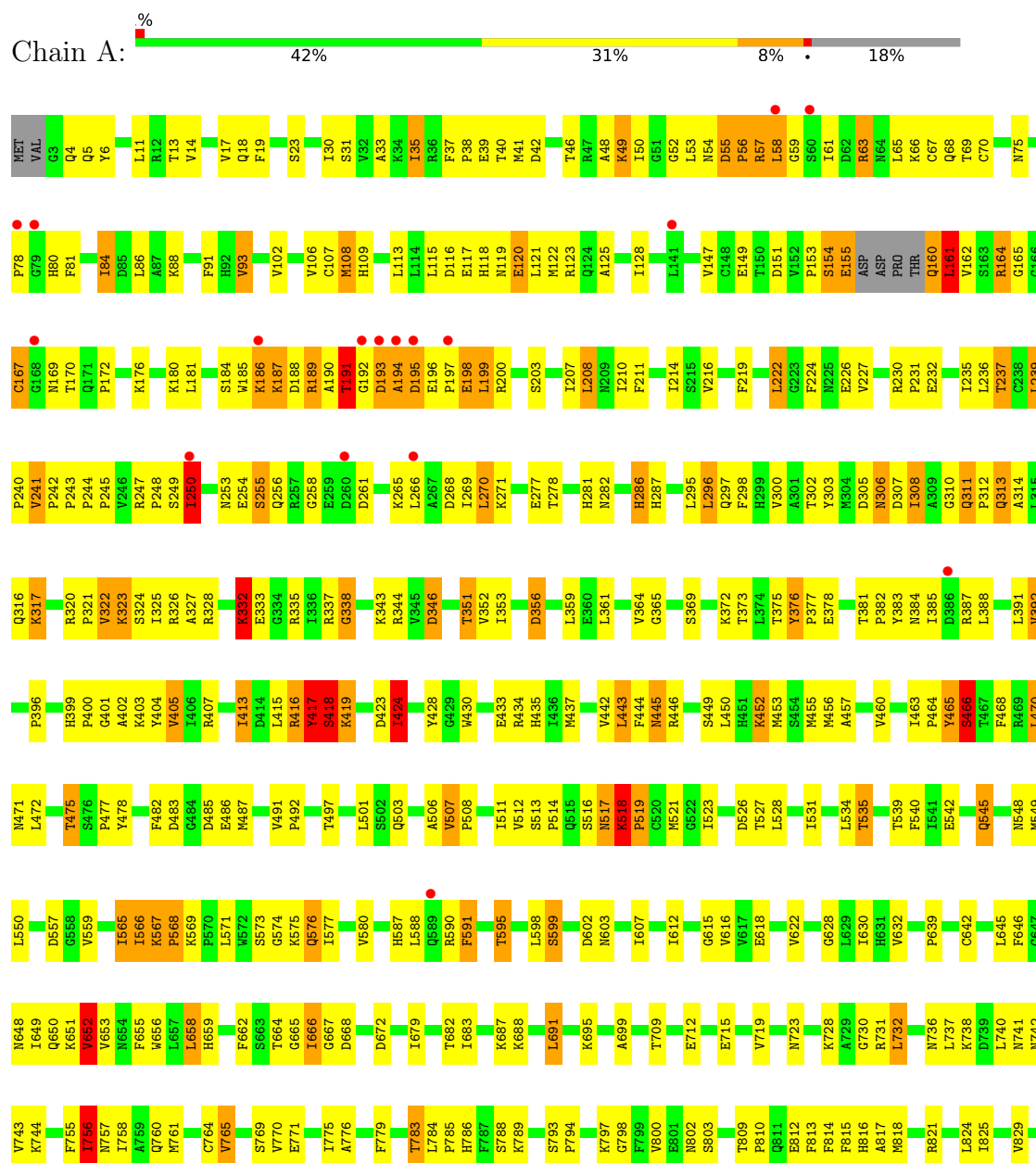
- Molecule 15 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

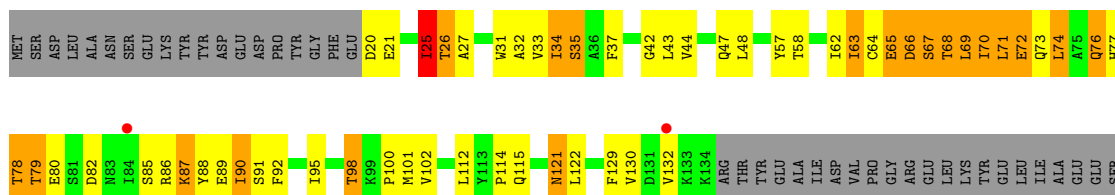
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	A	1	Total 1	Mg 1	0	0

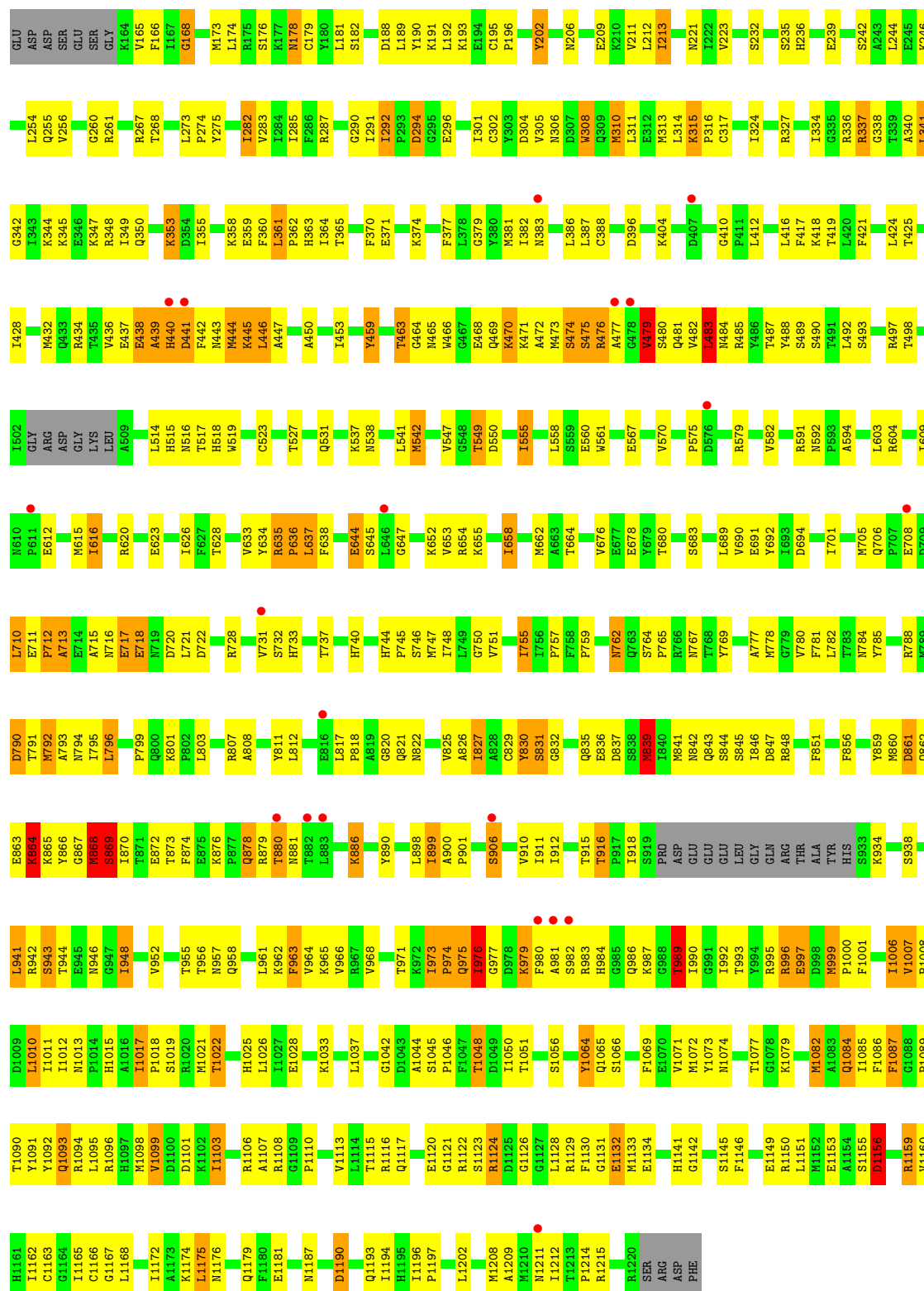
3 Residue-property plots [i](#)

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

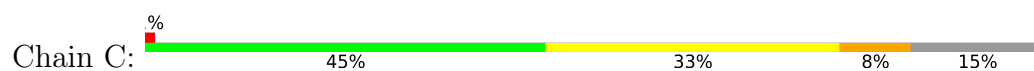
- Molecule 1: DNA-directed RNA polymerase II subunit RPB1

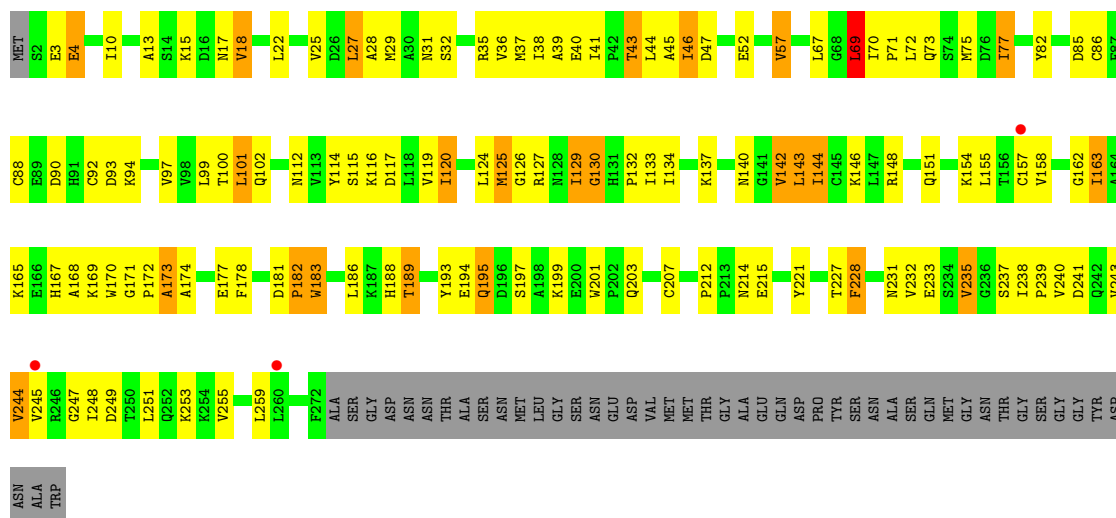


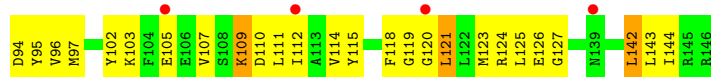




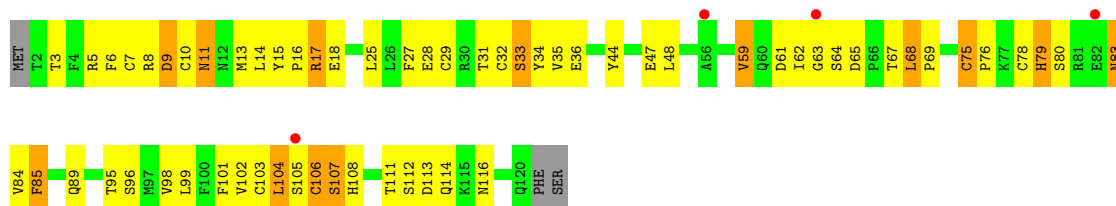
• Molecule 3: DNA-directed RNA polymerase II subunit RPB3







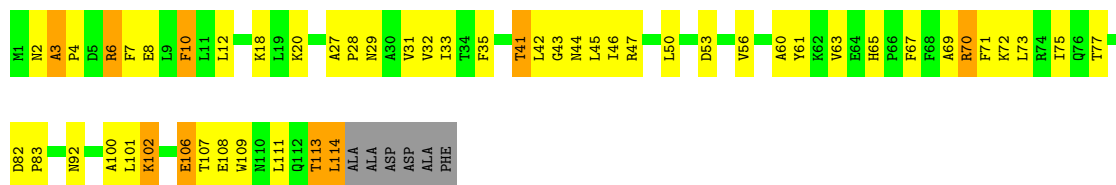
- Molecule 7: DNA-directed RNA polymerase II subunit RPB9



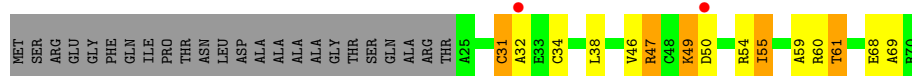
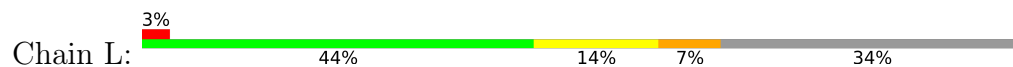
- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC5



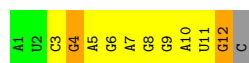
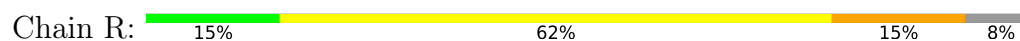
- Molecule 9: DNA-directed RNA polymerase II subunit RPB11



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



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

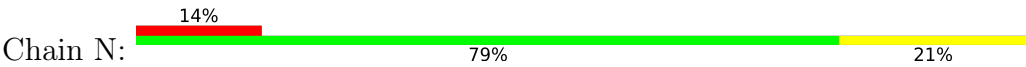


- Molecule 12: DNA (28-MER)





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



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	170.92Å 225.50Å 195.93Å 90.00° 101.21° 90.00°	Depositor
Resolution (Å)	50.00 – 3.42 50.00 – 3.42	Depositor EDS
% Data completeness (in resolution range)	91.7 (50.00-3.42) 91.8 (50.00-3.42)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.52 (at 3.40Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.282 , 0.292 0.270 , 0.278	Depositor DCC
R_{free} test set	4479 reflections (4.56%)	wwPDB-VP
Wilson B-factor (Å ²)	106.8	Xtriage
Anisotropy	0.267	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 97.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	29974	wwPDB-VP
Average B, all atoms (Å ²)	145.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.87% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.89	3/11438 (0.0%)	1.08	51/15465 (0.3%)
2	B	0.96	3/9348 (0.0%)	1.10	29/12611 (0.2%)
3	C	1.09	3/2174 (0.1%)	1.15	13/2946 (0.4%)
4	E	0.97	2/1793 (0.1%)	1.04	6/2413 (0.2%)
5	F	0.84	0/696	1.00	3/940 (0.3%)
6	H	0.89	0/1105	0.97	1/1495 (0.1%)
7	I	0.97	1/989 (0.1%)	1.04	9/1331 (0.7%)
8	J	1.03	0/541	1.12	1/727 (0.1%)
9	K	0.96	0/937	1.09	1/1265 (0.1%)
10	L	1.10	0/365	1.18	1/485 (0.2%)
11	R	0.53	0/292	0.90	0/455
12	T	0.59	0/634	1.29	6/975 (0.6%)
13	N	0.52	0/317	1.08	1/488 (0.2%)
All	All	0.93	12/30629 (0.0%)	1.09	122/41596 (0.3%)

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	989	THR	CA-CB	6.78	1.64	1.53
2	B	847	ASP	CG-OD2	6.13	1.37	1.25
1	A	756	ILE	CA-CB	6.03	1.62	1.54
7	I	102	VAL	CA-C	5.82	1.59	1.52
3	C	97	VAL	CA-CB	5.57	1.60	1.53
1	A	1299	VAL	CA-CB	5.52	1.61	1.54
3	C	195	GLN	C-O	5.32	1.30	1.24
4	E	31	THR	CA-CB	5.31	1.62	1.53
3	C	212	PRO	CA-C	5.20	1.54	1.51
2	B	996	ARG	CZ-NH1	5.09	1.39	1.32
4	E	9	ILE	CA-CB	5.06	1.60	1.54
1	A	250	ILE	CA-CB	5.03	1.61	1.54

All (122) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1156	ASP	N-CA-C	10.81	126.60	113.41
2	B	25	ILE	CB-CA-C	-9.42	95.96	111.32
3	C	183	TRP	N-CA-C	-8.73	96.76	109.59
1	A	93	VAL	N-CA-C	8.45	119.23	110.62
1	A	356	ASP	CA-C-N	7.88	127.60	119.56
1	A	356	ASP	C-N-CA	7.88	127.60	119.56
2	B	635	ARG	CA-C-N	7.86	129.66	119.84
2	B	635	ARG	C-N-CA	7.86	129.66	119.84
10	L	50	ASP	N-CA-C	7.69	122.00	111.54
4	E	52	ARG	CA-C-N	7.64	129.39	119.84
4	E	52	ARG	C-N-CA	7.64	129.39	119.84
1	A	1424	VAL	CB-CA-C	-7.35	102.62	111.81
1	A	776	ALA	N-CA-C	7.21	119.28	110.41
1	A	316	GLN	N-CA-C	7.15	122.04	111.96
1	A	88	LYS	CA-C-N	7.15	127.19	119.90
1	A	88	LYS	C-N-CA	7.15	127.19	119.90
7	I	102	VAL	N-CA-C	7.09	118.00	106.72
1	A	664	THR	CB-CA-C	-7.06	101.91	110.94
2	B	976	ILE	N-CA-C	7.03	123.96	109.34
3	C	173	ALA	N-CA-C	7.03	121.91	113.12
12	T	15	DA	P-O3'-C3'	6.76	130.34	120.20
2	B	361	LEU	CA-C-N	6.71	126.40	119.56
2	B	361	LEU	C-N-CA	6.71	126.40	119.56
9	K	3	ALA	N-CA-C	6.60	117.69	109.57
3	C	130	GLY	N-CA-C	6.55	124.05	115.40
3	C	195	GLN	N-CA-C	6.49	124.62	110.80
1	A	1316	VAL	CB-CA-C	-6.48	104.16	111.80
2	B	1021	MET	N-CA-C	6.42	120.52	111.92
5	F	138	LEU	CA-C-N	6.40	127.84	119.84
5	F	138	LEU	C-N-CA	6.40	127.84	119.84
1	A	247	ARG	CA-C-N	6.39	127.82	119.84
1	A	247	ARG	C-N-CA	6.39	127.82	119.84
7	I	68	LEU	CA-C-N	6.34	126.25	119.85
7	I	68	LEU	C-N-CA	6.34	126.25	119.85
1	A	1319	VAL	N-CA-C	6.33	114.91	109.02
3	C	193	TYR	N-CA-C	6.30	116.56	108.24
2	B	616	ILE	N-CA-C	6.23	115.70	106.85
6	H	91	ASP	N-CA-C	6.15	118.47	108.26
1	A	116	ASP	CB-CA-C	-6.14	98.22	111.11
1	A	296	LEU	N-CA-C	-6.10	107.07	114.75
1	A	506	ALA	CA-C-N	6.04	124.04	120.24
1	A	506	ALA	C-N-CA	6.04	124.04	120.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	241	VAL	CA-C-N	6.03	126.59	120.38
1	A	241	VAL	C-N-CA	6.03	126.59	120.38
12	T	22	DT	P-O3'-C3'	6.00	129.21	120.20
2	B	308	TRP	N-CA-C	5.96	117.45	111.07
4	E	182	ASP	CA-C-N	5.90	127.21	119.84
4	E	182	ASP	C-N-CA	5.90	127.21	119.84
1	A	117	GLU	CB-CA-C	-5.88	109.78	116.54
2	B	948	ILE	N-CA-C	5.86	116.04	107.37
1	A	1424	VAL	N-CA-C	5.83	115.96	110.30
7	I	15	TYR	CA-C-N	5.78	127.06	119.84
7	I	15	TYR	C-N-CA	5.78	127.06	119.84
1	A	199	LEU	N-CA-CB	5.77	122.49	112.27
2	B	876	LYS	CA-C-N	5.76	125.72	119.78
2	B	876	LYS	C-N-CA	5.76	125.72	119.78
2	B	856	PHE	N-CA-C	-5.76	101.50	110.42
1	A	652	VAL	CB-CA-C	-5.71	104.56	112.04
2	B	737	THR	N-CA-C	-5.68	98.69	110.80
7	I	65	ASP	CA-C-N	5.67	126.93	119.84
7	I	65	ASP	C-N-CA	5.67	126.93	119.84
2	B	861	ASP	N-CA-C	5.66	117.01	108.46
3	C	69	LEU	N-CA-C	5.65	118.98	111.75
1	A	286	HIS	N-CA-C	5.64	118.52	111.24
1	A	518	LYS	CB-CA-C	5.62	121.24	110.17
12	T	16	DC	O4'-C4'-C3'	-5.61	96.98	105.40
1	A	328	ARG	N-CA-C	-5.61	105.94	112.89
4	E	144	ILE	N-CA-C	5.53	116.30	110.72
2	B	165	VAL	N-CA-C	5.49	115.89	107.77
1	A	655	PHE	N-CA-C	-5.48	104.99	110.97
2	B	78	THR	CA-C-N	5.48	131.56	121.70
2	B	78	THR	C-N-CA	5.48	131.56	121.70
7	I	85	PHE	N-CA-C	5.48	117.12	108.96
2	B	801	LYS	CA-C-N	5.48	125.48	119.89
2	B	801	LYS	C-N-CA	5.48	125.48	119.89
1	A	977	LYS	CA-C-N	5.47	125.41	119.78
1	A	977	LYS	C-N-CA	5.47	125.41	119.78
2	B	868	MET	N-CA-CB	-5.45	103.18	111.19
2	B	1006	ILE	CB-CA-C	-5.44	102.99	111.26
1	A	376	TYR	CA-C-N	5.43	126.63	119.84
1	A	376	TYR	C-N-CA	5.43	126.63	119.84
1	A	996	ASN	N-CA-C	5.43	119.47	112.41
1	A	236	LEU	N-CA-C	5.40	118.05	109.24
3	C	39	ALA	N-CA-C	5.38	119.42	109.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1311	VAL	N-CA-C	5.37	115.78	107.78
13	N	10	DG	P-O3'-C3'	5.36	128.24	120.20
2	B	1064	TYR	N-CA-C	5.36	117.21	109.07
3	C	181	ASP	CA-C-N	5.35	126.53	119.84
3	C	181	ASP	C-N-CA	5.35	126.53	119.84
1	A	566	ILE	N-CA-C	-5.30	98.31	109.34
2	B	1010	LEU	N-CA-C	5.30	117.14	108.76
3	C	101	LEU	N-CA-C	5.30	117.45	108.02
7	I	25	LEU	N-CA-C	5.29	117.58	109.07
3	C	92	CYS	N-CA-C	5.28	115.00	108.19
1	A	507	VAL	CB-CA-C	-5.28	108.75	114.35
1	A	286	HIS	CA-C-N	5.26	131.16	121.70
1	A	286	HIS	C-N-CA	5.26	131.16	121.70
1	A	248	PRO	CB-CA-C	-5.25	102.89	111.56
1	A	1255	GLU	CB-CA-C	-5.25	103.14	111.48
1	A	491	VAL	CA-C-N	5.24	125.17	119.78
1	A	491	VAL	C-N-CA	5.24	125.17	119.78
4	E	115	ASN	N-CA-C	5.22	116.08	108.14
5	F	137	TYR	N-CA-C	5.22	117.75	109.24
12	T	22	DT	C4'-C3'-C2'	-5.22	94.57	102.40
2	B	1090	THR	N-CA-C	5.22	116.69	107.61
3	C	18	VAL	N-CA-C	5.22	114.30	106.42
1	A	783	THR	CB-CA-C	-5.21	101.54	110.24
12	T	6	DG	P-O3'-C3'	5.19	127.99	120.20
1	A	466	SER	N-CA-C	5.16	119.32	112.30
1	A	33	ALA	N-CA-C	5.16	117.48	108.76
2	B	1123	SER	N-CA-C	-5.16	106.58	112.92
1	A	1075	PRO	N-CA-C	-5.15	107.42	113.86
12	T	28	DT	O5'-C5'-C4'	5.14	118.50	110.80
1	A	894	GLU	N-CA-C	-5.13	105.58	111.07
1	A	519	PRO	N-CA-C	-5.09	101.98	112.47
1	A	942	PHE	N-CA-C	5.09	116.90	111.36
8	J	15	GLY	N-CA-C	5.07	120.02	113.27
1	A	1074	GLU	CA-C-N	-5.04	114.47	119.56
1	A	1074	GLU	C-N-CA	-5.04	114.47	119.56
3	C	174	ALA	CB-CA-C	-5.04	110.37	117.23
2	B	839	MET	N-CA-C	5.03	116.71	109.07
2	B	1155	SER	N-CA-C	5.01	121.47	110.80

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	11239	0	11313	708	0
2	B	9168	0	9179	496	0
3	C	2135	0	2090	103	0
4	E	1757	0	1781	44	0
5	F	684	0	703	26	0
6	H	1087	0	1062	55	0
7	I	971	0	930	55	0
8	J	532	0	544	30	0
9	K	919	0	929	47	0
10	L	363	0	387	11	0
11	R	260	0	132	38	0
12	T	566	0	316	13	0
13	N	284	0	161	5	0
14	A	2	0	0	1	0
14	B	1	0	0	0	0
14	C	1	0	0	0	0
14	I	2	0	0	2	0
14	J	1	0	0	1	0
14	L	1	0	0	0	0
15	A	1	0	0	0	0
All	All	29974	0	29527	1529	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 26.

All (1529) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1169:ILE:CB	1:A:1170:ILE:HB	1.41	1.47
2:B:863:GLU:CA	2:B:864:LYS:HB2	1.43	1.42
2:B:863:GLU:HA	2:B:864:LYS:CB	1.47	1.40
2:B:841:MET:HE1	2:B:980:PHE:CZ	1.61	1.34
1:A:1082:ASN:CA	1:A:1083:THR:HB	1.51	1.33
1:A:1082:ASN:HA	1:A:1083:THR:CB	1.54	1.33
2:B:338:GLY:CA	2:B:341:LEU:HD21	1.59	1.31

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:439:ALA:CB	2:B:440:HIS:HA	1.54	1.30
1:A:1168:GLU:HB2	1:A:1171:GLN:CB	1.63	1.26
2:B:864:LYS:O	2:B:864:LYS:HD3	1.35	1.23
1:A:55:ASP:OD1	1:A:59:GLY:HA3	1.40	1.22
11:R:8:G:O2'	11:R:9:G:H5'	1.37	1.22
1:A:1169:ILE:HB	1:A:1170:ILE:CB	1.69	1.21
2:B:439:ALA:HB3	2:B:440:HIS:CA	1.71	1.21
1:A:1168:GLU:CA	1:A:1171:GLN:HB2	1.70	1.20
1:A:1169:ILE:CA	1:A:1170:ILE:HB	1.68	1.20
1:A:1083:THR:N	1:A:1084:PHE:HA	1.52	1.18
2:B:78:THR:H	2:B:79:THR:HB	1.06	1.17
2:B:438:GLU:HB3	2:B:440:HIS:CD2	1.82	1.15
1:A:1169:ILE:H	1:A:1170:ILE:C	1.55	1.14
2:B:338:GLY:HA3	2:B:341:LEU:HD21	1.24	1.14
11:R:4:G:H2'	11:R:5:A:C8	1.84	1.12
1:A:198:GLU:CD	1:A:198:GLU:H	1.59	1.10
11:R:4:G:H2'	11:R:5:A:H8	0.95	1.10
1:A:1168:GLU:HA	1:A:1171:GLN:CB	1.82	1.10
2:B:445:LYS:HA	2:B:446:LEU:HB3	1.24	1.10
1:A:1168:GLU:CB	1:A:1171:GLN:CB	2.30	1.10
1:A:58:LEU:HD22	1:A:58:LEU:O	1.50	1.09
1:A:1079:MET:HE1	1:A:1359:ASP:HB2	1.31	1.09
1:A:154:SER:O	1:A:155:GLU:HB2	1.52	1.08
1:A:313:GLN:HG2	1:A:314:ALA:HB2	1.12	1.07
2:B:472:ALA:HB1	2:B:476:ARG:HG2	1.26	1.06
1:A:55:ASP:H	1:A:56:PRO:CD	1.68	1.06
1:A:1168:GLU:HB2	1:A:1171:GLN:HB3	1.07	1.06
5:F:93:ILE:HD11	5:F:134:ILE:HD11	1.35	1.06
1:A:1169:ILE:HG22	1:A:1170:ILE:HG12	1.38	1.05
1:A:1092:LYS:HB3	1:A:1094:VAL:N	1.70	1.04
1:A:1168:GLU:CB	1:A:1171:GLN:HB3	1.84	1.04
1:A:567:LYS:HB2	1:A:568:PRO:HD2	1.31	1.04
2:B:865:LYS:HA	2:B:870:ILE:O	1.57	1.03
1:A:196:GLU:N	1:A:197:PRO:HD3	1.70	1.03
3:C:142:VAL:HG22	3:C:143:LEU:H	1.20	1.02
1:A:310:GLY:CA	1:A:311:GLN:HB3	1.90	1.02
2:B:1187:ASN:HD21	2:B:1190:ASP:HB2	1.25	1.01
1:A:353:ILE:HD13	1:A:487:MET:HE2	1.42	1.01
1:A:1168:GLU:CA	1:A:1171:GLN:CB	2.38	1.01
2:B:472:ALA:HB1	2:B:476:ARG:CG	1.90	1.01
11:R:7:A:O2'	11:R:8:G:H5'	1.62	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:955:THR:HG22	2:B:956:THR:H	1.27	1.00
2:B:980:PHE:CE1	2:B:990:ILE:HD11	1.97	0.99
2:B:444:MET:HE3	2:B:446:LEU:HD13	1.44	0.99
1:A:1169:ILE:CB	1:A:1170:ILE:CB	2.30	0.98
2:B:841:MET:HE1	2:B:980:PHE:CE2	1.98	0.97
1:A:195:ASP:C	1:A:197:PRO:HD3	1.88	0.97
1:A:313:GLN:HG2	1:A:314:ALA:CB	1.95	0.97
1:A:1246:LYS:HD2	1:A:1246:LYS:O	1.65	0.96
1:A:161:LEU:HD22	1:A:162:VAL:N	1.80	0.96
1:A:192:GLY:O	1:A:193:ASP:HB3	1.64	0.96
1:A:1169:ILE:HB	1:A:1170:ILE:HB	0.98	0.96
1:A:1079:MET:CE	1:A:1359:ASP:HB2	1.95	0.95
1:A:567:LYS:CB	1:A:568:PRO:HD2	1.97	0.95
1:A:1083:THR:H	1:A:1084:PHE:HA	1.17	0.94
2:B:981:ALA:HB2	2:B:987:LYS:HA	1.50	0.94
6:H:109:LYS:HB3	6:H:111:LEU:H	1.32	0.94
1:A:1083:THR:HG22	1:A:1083:THR:O	1.64	0.94
1:A:1169:ILE:N	1:A:1170:ILE:HB	1.79	0.94
1:A:1169:ILE:N	1:A:1170:ILE:CB	2.30	0.94
1:A:1169:ILE:H	1:A:1170:ILE:CA	1.81	0.94
1:A:470:LEU:HD21	1:A:487:MET:HE1	1.50	0.93
1:A:1084:PHE:CE2	1:A:1092:LYS:HG2	2.03	0.93
2:B:983:ARG:HD2	2:B:1091:TYR:HD2	1.32	0.93
1:A:899:VAL:HB	1:A:929:LEU:HD11	1.51	0.92
1:A:187:LYS:HZ2	1:A:188:ASP:H	1.16	0.92
3:C:167:HIS:HD2	3:C:169:LYS:H	1.15	0.92
1:A:40:THR:N	1:A:41:MET:HB2	1.83	0.92
1:A:1178:ASP:CB	1:A:1179:GLU:HA	1.98	0.92
1:A:485:ASP:OD2	11:R:10:A:H4'	1.70	0.91
2:B:341:LEU:HD22	2:B:341:LEU:H	1.35	0.91
1:A:445:ASN:HB3	1:A:455:MET:HG2	1.52	0.91
1:A:40:THR:H	1:A:41:MET:HB2	1.31	0.91
1:A:310:GLY:N	1:A:311:GLN:HB3	1.85	0.91
1:A:58:LEU:HD11	1:A:244:PRO:HD3	1.52	0.90
2:B:864:LYS:HE2	2:B:864:LYS:HA	1.53	0.90
2:B:981:ALA:O	2:B:1092:TYR:CD2	2.24	0.90
2:B:445:LYS:CA	2:B:446:LEU:HB3	2.01	0.90
1:A:567:LYS:HB2	1:A:568:PRO:CD	2.00	0.90
1:A:1168:GLU:HA	1:A:1171:GLN:HB2	0.92	0.89
1:A:58:LEU:HD22	1:A:58:LEU:C	1.96	0.89
1:A:1173:HIS:NE2	1:A:1175:SER:HB3	1.88	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1173:HIS:CD2	1:A:1175:SER:HB3	2.08	0.89
1:A:575:LYS:HB3	1:A:612:ILE:HD11	1.52	0.89
1:A:118:HIS:CE1	1:A:155:GLU:HG2	2.08	0.88
7:I:10:CYS:HG	14:I:203:ZN:ZN	0.63	0.88
1:A:160:GLN:CD	1:A:160:GLN:N	2.30	0.88
1:A:310:GLY:H	1:A:311:GLN:HB3	1.37	0.88
1:A:198:GLU:CD	1:A:198:GLU:N	2.30	0.88
1:A:310:GLY:HA2	1:A:311:GLN:HB3	1.54	0.88
1:A:55:ASP:H	1:A:56:PRO:HD2	1.38	0.87
2:B:634:TYR:CE1	2:B:692:TYR:HD1	1.92	0.87
1:A:1169:ILE:CG2	1:A:1170:ILE:HG12	2.04	0.87
1:A:57:ARG:HB3	1:A:68:GLN:HB3	1.53	0.87
1:A:1092:LYS:HB3	1:A:1093:LYS:C	1.99	0.87
1:A:351:THR:OG1	2:B:1103:ILE:HG12	1.73	0.87
1:A:741:ASN:HD22	1:A:744:LYS:H	1.22	0.86
2:B:1162:ILE:HG22	2:B:1163:CYS:H	1.39	0.86
1:A:1168:GLU:HB2	1:A:1171:GLN:CG	2.04	0.86
2:B:78:THR:H	2:B:79:THR:CB	1.88	0.86
2:B:77:HIS:HB3	2:B:78:THR:HB	1.58	0.86
1:A:1083:THR:N	1:A:1084:PHE:CA	2.35	0.86
1:A:470:LEU:HD21	1:A:487:MET:CE	2.05	0.86
2:B:636:PRO:CB	2:B:637:LEU:HA	2.05	0.86
2:B:344:LYS:HB2	2:B:347:LYS:HB2	1.58	0.86
2:B:438:GLU:CB	2:B:440:HIS:CD2	2.58	0.86
1:A:668:ASP:HB3	1:A:743:VAL:HG23	1.59	0.85
7:I:105:SER:O	7:I:106:CYS:HB3	1.75	0.85
1:A:49:LYS:HB3	1:A:55:ASP:OD2	1.77	0.85
1:A:53:LEU:HD23	1:A:54:ASN:N	1.90	0.85
1:A:566:ILE:O	1:A:566:ILE:HG23	1.77	0.84
2:B:841:MET:CE	2:B:980:PHE:CZ	2.56	0.84
3:C:186:LEU:HB3	3:C:188:HIS:HD2	1.43	0.83
1:A:666:ILE:HD11	2:B:1026:LEU:HB3	1.60	0.83
1:A:1178:ASP:CG	1:A:1179:GLU:HA	2.02	0.83
2:B:1168:LEU:HD13	2:B:1208:MET:HE3	1.59	0.83
3:C:47:ASP:HA	10:L:69:ALA:HB3	1.58	0.83
1:A:1169:ILE:H	1:A:1170:ILE:CB	1.88	0.83
1:A:1170:ILE:HG22	1:A:1170:ILE:O	1.78	0.83
1:A:1169:ILE:N	1:A:1170:ILE:C	2.36	0.83
1:A:55:ASP:N	1:A:56:PRO:CD	2.40	0.82
2:B:996:ARG:HG3	2:B:1007:VAL:HG21	1.62	0.82
2:B:273:LEU:HD21	2:B:360:PHE:HD1	1.45	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:868:TYR:CE1	1:A:1064:VAL:HG11	2.15	0.82
6:H:109:LYS:HA	6:H:110:ASP:HB3	1.59	0.82
2:B:78:THR:N	2:B:79:THR:HB	1.92	0.82
11:R:3:C:H2'	11:R:4:G:C8	2.14	0.82
6:H:112:ILE:HG22	6:H:127:GLY:O	1.80	0.81
1:A:419:LYS:NZ	1:A:419:LYS:HB3	1.95	0.81
1:A:313:GLN:CG	1:A:314:ALA:HB2	2.05	0.81
5:F:93:ILE:HD11	5:F:134:ILE:CD1	2.10	0.81
2:B:338:GLY:CA	2:B:341:LEU:CD2	2.54	0.81
2:B:999:MET:HG3	2:B:1000:PRO:HD2	1.62	0.80
2:B:338:GLY:HA3	2:B:341:LEU:CD2	2.09	0.80
2:B:986:GLN:HE21	2:B:1022:THR:HG21	1.45	0.80
1:A:1170:ILE:O	1:A:1170:ILE:CG2	2.30	0.80
2:B:444:MET:HE3	2:B:446:LEU:CD1	2.12	0.79
1:A:1085:HIS:H	1:A:1085:HIS:CD2	1.96	0.79
3:C:167:HIS:CD2	3:C:169:LYS:H	1.98	0.79
1:A:58:LEU:HD21	1:A:244:PRO:HD2	1.63	0.79
2:B:865:LYS:CA	2:B:870:ILE:O	2.30	0.79
1:A:310:GLY:H	1:A:311:GLN:CB	1.95	0.79
1:A:1081:LEU:O	1:A:1083:THR:CB	2.30	0.79
2:B:759:PRO:HB3	2:B:767:ASN:HD21	1.48	0.79
1:A:1246:LYS:O	1:A:1246:LYS:CD	2.30	0.79
2:B:338:GLY:N	2:B:341:LEU:HD21	1.96	0.79
1:A:286:HIS:HB3	1:A:287:HIS:HB2	1.66	0.78
1:A:1173:HIS:CD2	1:A:1175:SER:CB	2.66	0.78
2:B:899:ILE:HD11	2:B:911:ILE:HG23	1.63	0.78
1:A:1079:MET:HE1	1:A:1359:ASP:CB	2.12	0.78
2:B:341:LEU:HB3	2:B:344:LYS:HE3	1.63	0.78
1:A:115:LEU:HD12	1:A:122:MET:HE3	1.65	0.78
1:A:445:ASN:CB	1:A:455:MET:HG2	2.14	0.78
1:A:335:ARG:HD2	2:B:1202:LEU:HD12	1.65	0.78
11:R:9:G:O2'	11:R:10:A:H5'	1.84	0.78
1:A:775:ILE:HB	1:A:797:LYS:O	1.84	0.77
1:A:58:LEU:O	1:A:58:LEU:CD2	2.32	0.77
3:C:3:GLU:HG3	3:C:4:GLU:H	1.48	0.77
3:C:57:VAL:HG21	8:J:57:ILE:HD11	1.66	0.77
1:A:187:LYS:HB2	1:A:187:LYS:NZ	1.99	0.77
1:A:193:ASP:O	1:A:194:ALA:CB	2.32	0.77
1:A:868:TYR:HE1	1:A:1064:VAL:HG11	1.49	0.77
2:B:843:GLN:HG2	2:B:993:THR:HB	1.64	0.77
2:B:636:PRO:HB3	2:B:637:LEU:HA	1.65	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:864:LYS:HG3	2:B:872:GLU:HB2	1.66	0.77
1:A:1082:ASN:CA	1:A:1083:THR:CB	2.30	0.77
1:A:1169:ILE:CG2	1:A:1170:ILE:CG1	2.63	0.77
2:B:715:ALA:H	2:B:716:ASN:HA	1.50	0.77
1:A:187:LYS:HD3	1:A:188:ASP:N	2.00	0.77
1:A:1245:PRO:O	1:A:1246:LYS:HG3	1.84	0.77
2:B:980:PHE:HE1	2:B:990:ILE:HD11	1.47	0.77
1:A:118:HIS:HB2	1:A:123:ARG:HG2	1.67	0.77
3:C:32:SER:O	3:C:36:VAL:HG12	1.84	0.76
1:A:55:ASP:H	1:A:56:PRO:HD3	1.48	0.76
1:A:886:ILE:HD11	1:A:943:LEU:HB3	1.66	0.76
7:I:78:CYS:O	7:I:79:HIS:HB2	1.84	0.76
11:R:4:G:C2'	11:R:5:A:H8	1.88	0.76
2:B:1162:ILE:HG22	2:B:1163:CYS:N	2.00	0.76
1:A:567:LYS:CB	1:A:568:PRO:CD	2.62	0.76
2:B:338:GLY:C	2:B:341:LEU:HD21	2.09	0.76
2:B:980:PHE:CE1	2:B:990:ILE:CD1	2.69	0.76
6:H:95:TYR:HE2	6:H:97:MET:HG3	1.50	0.76
1:A:588:LEU:HB3	1:A:607:ILE:HB	1.68	0.76
9:K:73:LEU:HD23	9:K:75:ILE:HD11	1.67	0.75
1:A:187:LYS:O	1:A:189:ARG:HG3	1.85	0.75
1:A:326:ARG:HG2	1:A:1406:VAL:HG21	1.68	0.75
1:A:1083:THR:O	1:A:1083:THR:CG2	2.34	0.75
2:B:983:ARG:HD2	2:B:1091:TYR:CD2	2.21	0.75
1:A:1169:ILE:HG22	1:A:1170:ILE:CG1	2.15	0.75
1:A:320:ARG:HB3	1:A:321:PRO:CD	2.17	0.75
1:A:457:ALA:O	1:A:507:VAL:HG23	1.86	0.75
1:A:1169:ILE:HB	1:A:1170:ILE:CG1	2.16	0.75
2:B:911:ILE:HG22	2:B:912:ILE:HG13	1.69	0.75
2:B:341:LEU:CB	2:B:344:LYS:HE3	2.17	0.74
2:B:759:PRO:HB3	2:B:767:ASN:ND2	2.02	0.74
2:B:1159:ARG:HD3	2:B:1193:GLN:HG3	1.70	0.74
1:A:351:THR:CG2	1:A:352:VAL:N	2.49	0.74
6:H:109:LYS:HB3	6:H:111:LEU:N	2.03	0.74
7:I:78:CYS:SG	14:I:204:ZN:ZN	1.75	0.74
8:J:45:CYS:SG	14:J:101:ZN:ZN	1.75	0.74
2:B:1120:GLU:HG2	2:B:1121:GLY:N	2.02	0.74
1:A:192:GLY:O	1:A:193:ASP:CB	2.36	0.73
1:A:423:ASP:O	1:A:424:ILE:HB	1.85	0.73
2:B:864:LYS:HD3	2:B:864:LYS:C	2.14	0.73
1:A:1083:THR:H	1:A:1084:PHE:CA	2.00	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1253:GLU:CG	1:A:1253:GLU:O	2.35	0.73
4:E:119:SER:HB2	13:N:12:DT:C5'	2.18	0.73
2:B:1056:SER:HB3	2:B:1066:SER:O	1.89	0.73
1:A:602:ASP:HB3	1:A:616:VAL:HG23	1.70	0.73
2:B:980:PHE:HE1	2:B:990:ILE:CD1	2.01	0.73
1:A:41:MET:HG3	1:A:42:ASP:H	1.52	0.72
1:A:648:ASN:O	1:A:652:VAL:HG23	1.89	0.72
1:A:1085:HIS:H	1:A:1085:HIS:HD2	1.38	0.72
5:F:101:ILE:HD13	5:F:120:ILE:HG22	1.70	0.72
1:A:1342:GLU:HG3	4:E:198:ILE:HD13	1.71	0.72
2:B:634:TYR:CE1	2:B:692:TYR:CD1	2.77	0.72
1:A:188:ASP:O	1:A:189:ARG:HG2	1.89	0.72
11:R:3:C:H2'	11:R:4:G:H8	1.51	0.72
1:A:53:LEU:HD23	1:A:53:LEU:C	2.13	0.72
2:B:114:PRO:HG2	2:B:181:LEU:HD11	1.70	0.72
1:A:472:LEU:O	1:A:475:THR:HB	1.89	0.72
2:B:472:ALA:CB	2:B:476:ARG:CG	2.66	0.72
1:A:187:LYS:HZ2	1:A:187:LYS:HB2	1.55	0.72
1:A:508:PRO:O	1:A:511:ILE:HG13	1.89	0.72
1:A:741:ASN:ND2	1:A:744:LYS:H	1.86	0.71
1:A:899:VAL:HG23	1:A:1029:ARG:HG2	1.72	0.71
1:A:118:HIS:HE1	1:A:155:GLU:HG2	1.53	0.71
1:A:1167:GLU:O	1:A:1170:ILE:HG22	1.89	0.71
1:A:1402:PHE:CD2	1:A:1403:GLU:HB2	2.26	0.71
2:B:85:SER:H	2:B:86:ARG:HB3	1.54	0.71
6:H:109:LYS:HA	6:H:110:ASP:CB	2.20	0.71
1:A:419:LYS:HB3	1:A:419:LYS:HZ3	1.54	0.71
1:A:1155:ASP:HB3	1:A:1241:ARG:HH21	1.56	0.71
2:B:515:HIS:HD2	2:B:517:THR:H	1.36	0.71
1:A:858:ASN:C	1:A:858:ASN:HD22	1.99	0.71
2:B:981:ALA:CB	2:B:987:LYS:HA	2.21	0.71
11:R:8:G:O2'	11:R:9:G:C5'	2.30	0.70
1:A:196:GLU:N	1:A:197:PRO:CD	2.50	0.70
1:A:401:GLY:C	1:A:435:HIS:CD2	2.69	0.70
2:B:470:LYS:HE2	2:B:470:LYS:HA	1.73	0.70
1:A:161:LEU:HD22	1:A:162:VAL:H	1.54	0.70
2:B:644:GLU:HG3	2:B:654:ARG:HH22	1.56	0.70
9:K:65:HIS:HD2	9:K:67:PHE:HB2	1.56	0.70
1:A:378:GLU:OE1	1:A:434:ARG:HD3	1.90	0.70
2:B:341:LEU:HD22	2:B:341:LEU:N	2.07	0.70
1:A:185:TRP:HE3	1:A:198:GLU:HG2	1.56	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:119:SER:CB	13:N:12:DT:H5''	2.21	0.70
1:A:249:SER:O	1:A:250:ILE:HG13	1.90	0.70
1:A:1253:GLU:O	1:A:1254:ALA:C	2.34	0.69
2:B:898:LEU:HD13	2:B:952:VAL:HG11	1.73	0.69
4:E:15:ALA:O	4:E:19:VAL:HG23	1.92	0.69
2:B:438:GLU:HB3	2:B:440:HIS:CG	2.26	0.69
2:B:872:GLU:HG2	2:B:916:THR:HB	1.74	0.69
2:B:956:THR:HA	2:B:961:LEU:O	1.91	0.69
2:B:439:ALA:HB3	2:B:440:HIS:HA	0.74	0.69
1:A:907:THR:HG22	1:A:908:LEU:H	1.58	0.69
1:A:573:SER:H	1:A:576:GLN:HG3	1.57	0.69
1:A:666:ILE:CD1	2:B:1026:LEU:HB3	2.22	0.69
1:A:779:PHE:CE1	1:A:785:PRO:HD3	2.28	0.69
2:B:341:LEU:O	2:B:344:LYS:HG2	1.92	0.69
2:B:878:GLN:HG2	2:B:879:ARG:H	1.57	0.69
2:B:976:ILE:O	2:B:990:ILE:HB	1.92	0.69
2:B:976:ILE:HG23	2:B:977:GLY:H	1.58	0.69
1:A:1080:THR:HG22	1:A:1080:THR:O	1.91	0.69
11:R:6:G:C2	11:R:7:A:N7	2.62	0.69
1:A:193:ASP:O	1:A:194:ALA:HB3	1.93	0.68
11:R:6:G:H2'	11:R:7:A:H8	1.56	0.68
1:A:58:LEU:C	1:A:58:LEU:CD2	2.66	0.68
1:A:91:PHE:H	1:A:297:GLN:HE22	1.39	0.68
2:B:710:LEU:HD13	2:B:733:HIS:HB3	1.75	0.68
2:B:778:MET:CE	2:B:1094:ARG:HD3	2.24	0.68
7:I:7:CYS:HB2	7:I:14:LEU:HD21	1.76	0.68
2:B:444:MET:C	2:B:445:LYS:HG3	2.18	0.68
5:F:111:LEU:H	5:F:111:LEU:HD22	1.59	0.68
1:A:666:ILE:N	1:A:666:ILE:HD12	2.07	0.68
2:B:715:ALA:N	2:B:716:ASN:HA	2.08	0.68
1:A:1246:LYS:HD2	1:A:1246:LYS:C	2.17	0.68
2:B:952:VAL:HG22	2:B:966:VAL:HG13	1.76	0.68
2:B:759:PRO:CB	2:B:767:ASN:HD21	2.07	0.68
1:A:1359:ASP:OD1	1:A:1359:ASP:O	2.12	0.67
3:C:99:LEU:HB2	3:C:157:CYS:HB2	1.75	0.67
2:B:636:PRO:CB	2:B:637:LEU:CA	2.71	0.67
6:H:38:LEU:HD11	6:H:123:MET:HE2	1.77	0.67
1:A:53:LEU:CD2	1:A:54:ASN:N	2.57	0.67
2:B:438:GLU:O	2:B:439:ALA:C	2.37	0.67
1:A:401:GLY:O	1:A:435:HIS:CD2	2.48	0.67
1:A:1092:LYS:CB	1:A:1093:LYS:C	2.66	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:64:CYS:O	2:B:65:GLU:HB3	1.94	0.67
1:A:1079:MET:SD	1:A:1359:ASP:CB	2.83	0.67
2:B:338:GLY:C	2:B:341:LEU:CD2	2.68	0.67
11:R:8:G:C2'	11:R:9:G:H5'	2.25	0.67
1:A:889:SER:HB2	1:A:892:ALA:H	1.60	0.67
3:C:57:VAL:CG2	8:J:57:ILE:HD11	2.24	0.67
3:C:182:PRO:HB3	3:C:207:CYS:SG	2.35	0.67
1:A:1084:PHE:CD2	1:A:1092:LYS:HG2	2.28	0.66
2:B:66:ASP:CG	2:B:66:ASP:O	2.38	0.66
2:B:906:SER:HA	2:B:946:ASN:CB	2.25	0.66
9:K:102:LYS:O	9:K:106:GLU:HG2	1.95	0.66
1:A:14:VAL:H	1:A:1432:GLN:HE22	1.40	0.66
2:B:459:TYR:C	2:B:459:TYR:CD2	2.74	0.66
11:R:6:G:C2	11:R:7:A:C5	2.83	0.66
2:B:445:LYS:HB3	2:B:447:ALA:HB3	1.77	0.66
6:H:12:VAL:HG13	6:H:26:ILE:HD11	1.77	0.66
1:A:55:ASP:N	1:A:56:PRO:HD2	2.04	0.66
2:B:637:LEU:CD1	2:B:740:HIS:HB3	2.25	0.66
2:B:1117:GLN:HG2	2:B:1156:ASP:OD2	1.95	0.66
1:A:1323:ASP:OD1	1:A:1325:THR:HG22	1.95	0.66
2:B:636:PRO:HB2	2:B:637:LEU:HB3	1.77	0.66
2:B:944:THR:HG21	2:B:1122:ARG:NH2	2.11	0.66
3:C:142:VAL:HG21	8:J:5:VAL:HG13	1.76	0.66
2:B:439:ALA:CB	2:B:440:HIS:CA	2.41	0.66
6:H:114:VAL:HG22	6:H:125:LEU:HB3	1.76	0.66
1:A:567:LYS:CG	1:A:568:PRO:HD2	2.26	0.66
1:A:188:ASP:O	1:A:189:ARG:CG	2.45	0.65
2:B:839:MET:HE3	2:B:1010:LEU:HD12	1.78	0.65
2:B:168:GLY:H	2:B:450:ALA:HB1	1.61	0.65
2:B:310:MET:O	2:B:313:MET:HB2	1.96	0.65
2:B:706:GLN:O	2:B:710:LEU:HB2	1.95	0.65
1:A:310:GLY:N	1:A:311:GLN:CB	2.55	0.65
12:T:15:DA:H2''	12:T:16:DC:O5'	1.96	0.65
1:A:185:TRP:HH2	1:A:200:ARG:HD2	1.61	0.65
1:A:1167:GLU:O	1:A:1170:ILE:CG2	2.45	0.65
2:B:202:TYR:CD1	2:B:209:GLU:HB3	2.31	0.65
2:B:981:ALA:O	2:B:1092:TYR:HD2	1.72	0.65
1:A:154:SER:O	1:A:155:GLU:CB	2.36	0.65
1:A:160:GLN:O	1:A:161:LEU:HB2	1.97	0.65
4:E:124:VAL:HB	4:E:125:PRO:HD3	1.78	0.65
1:A:189:ARG:NH2	1:A:196:GLU:O	2.30	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:511:ILE:HG12	1:A:521:MET:HE2	1.79	0.65
1:A:1081:LEU:C	1:A:1083:THR:OG1	2.40	0.65
1:A:1168:GLU:HA	1:A:1170:ILE:O	1.97	0.65
2:B:862:GLN:HG2	2:B:963:PHE:HD1	1.62	0.65
1:A:765:VAL:HG22	1:A:800:VAL:HB	1.79	0.65
1:A:1172:LEU:O	1:A:1174:PHE:N	2.30	0.65
1:A:351:THR:HG23	1:A:352:VAL:N	2.11	0.65
2:B:65:GLU:CG	2:B:66:ASP:H	2.09	0.65
2:B:445:LYS:HB3	2:B:447:ALA:H	1.61	0.65
11:R:7:A:O2'	11:R:8:G:C5'	2.40	0.65
1:A:118:HIS:CE1	1:A:155:GLU:CG	2.80	0.64
1:A:482:PHE:O	2:B:989:THR:HG23	1.97	0.64
1:A:793:SER:HB2	1:A:794:PRO:HD2	1.77	0.64
1:A:1444:MET:HB2	5:F:133:VAL:HG12	1.77	0.64
4:E:24:LYS:HB3	4:E:30:ILE:HD12	1.78	0.64
3:C:102:GLN:HG2	3:C:154:LYS:HD2	1.79	0.64
11:R:6:G:C6	11:R:7:A:N6	2.65	0.64
1:A:58:LEU:CD1	1:A:244:PRO:HD3	2.27	0.64
1:A:1082:ASN:N	1:A:1083:THR:HB	2.11	0.64
2:B:85:SER:N	2:B:86:ARG:HB3	2.11	0.64
3:C:142:VAL:HG22	3:C:143:LEU:N	1.98	0.64
1:A:56:PRO:O	1:A:58:LEU:N	2.30	0.64
1:A:517:ASN:O	1:A:518:LYS:HB3	1.96	0.64
1:A:738:LYS:NZ	3:C:194:GLU:HA	2.12	0.64
1:A:1168:GLU:HG3	1:A:1168:GLU:O	1.96	0.64
7:I:83:ASN:C	7:I:83:ASN:HD22	2.06	0.64
2:B:115:GLN:HA	2:B:115:GLN:OE1	1.97	0.64
2:B:955:THR:HG22	2:B:956:THR:N	2.07	0.64
9:K:69:ALA:O	9:K:70:ARG:HB3	1.95	0.64
2:B:1001:PHE:CE2	2:B:1073:TYR:HB2	2.33	0.64
1:A:1092:LYS:HB3	1:A:1094:VAL:H	1.62	0.64
2:B:444:MET:HG2	2:B:446:LEU:HD22	1.80	0.64
3:C:133:ILE:HD11	3:C:237:SER:HA	1.79	0.64
3:C:163:ILE:HD13	9:K:10:PHE:CE1	2.32	0.64
11:R:6:G:N3	11:R:7:A:C8	2.66	0.63
1:A:1161:THR:HG22	1:A:1163:ILE:H	1.64	0.63
2:B:1162:ILE:CG2	2:B:1163:CYS:H	2.10	0.63
1:A:1092:LYS:N	1:A:1093:LYS:HA	2.13	0.63
2:B:898:LEU:HD13	2:B:952:VAL:CG1	2.29	0.63
11:R:5:A:C2	11:R:6:G:C5	2.87	0.63
11:R:6:G:C4	11:R:7:A:N7	2.66	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:107:CYS:SG	14:A:1734:ZN:ZN	1.86	0.63
1:A:1092:LYS:CB	1:A:1093:LYS:CA	2.76	0.63
4:E:12:LEU:HD11	4:E:58:MET:HE1	1.79	0.63
1:A:567:LYS:NZ	6:H:46:LEU:HB2	2.13	0.63
1:A:569:LYS:HD2	3:C:221:TYR:HB2	1.79	0.63
1:A:630:ILE:HD12	1:A:630:ILE:H	1.64	0.63
2:B:515:HIS:H	2:B:518:HIS:CD2	2.16	0.63
2:B:1084:GLN:HG2	3:C:201:TRP:CH2	2.33	0.63
2:B:440:HIS:C	2:B:442:PHE:H	2.07	0.63
2:B:1077:THR:HG23	2:B:1079:LYS:H	1.62	0.63
1:A:672:ASP:H	1:A:736:ASN:HD21	1.47	0.63
1:A:886:ILE:HD11	1:A:943:LEU:CB	2.29	0.63
1:A:1111:MET:HG3	1:A:1114:PRO:HG3	1.80	0.63
1:A:1168:GLU:CB	1:A:1171:GLN:CG	2.71	0.63
1:A:55:ASP:OD1	1:A:59:GLY:CA	2.33	0.63
1:A:534:LEU:O	1:A:574:GLY:HA3	1.98	0.63
1:A:1168:GLU:O	1:A:1168:GLU:CG	2.47	0.63
2:B:341:LEU:H	2:B:341:LEU:CD2	2.11	0.63
1:A:809:THR:HB	1:A:810:PRO:HD2	1.79	0.62
3:C:127:ARG:HG3	3:C:129:ILE:CG2	2.29	0.62
1:A:153:PRO:HA	1:A:161:LEU:HD23	1.80	0.62
2:B:906:SER:HA	2:B:946:ASN:HB2	1.79	0.62
1:A:1178:ASP:HB2	1:A:1179:GLU:HA	1.78	0.62
2:B:71:LEU:HG	2:B:72:GLU:N	2.14	0.62
1:A:1079:MET:SD	1:A:1359:ASP:OD2	2.57	0.62
1:A:679:ILE:O	1:A:682:THR:HG22	2.00	0.62
1:A:731:ARG:HG3	1:A:755:PHE:CE1	2.34	0.62
2:B:459:TYR:C	2:B:459:TYR:HD2	2.08	0.62
2:B:980:PHE:O	2:B:981:ALA:HB3	1.99	0.62
3:C:241:ASP:O	3:C:244:VAL:HG13	1.99	0.62
9:K:46:ILE:O	9:K:50:LEU:HB2	1.98	0.62
11:R:6:G:H2'	11:R:7:A:C8	2.35	0.62
1:A:503:GLN:HE22	5:F:90:ARG:HH21	1.48	0.62
1:A:731:ARG:HG3	1:A:755:PHE:CZ	2.35	0.62
1:A:1246:LYS:CD	1:A:1246:LYS:C	2.73	0.62
1:A:310:GLY:CA	1:A:311:GLN:CB	2.71	0.61
1:A:1253:GLU:O	1:A:1253:GLU:HG2	2.00	0.61
1:A:1256:GLU:O	1:A:1257:ASP:HB2	1.98	0.61
2:B:790:ASP:OD2	2:B:790:ASP:N	2.33	0.61
1:A:1441:PHE:CZ	5:F:89:GLU:HA	2.35	0.61
2:B:190:TYR:CE1	8:J:62:ARG:HG2	2.35	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1172:ILE:HG22	2:B:1174:LYS:HG3	1.83	0.61
1:A:899:VAL:CG2	1:A:1029:ARG:HG2	2.29	0.61
2:B:1065:GLN:HG2	2:B:1069:PHE:HB2	1.82	0.61
2:B:515:HIS:H	2:B:518:HIS:HD2	1.49	0.61
5:F:114:GLU:OE2	5:F:119:ARG:HG3	2.01	0.61
2:B:444:MET:CE	2:B:446:LEU:HD13	2.27	0.61
3:C:15:LYS:HZ1	9:K:114:LEU:HD22	1.66	0.61
1:A:320:ARG:HE	1:A:320:ARG:HA	1.65	0.61
1:A:1167:GLU:C	1:A:1170:ILE:HG22	2.26	0.61
1:A:699:ALA:HB1	7:I:114:GLN:HG3	1.82	0.60
1:A:858:ASN:ND2	1:A:860:LEU:H	1.98	0.60
2:B:239:GLU:HG2	2:B:255:GLN:HG2	1.83	0.60
2:B:636:PRO:HB2	2:B:637:LEU:CA	2.31	0.60
2:B:864:LYS:O	2:B:864:LYS:CD	2.30	0.60
1:A:1081:LEU:C	1:A:1083:THR:CB	2.74	0.60
1:A:466:SER:O	2:B:1103:ILE:HD11	2.01	0.60
1:A:1179:GLU:O	1:A:1179:GLU:HG3	2.01	0.60
1:A:35:ILE:HG22	1:A:270:LEU:HD11	1.82	0.60
2:B:341:LEU:HG	2:B:344:LYS:HE3	1.83	0.60
2:B:744:HIS:HD2	2:B:746:SER:OG	1.85	0.60
2:B:944:THR:HG21	2:B:1122:ARG:HH22	1.66	0.60
1:A:1173:HIS:HD2	1:A:1175:SER:OG	1.85	0.60
4:E:79:TRP:HE1	4:E:81:GLU:HG3	1.67	0.60
6:H:114:VAL:CG2	6:H:125:LEU:HB3	2.31	0.60
1:A:102:VAL:HG11	1:A:211:PHE:HE1	1.67	0.60
1:A:535:THR:HG22	1:A:575:LYS:HG2	1.84	0.60
2:B:282:ILE:HD12	2:B:283:VAL:HG13	1.84	0.60
3:C:186:LEU:HB3	3:C:188:HIS:CD2	2.31	0.60
1:A:1079:MET:SD	1:A:1359:ASP:HB2	2.41	0.60
2:B:864:LYS:HA	2:B:864:LYS:CE	2.25	0.60
1:A:1169:ILE:CB	1:A:1170:ILE:CG1	2.77	0.60
2:B:274:PRO:O	2:B:275:TYR:HB2	2.01	0.60
7:I:98:VAL:HG11	7:I:113:ASP:HB2	1.84	0.60
6:H:4:THR:HA	6:H:60:ALA:HB2	1.84	0.59
1:A:542:GLU:OE1	1:A:569:LYS:NZ	2.35	0.59
1:A:628:GLY:O	1:A:632:VAL:HG23	2.01	0.59
2:B:195:CYS:HB3	2:B:782:LEU:HD22	1.83	0.59
2:B:445:LYS:CA	2:B:447:ALA:H	2.15	0.59
4:E:119:SER:HB2	13:N:12:DT:H5'	1.83	0.59
2:B:341:LEU:CG	2:B:344:LYS:HE3	2.32	0.59
10:L:32:ALA:HB3	10:L:55:ILE:HD11	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:516:ASN:H	2:B:516:ASN:HD22	1.48	0.59
6:H:109:LYS:CB	6:H:111:LEU:H	2.10	0.59
1:A:190:ALA:O	1:A:191:THR:HG23	2.01	0.59
1:A:492:PRO:HB3	1:A:497:THR:HG22	1.83	0.59
1:A:1118:VAL:HG23	1:A:1306:LEU:HB2	1.83	0.59
2:B:308:TRP:HA	2:B:311:LEU:HD12	1.84	0.59
2:B:865:LYS:O	2:B:866:TYR:CD2	2.55	0.59
4:E:119:SER:HB2	13:N:12:DT:H5"	1.84	0.59
5:F:101:ILE:HD13	5:F:120:ILE:CG2	2.33	0.59
1:A:413:ILE:N	1:A:413:ILE:HD12	2.18	0.59
1:A:1178:ASP:CB	1:A:1179:GLU:CA	2.77	0.59
1:A:58:LEU:HG	1:A:80:HIS:HB2	1.84	0.59
1:A:119:ASN:O	1:A:120:GLU:O	2.21	0.59
1:A:1081:LEU:C	1:A:1083:THR:HB	2.27	0.59
1:A:320:ARG:HB3	1:A:321:PRO:HD2	1.83	0.59
11:R:6:G:N3	11:R:7:A:N7	2.51	0.59
1:A:994:GLN:HE22	1:A:1023:ARG:HE	1.49	0.59
1:A:1172:LEU:O	1:A:1173:HIS:C	2.45	0.59
2:B:865:LYS:HD2	2:B:868:MET:HA	1.85	0.59
2:B:986:GLN:HE21	2:B:1022:THR:CG2	2.16	0.59
2:B:1084:GLN:CD	2:B:1084:GLN:H	2.11	0.58
1:A:1170:ILE:O	1:A:1171:GLN:HB2	2.02	0.58
2:B:778:MET:HE1	2:B:1094:ARG:HD3	1.86	0.58
1:A:361:LEU:HD12	1:A:471:ASN:HD22	1.67	0.58
6:H:118:PHE:CZ	6:H:142:LEU:HD23	2.38	0.58
1:A:1081:LEU:O	1:A:1083:THR:HB	1.96	0.58
1:A:1168:GLU:CB	1:A:1171:GLN:HG3	2.33	0.58
6:H:95:TYR:HD2	6:H:95:TYR:C	2.10	0.58
1:A:14:VAL:H	1:A:1432:GLN:NE2	2.02	0.58
1:A:599:SER:HB2	1:A:603:ASN:H	1.68	0.58
1:A:818:MET:HG2	2:B:514:LEU:O	2.04	0.58
3:C:99:LEU:HD23	3:C:120:ILE:HA	1.85	0.58
1:A:35:ILE:HG13	1:A:241:VAL:HG21	1.84	0.58
2:B:445:LYS:HA	2:B:446:LEU:CB	2.04	0.58
2:B:803:LEU:N	2:B:822:ASN:HD21	2.00	0.58
3:C:143:LEU:C	3:C:143:LEU:HD12	2.29	0.58
6:H:109:LYS:HG2	6:H:111:LEU:HD12	1.86	0.58
4:E:100:ILE:HG23	4:E:105:PHE:HB2	1.86	0.58
1:A:53:LEU:CD2	1:A:54:ASN:HB3	2.33	0.58
1:A:1223:ASP:O	1:A:1224:LEU:HB3	2.03	0.58
2:B:652:LYS:HB3	2:B:689:LEU:HD23	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:27:LEU:HD12	3:C:228:PHE:HE2	1.69	0.58
3:C:142:VAL:CG2	3:C:143:LEU:H	2.05	0.58
6:H:95:TYR:C	6:H:95:TYR:CD2	2.81	0.58
1:A:356:ASP:OD2	9:K:65:HIS:HE1	1.87	0.57
1:A:443:LEU:HD23	1:A:444:PHE:H	1.69	0.57
1:A:464:PRO:HB2	1:A:465:TYR:HD1	1.69	0.57
1:A:848:ILE:HD13	1:A:858:ASN:HB3	1.86	0.57
11:R:7:A:H2'	11:R:8:G:H8	1.69	0.57
2:B:438:GLU:HG2	2:B:440:HIS:NE2	2.19	0.57
1:A:53:LEU:HD23	1:A:54:ASN:HB3	1.86	0.57
1:A:1169:ILE:N	1:A:1170:ILE:CG2	2.67	0.57
2:B:628:THR:HG22	2:B:628:THR:O	2.03	0.57
8:J:3:VAL:HG21	8:J:18:TRP:HB2	1.85	0.57
10:L:46:VAL:HG12	10:L:47:ARG:H	1.69	0.57
1:A:809:THR:HB	1:A:810:PRO:CD	2.34	0.57
1:A:913:LEU:HD11	1:A:981:LEU:O	2.04	0.57
1:A:1178:ASP:OD2	1:A:1179:GLU:HA	2.04	0.57
2:B:706:GLN:HB2	2:B:710:LEU:HD23	1.87	0.57
7:I:103:CYS:HB3	7:I:108:HIS:HB3	1.85	0.57
1:A:527:THR:HG21	1:A:650:GLN:HG2	1.86	0.57
1:A:575:LYS:NZ	1:A:615:GLY:O	2.33	0.57
1:A:587:HIS:HE2	1:A:969:GLN:HG2	1.68	0.57
1:A:1085:HIS:CD2	1:A:1085:HIS:N	2.71	0.57
1:A:1089:VAL:O	1:A:1089:VAL:HG13	2.03	0.57
1:A:1169:ILE:N	1:A:1170:ILE:CA	2.51	0.57
1:A:1173:HIS:HD2	1:A:1175:SER:CB	2.16	0.57
2:B:878:GLN:O	2:B:879:ARG:NH2	2.36	0.57
3:C:112:ASN:HD21	3:C:146:LYS:HD3	1.68	0.57
4:E:157:SER:OG	4:E:160:GLU:HB2	2.05	0.57
12:T:26:DG:N3	12:T:27:DA:H1'	2.19	0.57
1:A:1178:ASP:HB2	1:A:1179:GLU:CA	2.35	0.57
1:A:324:SER:OG	1:A:325:ILE:N	2.36	0.57
1:A:900:ASP:HA	1:A:926:GLN:HE22	1.70	0.57
1:A:1015:VAL:HG12	1:A:1019:CYS:SG	2.44	0.57
2:B:274:PRO:HB2	2:B:359:GLU:HB3	1.87	0.57
1:A:979:SER:OG	1:A:980:ASP:N	2.38	0.57
2:B:383:ASN:O	2:B:387:LEU:HB2	2.04	0.57
12:T:26:DG:C2	12:T:27:DA:H1'	2.40	0.57
2:B:716:ASN:O	2:B:717:GLU:CB	2.53	0.57
2:B:863:GLU:CA	2:B:864:LYS:CB	2.30	0.57
2:B:976:ILE:HG23	2:B:977:GLY:N	2.20	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:GLU:HB3	1:A:41:MET:HB2	1.87	0.56
2:B:636:PRO:HB2	2:B:637:LEU:HA	1.87	0.56
1:A:1030:ARG:HG2	1:A:1034:GLU:OE2	2.05	0.56
7:I:63:GLY:HA3	7:I:104:LEU:HD11	1.86	0.56
9:K:73:LEU:CD2	9:K:75:ILE:HD11	2.34	0.56
12:T:25:DC:H2'	12:T:26:DG:H8	1.70	0.56
1:A:902:LEU:HG	1:A:926:GLN:HG3	1.87	0.56
1:A:1072:ILE:O	1:A:1075:PRO:HD2	2.05	0.56
2:B:716:ASN:O	2:B:717:GLU:HB2	2.04	0.56
2:B:980:PHE:CE1	2:B:990:ILE:CG1	2.89	0.56
1:A:645:LEU:O	1:A:646:PHE:C	2.48	0.56
2:B:980:PHE:CZ	2:B:990:ILE:HD11	2.40	0.56
12:T:26:DG:N2	12:T:27:DA:H1'	2.20	0.56
1:A:691:LEU:O	1:A:695:LYS:HB2	2.06	0.56
4:E:184:VAL:O	4:E:187:TYR:N	2.38	0.56
1:A:35:ILE:HG22	1:A:35:ILE:O	2.04	0.56
1:A:485:ASP:OD2	11:R:10:A:C4'	2.50	0.56
2:B:176:SER:O	2:B:182:SER:HB3	2.06	0.56
9:K:63:VAL:HG23	9:K:63:VAL:O	2.05	0.56
2:B:982:SER:HB3	2:B:1092:TYR:CZ	2.41	0.56
4:E:161:LYS:HD2	4:E:195:VAL:HG23	1.87	0.56
1:A:302:THR:HG21	1:A:314:ALA:HB3	1.88	0.56
1:A:444:PHE:CE2	1:A:470:LEU:HD23	2.40	0.56
1:A:901:LEU:HD12	1:A:926:GLN:HG2	1.87	0.56
2:B:315:LYS:HG2	7:I:13:MET:HE1	1.87	0.56
2:B:1001:PHE:HE1	3:C:178:PHE:HB3	1.71	0.56
1:A:1169:ILE:N	1:A:1170:ILE:HG22	2.21	0.56
2:B:63:ILE:HD12	2:B:421:PHE:CE2	2.41	0.56
2:B:865:LYS:CB	2:B:870:ILE:O	2.54	0.56
4:E:28:TYR:HA	4:E:64:PRO:HA	1.88	0.56
6:H:40:LEU:HD12	6:H:41:ASP:H	1.71	0.56
1:A:58:LEU:HD21	1:A:244:PRO:CD	2.36	0.56
1:A:587:HIS:NE2	1:A:969:GLN:HG2	2.20	0.56
1:A:255:SER:HA	1:A:256:GLN:C	2.31	0.55
1:A:298:PHE:CE1	1:A:313:GLN:HG3	2.41	0.55
1:A:566:ILE:O	1:A:566:ILE:CG2	2.50	0.55
1:A:765:VAL:CG2	1:A:800:VAL:HB	2.36	0.55
1:A:890:ASP:H	1:A:1296:GLY:HA3	1.70	0.55
2:B:635:ARG:HB2	2:B:636:PRO:HD2	1.88	0.55
2:B:65:GLU:HG2	2:B:66:ASP:N	2.21	0.55
2:B:102:VAL:HG12	2:B:112:LEU:HB2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1166:CYS:O	2:B:1215:ARG:HD2	2.06	0.55
1:A:981:LEU:HD21	1:A:1039:LYS:HA	1.86	0.55
1:A:1017:LEU:HB2	4:E:206:GLY:H	1.70	0.55
2:B:221:ASN:OD1	2:B:242:SER:HA	2.06	0.55
2:B:516:ASN:H	2:B:516:ASN:ND2	2.04	0.55
6:H:107:VAL:O	6:H:109:LYS:HG3	2.06	0.55
1:A:455:MET:HE1	2:B:1130:PHE:CE1	2.41	0.55
1:A:1192:LEU:HG	1:A:1193:LEU:N	2.21	0.55
2:B:445:LYS:CB	2:B:447:ALA:H	2.19	0.55
2:B:637:LEU:HD11	2:B:740:HIS:HB3	1.88	0.55
3:C:127:ARG:HG3	3:C:129:ILE:HG21	1.89	0.55
1:A:56:PRO:C	1:A:58:LEU:N	2.63	0.55
1:A:424:ILE:O	1:A:424:ILE:CG2	2.55	0.55
1:A:821:ARG:O	1:A:825:ILE:HG12	2.06	0.55
1:A:31:SER:HB2	1:A:81:PHE:O	2.07	0.55
1:A:161:LEU:HD22	1:A:161:LEU:C	2.28	0.55
1:A:540:PHE:HB3	1:A:571:LEU:HD23	1.88	0.55
1:A:1169:ILE:H	1:A:1170:ILE:CG2	2.20	0.55
2:B:63:ILE:HG12	2:B:95:ILE:HD12	1.89	0.55
2:B:880:THR:HB	2:B:934:LYS:HB2	1.89	0.55
11:R:3:C:H42	12:T:26:DG:H1	1.52	0.55
1:A:185:TRP:O	1:A:186:LYS:CB	2.54	0.55
1:A:404:TYR:HA	1:A:413:ILE:O	2.07	0.55
1:A:1134:ILE:O	1:A:1138:ILE:HG12	2.06	0.55
2:B:1120:GLU:HG2	2:B:1121:GLY:H	1.71	0.55
3:C:148:ARG:HH22	8:J:64:ASN:ND2	2.05	0.55
2:B:523:CYS:SG	2:B:750:GLY:N	2.79	0.55
3:C:43:THR:CG2	3:C:44:LEU:N	2.69	0.55
7:I:17:ARG:HH11	7:I:17:ARG:HB2	1.71	0.55
8:J:45:CYS:SG	8:J:46:CYS:SG	3.03	0.55
9:K:70:ARG:O	9:K:70:ARG:HG3	2.06	0.55
1:A:109:HIS:HB2	1:A:167:CYS:SG	2.47	0.55
1:A:567:LYS:CD	1:A:568:PRO:HD2	2.36	0.55
2:B:31:TRP:CE3	2:B:34:ILE:HD12	2.42	0.55
2:B:717:GLU:O	2:B:718:GLU:C	2.50	0.55
1:A:901:LEU:N	1:A:926:GLN:HE21	2.05	0.55
1:A:194:ALA:C	1:A:195:ASP:OD2	2.50	0.54
1:A:535:THR:O	1:A:575:LYS:HE2	2.07	0.54
1:A:917:SER:O	1:A:918:GLU:HG3	2.07	0.54
2:B:334:ILE:HG22	2:B:334:ILE:O	2.07	0.54
1:A:824:LEU:O	11:R:12:G:N2	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:836:TYR:CE2	1:A:840:ARG:HD2	2.42	0.54
1:A:1219:THR:HG21	1:A:1271:ILE:HD11	1.90	0.54
1:A:875:ALA:HA	1:A:878:ILE:HD12	1.90	0.54
1:A:913:LEU:HD12	1:A:914:GLU:H	1.73	0.54
2:B:868:MET:C	2:B:869:SER:OG	2.51	0.54
2:B:1084:GLN:HG2	3:C:201:TRP:CZ2	2.42	0.54
1:A:277:GLU:O	1:A:281:HIS:HD2	1.90	0.54
1:A:444:PHE:HE2	1:A:470:LEU:HD23	1.73	0.54
1:A:1092:LYS:HG3	1:A:1094:VAL:O	2.08	0.54
2:B:843:GLN:HG2	2:B:993:THR:CB	2.35	0.54
2:B:1149:GLU:C	2:B:1151:LEU:H	2.15	0.54
3:C:3:GLU:HG2	9:K:100:ALA:HB1	1.90	0.54
3:C:124:LEU:C	3:C:126:GLY:N	2.65	0.54
8:J:9:SER:OG	8:J:45:CYS:HB2	2.07	0.54
1:A:351:THR:HG22	1:A:352:VAL:O	2.08	0.54
1:A:369:SER:HB2	9:K:2:ASN:OD1	2.08	0.54
3:C:27:LEU:HD12	3:C:228:PHE:CE2	2.41	0.54
3:C:69:LEU:H	3:C:69:LEU:HD23	1.73	0.54
1:A:151:ASP:HB2	1:A:162:VAL:O	2.08	0.54
1:A:1169:ILE:CG2	1:A:1170:ILE:CB	2.86	0.54
2:B:65:GLU:CG	2:B:66:ASP:N	2.69	0.54
12:T:13:DA:H61	13:N:2:DT:C7	2.20	0.54
1:A:332:LYS:H	1:A:337:ARG:HB3	1.72	0.54
11:R:7:A:H2'	11:R:8:G:C8	2.43	0.54
1:A:834:THR:HG21	1:A:1077:THR:HA	1.90	0.54
2:B:363:HIS:O	2:B:364:ILE:HB	2.06	0.54
2:B:955:THR:HG23	10:L:54:ARG:O	2.08	0.54
2:B:981:ALA:C	2:B:1092:TYR:CE2	2.86	0.54
2:B:1163:CYS:HB3	2:B:1167:GLY:H	1.72	0.54
7:I:34:TYR:OH	7:I:36:GLU:HB3	2.07	0.54
8:J:3:VAL:HG21	8:J:18:TRP:CG	2.43	0.54
1:A:343:LYS:HZ1	2:B:1197:PRO:HB3	1.71	0.54
1:A:769:SER:OG	1:A:1085:HIS:CE1	2.60	0.54
2:B:784:ASN:CG	2:B:788:ARG:HD2	2.32	0.54
1:A:1253:GLU:O	1:A:1253:GLU:HG3	2.08	0.53
2:B:906:SER:HA	2:B:946:ASN:HB3	1.90	0.53
1:A:188:ASP:C	1:A:189:ARG:CG	2.80	0.53
1:A:351:THR:HG23	1:A:352:VAL:H	1.72	0.53
1:A:1319:VAL:HG12	1:A:1322:ILE:HG23	1.90	0.53
2:B:132:VAL:HG21	2:B:445:LYS:HZ1	1.72	0.53
3:C:52:GLU:HB3	3:C:154:LYS:HB3	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:K:6:ARG:C	9:K:8:GLU:H	2.16	0.53
1:A:871:ASP:OD1	1:A:1366:ARG:NH2	2.41	0.53
1:A:1084:PHE:N	1:A:1084:PHE:CD1	2.74	0.53
1:A:1259:MET:O	1:A:1262:LYS:N	2.40	0.53
2:B:445:LYS:HB3	2:B:447:ALA:CB	2.38	0.53
2:B:982:SER:OG	2:B:983:ARG:N	2.30	0.53
3:C:165:LYS:O	9:K:6:ARG:NH1	2.40	0.53
6:H:93:TYR:CD1	6:H:143:LEU:HD23	2.42	0.53
1:A:907:THR:HG22	1:A:908:LEU:N	2.22	0.53
1:A:53:LEU:HD23	1:A:54:ASN:CA	2.38	0.53
1:A:549:MET:HE1	1:A:656:TRP:HD1	1.73	0.53
1:A:630:ILE:HD12	1:A:630:ILE:N	2.23	0.53
1:A:1030:ARG:C	1:A:1032:LEU:H	2.16	0.53
1:A:1079:MET:CE	1:A:1359:ASP:CB	2.78	0.53
1:A:658:LEU:HG	1:A:659:HIS:CD2	2.44	0.53
1:A:1220:PHE:O	1:A:1221:LYS:HB2	2.09	0.53
2:B:560:GLU:O	2:B:561:TRP:CD1	2.62	0.53
1:A:1094:VAL:HA	1:A:1113:THR:HG21	1.90	0.53
3:C:45:ALA:HA	3:C:72:LEU:HD12	1.90	0.53
1:A:53:LEU:HD23	1:A:54:ASN:CB	2.38	0.53
1:A:302:THR:HG23	1:A:306:ASN:HB3	1.91	0.53
3:C:94:LYS:HE2	3:C:125:MET:HE1	1.90	0.53
1:A:1092:LYS:CB	1:A:1093:LYS:HA	2.39	0.53
1:A:14:VAL:HB	1:A:1432:GLN:HE22	1.73	0.53
1:A:402:ALA:O	1:A:415:LEU:HD12	2.09	0.53
3:C:102:GLN:HG2	3:C:154:LYS:CD	2.38	0.53
4:E:79:TRP:NE1	4:E:81:GLU:HG3	2.23	0.53
7:I:14:LEU:HB3	7:I:27:PHE:HB3	1.89	0.53
8:J:10:CYS:SG	8:J:46:CYS:SG	3.07	0.53
1:A:423:ASP:O	1:A:424:ILE:CB	2.55	0.52
1:A:573:SER:O	1:A:576:GLN:HB2	2.09	0.52
1:A:1081:LEU:O	1:A:1083:THR:HG21	2.09	0.52
1:A:1092:LYS:HB3	1:A:1093:LYS:CA	2.39	0.52
2:B:338:GLY:H	2:B:341:LEU:HD21	1.73	0.52
2:B:793:ALA:C	2:B:794:ASN:HD22	2.17	0.52
3:C:73:GLN:HE21	3:C:75:MET:N	2.07	0.52
6:H:8:ASP:HB3	6:H:10:PHE:CE1	2.45	0.52
1:A:565:ILE:HG23	1:A:567:LYS:HG2	1.91	0.52
2:B:64:CYS:O	2:B:65:GLU:CB	2.55	0.52
5:F:99:LEU:HD13	5:F:99:LEU:O	2.09	0.52
1:A:449:SER:OG	2:B:1134:GLU:OE2	2.23	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:842:ASN:HD22	2:B:845:SER:HB3	1.73	0.52
6:H:26:ILE:HG22	6:H:40:LEU:O	2.09	0.52
6:H:36:CYS:HA	6:H:126:GLU:O	2.09	0.52
1:A:265:LYS:HA	1:A:268:ASP:HB2	1.91	0.52
1:A:470:LEU:CD2	1:A:487:MET:HE1	2.32	0.52
1:A:1082:ASN:HA	1:A:1083:THR:HB	0.66	0.52
7:I:80:SER:HB3	7:I:105:SER:HB2	1.91	0.52
1:A:343:LYS:HE2	2:B:1151:LEU:HD23	1.91	0.52
1:A:388:LEU:HA	1:A:391:LEU:HD12	1.91	0.52
2:B:273:LEU:HD21	2:B:360:PHE:CD1	2.36	0.52
2:B:567:GLU:H	2:B:567:GLU:CD	2.17	0.52
2:B:865:LYS:HG2	2:B:867:GLY:C	2.34	0.52
5:F:82:THR:HG22	5:F:84:TYR:H	1.75	0.52
1:A:548:ASN:OD1	9:K:60:ALA:HB1	2.09	0.52
1:A:874:ASP:N	1:A:1058:VAL:HG23	2.25	0.52
4:E:88:VAL:HG21	4:E:116:ILE:HD13	1.92	0.52
4:E:180:ARG:HB2	4:E:215:MET:OXT	2.10	0.52
7:I:80:SER:CB	7:I:105:SER:HB2	2.39	0.52
7:I:111:THR:HG22	7:I:113:ASP:H	1.74	0.52
1:A:567:LYS:HZ2	6:H:46:LEU:HB2	1.74	0.52
1:A:1281:ARG:HG3	1:A:1281:ARG:O	2.09	0.52
2:B:85:SER:CA	2:B:86:ARG:HB3	2.40	0.52
2:B:712:PRO:O	2:B:713:ALA:HB2	2.10	0.52
1:A:382:PRO:HG3	1:A:428:TYR:CE2	2.45	0.52
1:A:567:LYS:HD3	1:A:568:PRO:HD2	1.91	0.52
1:A:890:ASP:OD2	1:A:1296:GLY:HA2	2.09	0.52
2:B:434:ARG:HA	2:B:437:GLU:HG3	1.92	0.52
2:B:879:ARG:HA	2:B:879:ARG:CZ	2.38	0.52
3:C:71:PRO:O	3:C:133:ILE:HG13	2.09	0.52
7:I:111:THR:HG22	7:I:112:SER:N	2.25	0.52
6:H:62:SER:O	6:H:63:LEU:O	2.27	0.52
1:A:507:VAL:HG12	1:A:521:MET:HE1	1.92	0.52
3:C:69:LEU:N	3:C:69:LEU:CD2	2.73	0.52
3:C:259:LEU:HD21	9:K:92:ASN:OD1	2.10	0.52
1:A:346:ASP:OD1	1:A:346:ASP:N	2.43	0.51
1:A:452:LYS:HB2	2:B:1141:HIS:CE1	2.44	0.51
2:B:428:ILE:O	2:B:432:MET:HG3	2.10	0.51
2:B:464:GLY:HA3	2:B:479:VAL:O	2.10	0.51
3:C:249:ASP:O	3:C:253:LYS:HG3	2.10	0.51
11:R:11:U:H5'	11:R:12:G:OP2	2.09	0.51
1:A:153:PRO:C	1:A:155:GLU:H	2.17	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:487:THR:HG22	2:B:488:TYR:N	2.24	0.51
2:B:616:ILE:HD12	2:B:616:ILE:N	2.25	0.51
2:B:636:PRO:O	2:B:691:GLU:O	2.26	0.51
6:H:96:VAL:HG12	6:H:97:MET:N	2.25	0.51
1:A:1407:GLU:CD	1:A:1407:GLU:H	2.18	0.51
2:B:475:SER:O	2:B:477:ALA:N	2.44	0.51
2:B:712:PRO:HD2	2:B:713:ALA:H	1.76	0.51
9:K:10:PHE:N	9:K:10:PHE:CD2	2.78	0.51
1:A:56:PRO:C	1:A:58:LEU:H	2.18	0.51
1:A:172:PRO:HD3	1:A:185:TRP:HE1	1.75	0.51
1:A:353:ILE:HD13	1:A:487:MET:CE	2.27	0.51
1:A:666:ILE:CD1	1:A:666:ILE:N	2.72	0.51
2:B:979:LYS:HG2	2:B:1095:LEU:HD12	1.93	0.51
3:C:100:THR:HG22	3:C:119:VAL:HB	1.93	0.51
1:A:1254:ALA:O	1:A:1255:GLU:CG	2.59	0.51
2:B:780:VAL:HG12	2:B:817:LEU:HD23	1.91	0.51
7:I:16:PRO:HG3	7:I:27:PHE:CE2	2.46	0.51
2:B:341:LEU:HB3	2:B:344:LYS:CE	2.36	0.51
2:B:444:MET:O	2:B:445:LYS:HG3	2.10	0.51
2:B:1181:GLU:HA	2:B:1187:ASN:O	2.10	0.51
5:F:73:ALA:HB2	5:F:143:PHE:CZ	2.46	0.51
1:A:662:PHE:HB3	2:B:829:CYS:SG	2.51	0.51
2:B:417:PHE:CE1	2:B:453:ILE:HD13	2.46	0.51
2:B:784:ASN:OD1	2:B:788:ARG:HD2	2.11	0.51
3:C:47:ASP:HA	10:L:69:ALA:CB	2.34	0.51
4:E:9:ILE:HD12	4:E:53:PRO:HG3	1.93	0.51
4:E:179:GLN:O	4:E:182:ASP:HB2	2.11	0.51
8:J:3:VAL:HG21	8:J:18:TRP:CB	2.40	0.51
2:B:841:MET:HE1	2:B:980:PHE:CE1	2.33	0.51
10:L:60:ARG:HG3	10:L:61:THR:H	1.75	0.51
1:A:779:PHE:CZ	2:B:517:THR:HA	2.46	0.51
2:B:515:HIS:CD2	2:B:517:THR:H	2.24	0.51
1:A:1193:LEU:HD21	1:A:1267:MET:HE2	1.93	0.51
2:B:886:LYS:HB2	2:B:890:TYR:OH	2.11	0.51
2:B:1174:LYS:HB2	2:B:1179:GLN:O	2.11	0.51
11:R:6:G:C2	11:R:7:A:C8	2.98	0.51
1:A:738:LYS:HZ1	3:C:194:GLU:HA	1.75	0.50
2:B:87:LYS:NZ	2:B:436:VAL:HG11	2.26	0.50
3:C:82:TYR:HB2	3:C:85:ASP:OD2	2.11	0.50
1:A:392:VAL:HG11	1:A:424:ILE:HG21	1.92	0.50
2:B:440:HIS:C	2:B:442:PHE:N	2.68	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:941:LEU:HD22	2:B:942:ARG:H	1.76	0.50
3:C:148:ARG:HH22	8:J:64:ASN:HD22	1.59	0.50
6:H:44:VAL:HG13	6:H:48:PRO:HA	1.92	0.50
7:I:5:ARG:HG3	7:I:6:PHE:H	1.76	0.50
9:K:47:ARG:HD2	9:K:60:ALA:HA	1.93	0.50
1:A:160:GLN:N	1:A:160:GLN:OE1	2.43	0.50
2:B:488:TYR:C	2:B:490:SER:H	2.19	0.50
3:C:133:ILE:CD1	3:C:237:SER:HA	2.42	0.50
8:J:43:ARG:HH11	8:J:43:ARG:HB3	1.76	0.50
8:J:44:TYR:CD1	8:J:44:TYR:C	2.89	0.50
1:A:765:VAL:HG13	1:A:802:ASN:O	2.12	0.50
2:B:464:GLY:CA	2:B:479:VAL:O	2.60	0.50
2:B:982:SER:O	2:B:1093:GLN:HG3	2.12	0.50
7:I:83:ASN:O	7:I:83:ASN:ND2	2.43	0.50
1:A:1236:LEU:C	1:A:1237:ILE:HG13	2.35	0.50
1:A:1429:ILE:HG22	1:A:1429:ILE:O	2.12	0.50
2:B:1142:GLY:HA3	5:F:88:TYR:HE2	1.77	0.50
3:C:228:PHE:CD1	3:C:228:PHE:N	2.80	0.50
3:C:244:VAL:O	3:C:248:ILE:HG13	2.11	0.50
4:E:161:LYS:HD2	4:E:195:VAL:CG2	2.42	0.50
6:H:142:LEU:HD12	6:H:142:LEU:C	2.37	0.50
1:A:338:GLY:HA2	2:B:1129:ARG:HH22	1.76	0.50
1:A:1449:SER:HA	1:A:1450:LEU:C	2.37	0.50
2:B:620:ARG:NE	7:I:89:GLN:HE22	2.10	0.50
2:B:791:THR:O	2:B:792:MET:HB2	2.10	0.50
3:C:162:GLY:HA3	3:C:170:TRP:CE2	2.46	0.50
7:I:78:CYS:O	7:I:79:HIS:CB	2.59	0.50
1:A:125:ALA:O	1:A:128:ILE:HG22	2.12	0.50
1:A:242:PRO:HG3	2:B:1209:ALA:HB1	1.94	0.50
1:A:323:LYS:O	1:A:324:SER:HB3	2.11	0.50
1:A:567:LYS:HE2	6:H:95:TYR:CZ	2.47	0.50
1:A:1146:VAL:O	1:A:1197:LEU:HD23	2.12	0.50
2:B:115:GLN:HG2	2:B:193:LYS:HB2	1.94	0.50
5:F:76:LYS:O	5:F:77:ASP:O	2.30	0.50
1:A:526:ASP:HB2	2:B:835:GLN:CD	2.37	0.50
1:A:715:GLU:O	1:A:719:VAL:HG23	2.12	0.50
1:A:775:ILE:HB	1:A:797:LYS:C	2.36	0.50
1:A:1081:LEU:C	1:A:1083:THR:HG1	2.18	0.50
1:A:1410:PHE:HD2	2:B:1212:ILE:HD11	1.77	0.50
2:B:662:MET:C	2:B:664:THR:H	2.19	0.50
2:B:830:TYR:O	2:B:831:SER:OG	2.28	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:482:PHE:CE1	2:B:836:GLU:HB2	2.47	0.49
1:A:531:ILE:HG12	1:A:531:ILE:O	2.12	0.49
1:A:668:ASP:OD2	1:A:742:ASN:HB2	2.12	0.49
1:A:873:MET:HE3	1:A:957:PRO:HG2	1.94	0.49
1:A:1167:GLU:O	1:A:1170:ILE:O	2.30	0.49
1:A:1392:SER:O	1:A:1393:ASN:C	2.54	0.49
2:B:71:LEU:HG	2:B:72:GLU:HB2	1.93	0.49
2:B:308:TRP:O	2:B:311:LEU:N	2.45	0.49
2:B:558:LEU:C	2:B:560:GLU:H	2.19	0.49
2:B:964:VAL:HG12	2:B:965:LYS:N	2.26	0.49
4:E:185:ALA:HA	4:E:190:LEU:HD23	1.92	0.49
2:B:791:THR:O	2:B:792:MET:CB	2.59	0.49
7:I:10:CYS:O	7:I:11:ASN:HB3	2.12	0.49
9:K:32:VAL:O	9:K:32:VAL:HG13	2.12	0.49
1:A:249:SER:C	1:A:250:ILE:HG13	2.36	0.49
1:A:719:VAL:O	1:A:723:ASN:ND2	2.45	0.49
1:A:1227:ILE:HG22	1:A:1228:TRP:H	1.77	0.49
3:C:241:ASP:HB3	9:K:109:TRP:CZ2	2.47	0.49
4:E:205:SER:O	4:E:206:GLY:C	2.56	0.49
2:B:386:LEU:C	2:B:388:CYS:H	2.19	0.49
2:B:440:HIS:O	2:B:442:PHE:N	2.45	0.49
3:C:67:LEU:HD11	3:C:155:LEU:HD13	1.94	0.49
4:E:94:LYS:HE2	4:E:94:LYS:HA	1.95	0.49
1:A:1002:GLY:HA3	1:A:1007:ILE:HG21	1.94	0.49
1:A:1092:LYS:H	1:A:1093:LYS:HA	1.78	0.49
1:A:1119:TYR:CD1	1:A:1326:ARG:HB3	2.48	0.49
2:B:301:ILE:HG22	2:B:302:CYS:N	2.27	0.49
2:B:980:PHE:CE1	2:B:990:ILE:HG13	2.48	0.49
1:A:1081:LEU:O	1:A:1083:THR:OG1	2.30	0.49
1:A:1364:ASN:OD1	1:A:1366:ARG:HD2	2.13	0.49
2:B:340:ALA:O	2:B:342:GLY:N	2.44	0.49
2:B:541:LEU:HB2	2:B:747:MET:HE3	1.95	0.49
2:B:807:ARG:HG2	2:B:1045:SER:OG	2.12	0.49
7:I:103:CYS:CB	7:I:108:HIS:HB3	2.42	0.49
8:J:44:TYR:HA	8:J:47:ARG:HB2	1.95	0.49
1:A:39:GLU:HB3	1:A:41:MET:CB	2.41	0.49
1:A:295:LEU:HA	1:A:298:PHE:HB3	1.94	0.49
1:A:313:GLN:HG2	1:A:314:ALA:CA	2.42	0.49
1:A:1131:ALA:HA	1:A:1134:ILE:HD12	1.94	0.49
1:A:413:ILE:N	1:A:413:ILE:CD1	2.75	0.49
1:A:465:TYR:N	1:A:465:TYR:CD1	2.81	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:590:ARG:O	1:A:591:PHE:HB2	2.13	0.49
3:C:233:GLU:OE1	8:J:12:LYS:HG3	2.13	0.49
7:I:85:PHE:HB3	7:I:101:PHE:CD2	2.48	0.49
12:T:26:DG:H21	12:T:27:DA:H1'	1.78	0.49
1:A:198:GLU:N	1:A:198:GLU:OE2	2.39	0.49
1:A:873:MET:C	1:A:1058:VAL:HG23	2.37	0.49
1:A:1081:LEU:O	1:A:1083:THR:CG2	2.60	0.49
6:H:4:THR:HA	6:H:60:ALA:CB	2.43	0.49
1:A:188:ASP:C	1:A:189:ARG:HG3	2.38	0.49
1:A:523:ILE:HG23	1:A:527:THR:OG1	2.13	0.49
1:A:1406:VAL:HG12	1:A:1410:PHE:CE1	2.48	0.49
1:A:1443:VAL:C	1:A:1444:MET:HG2	2.38	0.49
2:B:620:ARG:HE	7:I:89:GLN:HE22	1.60	0.49
3:C:129:ILE:HG13	3:C:130:GLY:N	2.28	0.49
8:J:36:LEU:HD13	8:J:47:ARG:HG2	1.94	0.49
9:K:61:TYR:HA	9:K:72:LYS:O	2.13	0.49
1:A:118:HIS:NE2	1:A:155:GLU:CG	2.76	0.48
1:A:814:PHE:O	1:A:817:ALA:HB3	2.13	0.48
1:A:1017:LEU:HB2	4:E:205:SER:HA	1.95	0.48
2:B:287:ARG:HA	2:B:291:ILE:O	2.13	0.48
2:B:464:GLY:HA2	2:B:480:SER:HB3	1.95	0.48
3:C:251:LEU:O	3:C:255:VAL:HG23	2.12	0.48
5:F:133:VAL:HG13	5:F:133:VAL:O	2.12	0.48
6:H:38:LEU:HD13	6:H:125:LEU:HD13	1.95	0.48
7:I:10:CYS:SG	7:I:11:ASN:N	2.85	0.48
1:A:18:GLN:O	2:B:1215:ARG:HG2	2.13	0.48
1:A:185:TRP:O	1:A:186:LYS:CG	2.61	0.48
2:B:859:TYR:OH	2:B:941:LEU:HD22	2.13	0.48
5:F:93:ILE:CD1	5:F:134:ILE:HD11	2.26	0.48
6:H:78:SER:O	6:H:79:TRP:C	2.56	0.48
1:A:351:THR:HG22	1:A:352:VAL:N	2.28	0.48
1:A:1287:TYR:CD2	1:A:1305:VAL:HG21	2.48	0.48
2:B:794:ASN:C	2:B:795:ILE:HD12	2.38	0.48
3:C:241:ASP:HB3	9:K:109:TRP:CE2	2.48	0.48
5:F:97:ARG:HD2	5:F:101:ILE:HG13	1.96	0.48
1:A:296:LEU:O	1:A:300:VAL:HG23	2.13	0.48
1:A:402:ALA:HB2	1:A:434:ARG:HA	1.94	0.48
1:A:1057:VAL:HG12	1:A:1058:VAL:O	2.12	0.48
2:B:1098:MET:O	2:B:1099:VAL:C	2.55	0.48
3:C:35:ARG:NH1	9:K:41:THR:OG1	2.47	0.48
4:E:29:PHE:C	4:E:30:ILE:HG13	2.38	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:107:CYS:SG	1:A:108:MET:N	2.86	0.48
1:A:1340:GLY:H	4:E:183:PRO:HG2	1.78	0.48
9:K:7:PHE:CD1	9:K:7:PHE:C	2.91	0.48
1:A:591:PHE:HA	1:A:595:THR:HG21	1.95	0.48
1:A:738:LYS:HZ3	3:C:194:GLU:HA	1.78	0.48
1:A:942:PHE:C	1:A:942:PHE:CD2	2.90	0.48
2:B:64:CYS:SG	2:B:65:GLU:N	2.86	0.48
2:B:1175:LEU:HD23	2:B:1176:ASN:N	2.29	0.48
8:J:43:ARG:HB3	8:J:43:ARG:NH1	2.29	0.48
10:L:32:ALA:CB	10:L:55:ILE:HD11	2.44	0.48
1:A:17:VAL:HB	1:A:1419:ASP:HB3	1.94	0.48
1:A:575:LYS:HB3	1:A:612:ILE:CD1	2.36	0.48
2:B:31:TRP:O	2:B:32:ALA:C	2.57	0.48
3:C:167:HIS:CD2	3:C:168:ALA:N	2.81	0.48
1:A:46:THR:C	1:A:48:ALA:H	2.21	0.48
1:A:244:PRO:HB2	1:A:245:PRO:HD3	1.95	0.48
1:A:784:LEU:HB3	1:A:786:HIS:HD2	1.78	0.48
2:B:35:SER:HB3	2:B:811:TYR:CE2	2.49	0.48
2:B:337:ARG:NH1	2:B:344:LYS:NZ	2.62	0.48
2:B:745:PRO:C	2:B:747:MET:N	2.70	0.48
2:B:820:GLY:N	2:B:1091:TYR:OH	2.47	0.48
3:C:29:MET:HE2	9:K:45:LEU:HD11	1.95	0.48
1:A:1119:TYR:HD1	1:A:1326:ARG:HB3	1.79	0.48
1:A:1376:THR:HG22	4:E:212:ARG:HH22	1.78	0.48
2:B:717:GLU:O	2:B:720:ASP:N	2.47	0.48
2:B:868:MET:O	2:B:869:SER:OG	2.30	0.48
9:K:65:HIS:CD2	9:K:67:PHE:HB2	2.43	0.48
1:A:402:ALA:HA	1:A:435:HIS:HD2	1.79	0.48
1:A:417:TYR:HB2	1:A:418:SER:H	1.52	0.48
1:A:877:HIS:C	1:A:878:ILE:HG13	2.38	0.48
1:A:900:ASP:HA	1:A:926:GLN:NE2	2.28	0.48
1:A:1171:GLN:CD	1:A:1171:GLN:O	2.57	0.48
2:B:25:ILE:HD11	2:B:653:VAL:HB	1.95	0.48
8:J:11:GLY:O	8:J:12:LYS:C	2.56	0.48
1:A:1188:GLN:O	1:A:1244:ARG:HD3	2.14	0.47
1:A:1447:GLU:C	1:A:1449:SER:H	2.22	0.47
2:B:129:PHE:CE2	2:B:166:PHE:HB2	2.49	0.47
2:B:445:LYS:CA	2:B:446:LEU:CB	2.78	0.47
2:B:636:PRO:HB2	2:B:637:LEU:CB	2.41	0.47
2:B:1017:ILE:HB	2:B:1018:PRO:HD3	1.96	0.47
2:B:1106:ARG:HH11	2:B:1126:GLY:HA2	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:62:ALA:N	4:E:78:LEU:O	2.47	0.47
5:F:118:LEU:O	5:F:122:MET:HG3	2.14	0.47
1:A:444:PHE:HE2	1:A:470:LEU:CD2	2.26	0.47
1:A:540:PHE:CE1	6:H:43:ASN:ND2	2.82	0.47
1:A:1243:VAL:HG13	1:A:1244:ARG:HB2	1.95	0.47
2:B:860:MET:SD	2:B:861:ASP:N	2.88	0.47
7:I:32:CYS:SG	7:I:33:SER:N	2.86	0.47
1:A:6:TYR:O	2:B:1175:LEU:HD21	2.14	0.47
1:A:598:LEU:HB3	6:H:25:ARG:HH12	1.78	0.47
7:I:105:SER:O	7:I:106:CYS:CB	2.52	0.47
1:A:208:LEU:HB2	1:A:235:ILE:HD11	1.96	0.47
2:B:485:ARG:HG2	2:B:485:ARG:HH11	1.79	0.47
3:C:238:ILE:HG22	3:C:239:PRO:O	2.14	0.47
1:A:53:LEU:CD2	1:A:54:ASN:CB	2.91	0.47
1:A:184:SER:HB2	1:A:199:LEU:HD23	1.97	0.47
1:A:1172:LEU:C	1:A:1174:PHE:N	2.72	0.47
2:B:910:VAL:HG13	2:B:938:SER:OG	2.13	0.47
1:A:679:ILE:HA	1:A:682:THR:HG22	1.97	0.47
2:B:438:GLU:HG2	2:B:440:HIS:CD2	2.49	0.47
2:B:1103:ILE:O	2:B:1122:ARG:NH1	2.47	0.47
3:C:167:HIS:CD2	3:C:167:HIS:C	2.91	0.47
1:A:4:GLN:O	1:A:5:GLN:HG3	2.14	0.47
1:A:67:CYS:O	1:A:70:CYS:HB2	2.14	0.47
1:A:470:LEU:HD21	1:A:487:MET:HE3	1.89	0.47
1:A:1436:ILE:O	1:A:1437:GLY:C	2.56	0.47
2:B:69:LEU:H	2:B:90:ILE:HG22	1.79	0.47
2:B:591:ARG:O	2:B:592:ASN:HB3	2.14	0.47
2:B:680:THR:O	2:B:683:SER:OG	2.32	0.47
4:E:27:GLY:O	4:E:65:THR:HG22	2.15	0.47
6:H:142:LEU:HD12	6:H:143:LEU:N	2.29	0.47
11:R:6:G:N1	11:R:7:A:C5	2.83	0.47
1:A:91:PHE:H	1:A:297:GLN:NE2	2.10	0.47
1:A:302:THR:O	1:A:324:SER:HB2	2.15	0.47
1:A:306:ASN:HB2	1:A:313:GLN:OE1	2.15	0.47
1:A:1253:GLU:O	1:A:1255:GLU:HG2	2.14	0.47
1:A:1428:VAL:C	1:A:1430:LEU:H	2.23	0.47
2:B:999:MET:HG2	2:B:1007:VAL:HG13	1.95	0.47
2:B:1082:MET:HA	3:C:189:THR:HA	1.97	0.47
7:I:99:LEU:O	7:I:111:THR:HG23	2.15	0.47
1:A:203:SER:O	1:A:207:ILE:HG13	2.15	0.47
1:A:254:GLU:HG3	2:B:918:ILE:HG21	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:445:LYS:HA	2:B:447:ALA:H	1.79	0.47
3:C:183:TRP:H	3:C:183:TRP:CD1	2.31	0.47
4:E:36:GLU:O	4:E:38:PRO:HD3	2.15	0.47
1:A:1116:LEU:HD13	1:A:1329:THR:OG1	2.15	0.47
1:A:1169:ILE:H	1:A:1170:ILE:HG22	1.78	0.47
2:B:232:SER:C	2:B:261:ARG:HH21	2.22	0.47
9:K:18:LYS:HD3	9:K:18:LYS:O	2.14	0.47
11:R:5:A:N3	11:R:6:G:C8	2.83	0.47
1:A:147:VAL:HG12	1:A:170:THR:HG22	1.97	0.46
1:A:203:SER:O	1:A:207:ILE:CD1	2.63	0.46
1:A:265:LYS:HE2	1:A:303:TYR:HA	1.97	0.46
1:A:317:LYS:HD2	1:A:317:LYS:N	2.30	0.46
1:A:1253:GLU:O	1:A:1254:ALA:O	2.33	0.46
1:A:1444:MET:HB2	5:F:133:VAL:CG1	2.45	0.46
2:B:98:THR:HG21	2:B:101:MET:HE2	1.96	0.46
2:B:973:ILE:O	2:B:975:GLN:N	2.48	0.46
8:J:37:SER:OG	8:J:47:ARG:NH2	2.48	0.46
9:K:43:GLY:HA2	9:K:71:PHE:CE1	2.51	0.46
1:A:13:THR:HG22	1:A:14:VAL:N	2.30	0.46
1:A:1044:TRP:O	1:A:1045:VAL:C	2.58	0.46
1:A:1245:PRO:O	1:A:1246:LYS:CG	2.61	0.46
7:I:11:ASN:CG	7:I:11:ASN:O	2.58	0.46
7:I:75:CYS:SG	7:I:103:CYS:CB	3.03	0.46
10:L:38:LEU:HD21	10:L:49:LYS:H	1.79	0.46
2:B:26:THR:HB	2:B:27:ALA:H	1.58	0.46
6:H:47:PHE:HB3	6:H:95:TYR:CD1	2.51	0.46
1:A:75:ASN:HA	2:B:1116:ARG:HH22	1.79	0.46
1:A:84:ILE:HG22	1:A:239:LEU:O	2.15	0.46
1:A:356:ASP:HB3	1:A:359:LEU:HD12	1.96	0.46
1:A:1144:LYS:HD2	1:A:1269:GLU:HG2	1.97	0.46
2:B:31:TRP:O	2:B:34:ILE:N	2.48	0.46
2:B:31:TRP:CZ3	2:B:34:ILE:HD12	2.49	0.46
2:B:63:ILE:HD12	2:B:421:PHE:CZ	2.50	0.46
2:B:487:THR:CG2	2:B:488:TYR:N	2.78	0.46
2:B:825:VAL:HG23	2:B:1010:LEU:HG	1.98	0.46
2:B:982:SER:O	2:B:983:ARG:HG3	2.15	0.46
6:H:105:GLU:HB2	6:H:115:TYR:HE1	1.81	0.46
6:H:109:LYS:HD3	6:H:111:LEU:HB2	1.98	0.46
7:I:68:LEU:HA	7:I:69:PRO:HD3	1.72	0.46
1:A:443:LEU:HD23	1:A:444:PHE:N	2.30	0.46
1:A:517:ASN:O	1:A:518:LYS:CB	2.62	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:873:MET:HG2	1:A:957:PRO:HG3	1.97	0.46
1:A:1098:VAL:N	1:A:1099:PRO:CD	2.79	0.46
2:B:100:PRO:HD3	2:B:178:ASN:O	2.16	0.46
2:B:1037:LEU:HD11	2:B:1064:TYR:CE1	2.51	0.46
3:C:75:MET:C	3:C:77:ILE:H	2.23	0.46
6:H:41:ASP:HB2	6:H:121:LEU:HB3	1.96	0.46
1:A:61:ILE:O	1:A:63:ARG:NH2	2.49	0.46
1:A:423:ASP:CG	1:A:424:ILE:H	2.24	0.46
1:A:649:ILE:O	1:A:653:VAL:HG23	2.16	0.46
1:A:769:SER:OG	1:A:1085:HIS:HE1	1.99	0.46
1:A:1189:SER:HB3	1:A:1241:ARG:HB3	1.98	0.46
3:C:93:ASP:O	3:C:127:ARG:NH2	2.48	0.46
4:E:45:LYS:HD3	4:E:46:TYR:HE1	1.81	0.46
4:E:153:HIS:O	4:E:154:ILE:HD13	2.15	0.46
7:I:106:CYS:O	7:I:107:SER:HB2	2.16	0.46
1:A:190:ALA:C	1:A:191:THR:OG1	2.59	0.46
1:A:375:THR:OG1	1:A:433:GLU:HB3	2.16	0.46
1:A:407:ARG:HG2	1:A:430:TRP:CH2	2.51	0.46
1:A:453:MET:HB3	1:A:477:PRO:HB3	1.98	0.46
2:B:122:LEU:HD22	2:B:958:GLN:HG3	1.97	0.46
2:B:361:LEU:HD21	2:B:377:PHE:CD2	2.51	0.46
2:B:715:ALA:HB3	2:B:716:ASN:C	2.41	0.46
2:B:794:ASN:HD22	2:B:794:ASN:N	2.14	0.46
1:A:622:VAL:O	1:A:630:ILE:HD11	2.16	0.46
2:B:1175:LEU:HD23	2:B:1176:ASN:H	1.81	0.46
8:J:35:ALA:O	8:J:39:LEU:HD13	2.16	0.46
1:A:757:ASN:O	1:A:761:MET:HG3	2.15	0.46
1:A:883:LEU:HD23	1:A:1021:LEU:HD13	1.97	0.46
1:A:1116:LEU:CD2	1:A:1311:VAL:HA	2.46	0.46
2:B:547:VAL:HG12	2:B:612:GLU:OE2	2.16	0.46
2:B:604:ARG:HD2	2:B:615:MET:HE2	1.98	0.46
2:B:1074:ASN:HB3	2:B:1077:THR:HG22	1.98	0.46
2:B:1187:ASN:ND2	2:B:1190:ASP:HB2	2.09	0.46
3:C:114:TYR:CD2	3:C:140:ASN:HB3	2.51	0.46
3:C:127:ARG:HG3	3:C:129:ILE:HG22	1.98	0.46
2:B:386:LEU:C	2:B:388:CYS:N	2.71	0.46
2:B:658:ILE:HD12	2:B:658:ILE:HA	1.87	0.46
4:E:45:LYS:HD3	4:E:46:TYR:CE1	2.51	0.46
11:R:7:A:C2	11:R:8:G:C5	3.04	0.45
1:A:286:HIS:HB3	1:A:287:HIS:CB	2.43	0.45
1:A:812:GLU:O	1:A:813:PHE:C	2.59	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1168:GLU:CA	1:A:1170:ILE:HG22	2.47	0.45
1:A:1344:GLY:O	1:A:1345:ARG:C	2.58	0.45
2:B:345:LYS:HG2	2:B:348:ARG:HH21	1.82	0.45
2:B:350:GLN:OE1	2:B:353:LYS:HE2	2.16	0.45
2:B:498:THR:HB	2:B:537:LYS:HB2	1.98	0.45
7:I:75:CYS:HA	7:I:76:PRO:HD3	1.77	0.45
12:T:26:DG:C2	12:T:27:DA:C8	3.04	0.45
1:A:53:LEU:C	1:A:53:LEU:CD2	2.83	0.45
1:A:756:ILE:O	1:A:760:GLN:HG2	2.16	0.45
1:A:789:LYS:HE2	7:I:67:THR:HB	1.97	0.45
1:A:862:ASN:OD1	4:E:174:GLN:HA	2.16	0.45
3:C:46:ILE:HG23	3:C:157:CYS:HB3	1.97	0.45
1:A:298:PHE:HE1	1:A:313:GLN:HG3	1.80	0.45
1:A:381:THR:C	1:A:383:TYR:N	2.74	0.45
1:A:557:ASP:OD1	1:A:559:VAL:HB	2.17	0.45
1:A:1168:GLU:HB3	1:A:1171:GLN:HG3	1.98	0.45
1:A:1364:ASN:O	1:A:1365:TYR:C	2.58	0.45
2:B:438:GLU:CG	2:B:440:HIS:CD2	2.99	0.45
3:C:172:PRO:C	3:C:235:VAL:HG23	2.41	0.45
1:A:242:PRO:HA	1:A:243:PRO:HD3	1.90	0.45
1:A:402:ALA:HA	1:A:435:HIS:CD2	2.52	0.45
1:A:1116:LEU:HB2	1:A:1308:THR:HB	1.98	0.45
1:A:1254:ALA:C	1:A:1256:GLU:N	2.72	0.45
2:B:821:GLN:HE22	2:B:851:PHE:H	1.65	0.45
3:C:124:LEU:O	3:C:126:GLY:N	2.49	0.45
1:A:365:GLY:O	1:A:468:PHE:HA	2.17	0.45
1:A:815:PHE:O	1:A:818:MET:N	2.50	0.45
1:A:1098:VAL:N	1:A:1099:PRO:HD2	2.31	0.45
1:A:1272:THR:C	1:A:1273:LEU:HD12	2.41	0.45
2:B:745:PRO:C	2:B:747:MET:H	2.23	0.45
2:B:803:LEU:H	2:B:822:ASN:HD21	1.65	0.45
3:C:70:ILE:HD11	3:C:144:ILE:HD12	1.97	0.45
1:A:19:PHE:O	1:A:1416:ALA:HA	2.17	0.45
1:A:37:PHE:HB2	1:A:52:GLY:HA3	1.99	0.45
1:A:219:PHE:O	1:A:222:LEU:HD12	2.17	0.45
1:A:858:ASN:C	1:A:858:ASN:ND2	2.68	0.45
1:A:889:SER:C	1:A:891:ALA:N	2.73	0.45
2:B:839:MET:CE	2:B:1010:LEU:HD12	2.46	0.45
5:F:130:ILE:HA	5:F:131:PRO:HD3	1.79	0.45
1:A:86:LEU:HB2	1:A:237:THR:O	2.16	0.45
1:A:917:SER:C	1:A:919:ILE:H	2.23	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:921:GLY:O	1:A:922:ASP:HB3	2.17	0.45
1:A:1021:LEU:HD11	1:A:1025:ARG:HE	1.82	0.45
1:A:1063:MET:SD	1:A:1436:ILE:HG12	2.57	0.45
2:B:344:LYS:HG3	2:B:348:ARG:HB3	1.98	0.45
2:B:603:LEU:HB2	2:B:609:ILE:HG12	1.98	0.45
2:B:728:ARG:HH21	2:B:1048:THR:H	1.65	0.45
2:B:982:SER:O	2:B:1093:GLN:CG	2.65	0.45
3:C:13:ALA:HA	3:C:17:ASN:O	2.16	0.45
3:C:43:THR:HG23	3:C:44:LEU:N	2.32	0.45
8:J:32:GLU:O	8:J:36:LEU:HG	2.16	0.45
1:A:189:ARG:CZ	1:A:196:GLU:O	2.64	0.45
1:A:391:LEU:HD23	1:A:400:PRO:C	2.41	0.45
1:A:728:LYS:HE2	1:A:728:LYS:HB2	1.71	0.45
1:A:848:ILE:HD12	1:A:864:ILE:HG13	1.98	0.45
1:A:1082:ASN:N	1:A:1083:THR:CB	2.76	0.45
1:A:1152:ILE:HB	7:I:44:TYR:HB3	1.98	0.45
2:B:48:LEU:HD23	2:B:173:MET:SD	2.57	0.45
2:B:63:ILE:HD12	2:B:63:ILE:HA	1.65	0.45
2:B:282:ILE:HD12	2:B:283:VAL:N	2.32	0.45
2:B:620:ARG:NH1	7:I:68:LEU:HD21	2.32	0.45
2:B:757:PRO:HB3	2:B:1044:ALA:HB1	1.97	0.45
3:C:124:LEU:O	3:C:125:MET:C	2.60	0.45
5:F:73:ALA:O	5:F:74:ILE:C	2.60	0.45
7:I:83:ASN:C	7:I:83:ASN:ND2	2.72	0.45
1:A:1017:LEU:HD12	4:E:206:GLY:H	1.82	0.45
1:A:1089:VAL:O	1:A:1089:VAL:CG1	2.61	0.45
2:B:493:SER:HA	2:B:751:VAL:HG11	1.99	0.45
2:B:830:TYR:CE2	2:B:1000:PRO:HD3	2.51	0.45
2:B:879:ARG:HA	2:B:879:ARG:NE	2.32	0.45
1:A:224:PHE:CZ	1:A:231:PRO:HG3	2.52	0.44
1:A:405:VAL:O	1:A:413:ILE:HD13	2.17	0.44
1:A:528:LEU:HA	1:A:531:ILE:HG22	1.99	0.44
2:B:71:LEU:H	2:B:88:TYR:HA	1.82	0.44
9:K:35:PHE:H	9:K:35:PHE:HD1	1.65	0.44
9:K:108:GLU:O	9:K:111:LEU:HB2	2.17	0.44
1:A:1261:LYS:O	1:A:1264:GLU:HG3	2.17	0.44
1:A:1378:GLN:OE1	1:A:1382:THR:HG21	2.17	0.44
6:H:80:ARG:O	6:H:81:PRO:O	2.35	0.44
1:A:372:LYS:HA	1:A:435:HIS:ND1	2.33	0.44
1:A:419:LYS:HB3	1:A:419:LYS:HZ2	1.81	0.44
1:A:492:PRO:HB3	1:A:497:THR:CG2	2.46	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:847:ASP:HB3	1:A:1424:VAL:HG23	1.99	0.44
2:B:70:ILE:HB	2:B:71:LEU:HA	1.99	0.44
2:B:315:LYS:N	2:B:316:PRO:CD	2.80	0.44
2:B:358:LYS:O	2:B:362:PRO:HG3	2.17	0.44
2:B:655:LYS:O	2:B:658:ILE:HG22	2.17	0.44
2:B:980:PHE:O	2:B:981:ALA:CB	2.64	0.44
9:K:29:ASN:ND2	9:K:77:THR:O	2.51	0.44
1:A:1105:LEU:HD22	1:A:1384:VAL:HG21	2.00	0.44
1:A:1260:LEU:HD13	1:A:1260:LEU:O	2.17	0.44
2:B:62:ILE:HG23	2:B:418:LYS:HG3	2.00	0.44
2:B:76:GLN:HA	2:B:82:ASP:HA	1.98	0.44
2:B:235:SER:OG	2:B:236:HIS:HD2	2.01	0.44
2:B:519:TRP:HZ2	2:B:705:MET:HE1	1.82	0.44
2:B:999:MET:HG2	2:B:1008:PRO:HD2	2.00	0.44
9:K:82:ASP:OD1	9:K:83:PRO:HD2	2.17	0.44
1:A:253:ASN:HA	1:A:254:GLU:HA	1.77	0.44
1:A:302:THR:HA	1:A:305:ASP:O	2.17	0.44
1:A:917:SER:C	1:A:919:ILE:N	2.75	0.44
1:A:1017:LEU:HD12	4:E:206:GLY:N	2.32	0.44
1:A:1189:SER:HB2	1:A:1242:VAL:O	2.18	0.44
1:A:1434:ALA:HB3	1:A:1436:ILE:HD12	2.00	0.44
2:B:973:ILE:CG2	2:B:974:PRO:HD2	2.48	0.44
2:B:999:MET:HE2	2:B:1011:ILE:HD11	1.99	0.44
3:C:70:ILE:HA	3:C:71:PRO:HD3	1.83	0.44
3:C:173:ALA:O	3:C:233:GLU:O	2.35	0.44
4:E:52:ARG:HA	4:E:53:PRO:HD3	1.71	0.44
4:E:94:LYS:O	4:E:98:ILE:HG12	2.17	0.44
7:I:5:ARG:HG3	7:I:6:PHE:N	2.33	0.44
7:I:17:ARG:HB2	7:I:17:ARG:NH1	2.31	0.44
9:K:56:VAL:HA	9:K:77:THR:HG22	1.99	0.44
1:A:48:ALA:O	1:A:49:LYS:HD2	2.17	0.44
1:A:49:LYS:H	1:A:50:ILE:HA	1.83	0.44
1:A:198:GLU:OE1	1:A:198:GLU:O	2.35	0.44
1:A:497:THR:HG23	2:B:1146:PHE:HD1	1.82	0.44
1:A:877:HIS:O	1:A:878:ILE:HG13	2.17	0.44
1:A:956:LEU:HD23	1:A:956:LEU:HA	1.61	0.44
1:A:1092:LYS:CG	1:A:1094:VAL:O	2.66	0.44
2:B:826:ALA:O	2:B:1011:ILE:HA	2.17	0.44
7:I:84:VAL:HG22	7:I:85:PHE:N	2.33	0.44
1:A:37:PHE:HB3	1:A:39:GLU:OE1	2.18	0.44
1:A:305:ASP:OD1	1:A:306:ASN:N	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1195:LEU:HB2	1:A:1238:ILE:HB	1.99	0.44
1:A:1255:GLU:O	1:A:1255:GLU:HG3	2.10	0.44
2:B:189:LEU:O	2:B:192:LEU:N	2.51	0.44
2:B:344:LYS:CB	2:B:347:LYS:HB2	2.39	0.44
2:B:788:ARG:NH1	2:B:790:ASP:OD1	2.51	0.44
2:B:826:ALA:HB2	2:B:1087:PHE:HD1	1.83	0.44
3:C:29:MET:HE3	3:C:29:MET:HB2	1.83	0.44
3:C:112:ASN:ND2	3:C:146:LYS:HD3	2.33	0.44
1:A:58:LEU:O	1:A:58:LEU:HD13	2.18	0.44
1:A:709:THR:HB	1:A:712:GLU:H	1.83	0.44
1:A:719:VAL:HG12	1:A:723:ASN:HD21	1.82	0.44
1:A:848:ILE:CD1	1:A:858:ASN:HB3	2.47	0.44
1:A:1163:ILE:HA	1:A:1164:PRO:HD3	1.80	0.44
1:A:1319:VAL:O	1:A:1322:ILE:HD12	2.18	0.44
2:B:73:GLN:HG3	2:B:86:ARG:HG3	1.98	0.44
2:B:863:GLU:CB	2:B:864:LYS:HB2	2.36	0.44
2:B:1131:GLY:O	2:B:1132:GLU:C	2.60	0.44
6:H:38:LEU:CD1	6:H:123:MET:HE2	2.47	0.44
7:I:75:CYS:SG	7:I:78:CYS:SG	3.16	0.44
7:I:75:CYS:HB2	7:I:78:CYS:SG	2.57	0.44
11:R:8:G:C2'	11:R:9:G:C5'	2.96	0.44
1:A:730:GLY:C	1:A:732:LEU:H	2.26	0.44
1:A:1064:VAL:HG12	1:A:1064:VAL:O	2.18	0.44
2:B:57:TYR:O	2:B:58:THR:C	2.60	0.44
2:B:121:ASN:N	2:B:121:ASN:HD22	2.16	0.44
2:B:983:ARG:C	2:B:984:HIS:CG	2.96	0.44
2:B:995:ARG:HB3	2:B:997:GLU:OE2	2.17	0.44
5:F:133:VAL:O	5:F:133:VAL:CG1	2.66	0.44
1:A:239:LEU:HD13	1:A:240:PRO:HD2	2.00	0.43
1:A:323:LYS:HG3	1:A:327:ALA:HB3	2.00	0.43
2:B:472:ALA:CB	2:B:476:ARG:HD3	2.48	0.43
6:H:80:ARG:O	6:H:81:PRO:C	2.61	0.43
9:K:35:PHE:CD1	9:K:35:PHE:N	2.85	0.43
12:T:18:DA:H2'	12:T:19:DT:C6	2.53	0.43
1:A:185:TRP:HH2	1:A:200:ARG:CD	2.28	0.43
1:A:591:PHE:HD2	1:A:595:THR:HB	1.83	0.43
2:B:256:VAL:HG11	2:B:382:ILE:HD13	1.98	0.43
2:B:444:MET:CG	2:B:446:LEU:HD22	2.46	0.43
2:B:848:ARG:HH22	2:B:996:ARG:NH1	2.16	0.43
7:I:62:ILE:C	7:I:64:SER:H	2.26	0.43
8:J:50:ILE:HD13	8:J:50:ILE:HA	1.74	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:55:ASP:O	1:A:56:PRO:C	2.59	0.43
2:B:1033:LYS:HA	2:B:1089:PRO:HG2	2.00	0.43
3:C:41:ILE:HD11	3:C:243:VAL:HG13	2.00	0.43
8:J:38:ARG:HH11	8:J:38:ARG:HB2	1.82	0.43
10:L:31:CYS:SG	10:L:34:CYS:HB2	2.59	0.43
1:A:185:TRP:O	1:A:186:LYS:HB2	2.18	0.43
1:A:1147:THR:HB	7:I:48:LEU:HD12	2.01	0.43
1:A:1269:GLU:O	1:A:1270:ASN:CB	2.66	0.43
2:B:745:PRO:O	2:B:748:ILE:HG12	2.19	0.43
2:B:778:MET:HE2	2:B:1094:ARG:HD3	2.00	0.43
2:B:827:ILE:HD11	2:B:1086:PHE:CD2	2.53	0.43
2:B:866:TYR:HA	2:B:867:GLY:HA2	1.79	0.43
2:B:957:ASN:HB3	2:B:961:LEU:HG	2.00	0.43
3:C:137:LYS:HB3	3:C:137:LYS:HE3	1.82	0.43
5:F:77:ASP:O	5:F:78:GLN:O	2.37	0.43
8:J:19:GLU:O	8:J:20:SER:C	2.61	0.43
1:A:56:PRO:O	1:A:57:ARG:C	2.59	0.43
1:A:153:PRO:C	1:A:155:GLU:N	2.76	0.43
1:A:310:GLY:H	1:A:311:GLN:HB2	1.79	0.43
1:A:416:ARG:HB3	1:A:417:TYR:CE1	2.54	0.43
1:A:840:ARG:O	1:A:841:LEU:C	2.60	0.43
1:A:1398:MET:C	1:A:1400:CYS:N	2.73	0.43
2:B:211:VAL:O	2:B:480:SER:HA	2.19	0.43
2:B:291:ILE:HD12	2:B:291:ILE:N	2.33	0.43
2:B:471:LYS:HA	2:B:472:ALA:HA	1.67	0.43
2:B:549:THR:HG22	2:B:550:ASP:H	1.84	0.43
2:B:831:SER:OG	2:B:832:GLY:N	2.52	0.43
2:B:841:MET:CE	2:B:980:PHE:CE2	2.87	0.43
2:B:981:ALA:O	2:B:1092:TYR:CE2	2.69	0.43
4:E:22:MET:O	4:E:26:ARG:HG2	2.18	0.43
4:E:136:ASN:O	4:E:137:GLU:C	2.61	0.43
1:A:193:ASP:O	1:A:193:ASP:OD2	2.36	0.43
1:A:356:ASP:HB3	1:A:359:LEU:HB2	2.00	0.43
1:A:737:LEU:HD23	1:A:737:LEU:HA	1.79	0.43
2:B:1106:ARG:NH1	2:B:1110:PRO:HD2	2.33	0.43
6:H:102:TYR:O	6:H:103:LYS:HB2	2.18	0.43
7:I:17:ARG:HH11	7:I:17:ARG:CB	2.31	0.43
2:B:26:THR:HG22	2:B:708:GLU:OE1	2.18	0.43
2:B:1101:ASP:HA	2:B:1122:ARG:HH22	1.84	0.43
1:A:913:LEU:HG	1:A:915:SER:H	1.83	0.43
2:B:473:MET:HA	2:B:474:SER:HA	1.59	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:803:LEU:O	2:B:1042:GLY:HA3	2.18	0.43
3:C:115:SER:C	3:C:117:ASP:N	2.76	0.43
8:J:43:ARG:HG3	8:J:46:CYS:SG	2.59	0.43
9:K:113:THR:O	9:K:114:LEU:HB2	2.18	0.43
11:R:6:G:O6	11:R:7:A:N6	2.52	0.43
1:A:49:LYS:CB	1:A:55:ASP:OD2	2.58	0.43
1:A:58:LEU:O	1:A:58:LEU:CG	2.65	0.43
1:A:540:PHE:CB	1:A:571:LEU:HD23	2.49	0.43
1:A:1039:LYS:HD3	1:A:1039:LYS:C	2.44	0.43
1:A:1172:LEU:O	1:A:1172:LEU:HG	2.19	0.43
2:B:363:HIS:C	2:B:365:THR:H	2.26	0.43
2:B:469:GLN:O	2:B:470:LYS:HB2	2.19	0.43
3:C:178:PHE:C	3:C:178:PHE:CD2	2.97	0.43
1:A:577:ILE:O	1:A:580:VAL:HB	2.19	0.43
1:A:665:GLY:O	1:A:668:ASP:HB2	2.19	0.43
1:A:919:ILE:HD13	1:A:919:ILE:HA	1.84	0.43
1:A:1158:PRO:HG3	1:A:1188:GLN:HE21	1.84	0.43
2:B:213:ILE:HD11	2:B:481:GLN:OE1	2.19	0.43
2:B:474:SER:O	2:B:475:SER:O	2.36	0.43
2:B:984:HIS:CE1	2:B:1025:HIS:HA	2.54	0.43
2:B:1013:ASN:C	2:B:1015:HIS:H	2.27	0.43
3:C:130:GLY:O	3:C:132:PRO:HD3	2.19	0.43
8:J:6:ARG:HG2	8:J:11:GLY:O	2.19	0.43
1:A:313:GLN:C	1:A:313:GLN:CD	2.87	0.42
1:A:1166:ASP:HB3	1:A:1169:ILE:HD13	2.00	0.42
2:B:628:THR:O	2:B:628:THR:CG2	2.67	0.42
2:B:796:LEU:HB3	2:B:799:PRO:HG3	1.99	0.42
2:B:1056:SER:CB	2:B:1066:SER:O	2.62	0.42
3:C:177:GLU:HB2	3:C:231:ASN:HB3	2.00	0.42
9:K:3:ALA:HA	9:K:4:PRO:HD3	1.87	0.42
1:A:207:ILE:O	1:A:210:ILE:HB	2.19	0.42
1:A:464:PRO:HD2	9:K:67:PHE:CD1	2.54	0.42
1:A:883:LEU:O	1:A:885:THR:N	2.42	0.42
1:A:1092:LYS:HA	1:A:1092:LYS:HD3	1.29	0.42
2:B:67:SER:O	2:B:68:THR:C	2.62	0.42
2:B:324:ILE:O	2:B:324:ILE:HG22	2.19	0.42
2:B:942:ARG:HD3	2:B:942:ARG:HA	1.85	0.42
2:B:1149:GLU:C	2:B:1151:LEU:N	2.77	0.42
9:K:53:ASP:HB3	9:K:56:VAL:HG23	2.01	0.42
11:R:8:G:H2'	11:R:9:G:H8	1.83	0.42
1:A:1396:ALA:O	1:A:1400:CYS:HB3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:24:CYS:O	6:H:41:ASP:HA	2.19	0.42
9:K:27:ALA:HA	9:K:28:PRO:HD3	1.83	0.42
9:K:44:ASN:HA	9:K:61:TYR:CE2	2.54	0.42
11:R:6:G:N1	11:R:7:A:C6	2.87	0.42
1:A:230:ARG:HA	1:A:231:PRO:HD3	1.85	0.42
1:A:376:TYR:HA	1:A:377:PRO:HD2	1.87	0.42
1:A:650:GLN:O	1:A:651:LYS:C	2.61	0.42
1:A:1082:ASN:C	1:A:1084:PHE:HA	2.35	0.42
1:A:1329:THR:HG23	1:A:1331:SER:H	1.84	0.42
2:B:634:TYR:HE1	2:B:692:TYR:CD1	2.32	0.42
2:B:827:ILE:CD1	2:B:1086:PHE:HD2	2.31	0.42
2:B:1168:LEU:HD13	2:B:1208:MET:CE	2.40	0.42
3:C:31:ASN:ND2	3:C:35:ARG:HD2	2.35	0.42
11:R:7:A:C2	11:R:8:G:C4	3.08	0.42
1:A:344:ARG:NH1	2:B:1129:ARG:HB2	2.35	0.42
1:A:943:LEU:C	1:A:945:GLU:H	2.26	0.42
1:A:1004:ASN:OD1	1:A:1004:ASN:C	2.63	0.42
1:A:1278:ASN:HD22	1:A:1312:ASN:HB2	1.85	0.42
1:A:1349:TYR:HA	1:A:1372:VAL:HG21	2.01	0.42
6:H:142:LEU:C	6:H:143:LEU:HD12	2.44	0.42
1:A:668:ASP:HB3	1:A:743:VAL:CG2	2.42	0.42
1:A:1319:VAL:O	1:A:1322:ILE:CD1	2.68	0.42
1:A:1437:GLY:HA3	5:F:88:TYR:CD2	2.54	0.42
2:B:314:LEU:C	2:B:316:PRO:HD2	2.44	0.42
2:B:762:ASN:HD22	2:B:762:ASN:HA	1.63	0.42
2:B:874:PHE:HD1	2:B:962:LYS:HE2	1.85	0.42
2:B:975:GLN:HG2	2:B:976:ILE:H	1.85	0.42
12:T:27:DA:H2'	12:T:27:DA:N3	2.34	0.42
1:A:286:HIS:CB	1:A:287:HIS:HB2	2.44	0.42
1:A:889:SER:O	1:A:890:ASP:C	2.62	0.42
2:B:67:SER:HB2	2:B:92:PHE:HD1	1.85	0.42
2:B:195:CYS:HA	2:B:196:PRO:HD3	1.93	0.42
2:B:363:HIS:C	2:B:365:THR:N	2.77	0.42
3:C:171:GLY:HA2	3:C:172:PRO:HD3	1.66	0.42
9:K:31:VAL:HG12	9:K:32:VAL:N	2.34	0.42
1:A:193:ASP:O	1:A:194:ALA:HB2	2.18	0.42
1:A:387:ARG:HH11	1:A:437:MET:HE1	1.84	0.42
1:A:464:PRO:HD2	9:K:67:PHE:HD1	1.85	0.42
1:A:963:ILE:HD12	1:A:1049:ILE:HG13	2.01	0.42
1:A:1066:VAL:O	1:A:1067:LEU:C	2.63	0.42
2:B:441:ASP:C	2:B:443:ASN:H	2.26	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:86:CYS:C	3:C:88:CYS:N	2.78	0.42
7:I:106:CYS:SG	7:I:107:SER:N	2.92	0.42
1:A:40:THR:H	1:A:41:MET:CB	2.16	0.42
1:A:598:LEU:HD21	6:H:124:ARG:HB2	2.01	0.42
1:A:1167:GLU:C	1:A:1170:ILE:CG2	2.90	0.42
1:A:1212:VAL:O	1:A:1216:ILE:HG13	2.20	0.42
1:A:1259:MET:HE2	1:A:1259:MET:HB2	1.72	0.42
2:B:542:MET:SD	2:B:747:MET:HE2	2.60	0.42
2:B:744:HIS:HA	2:B:745:PRO:HD3	1.91	0.42
3:C:37:MET:O	3:C:38:ILE:C	2.62	0.42
6:H:12:VAL:CG1	6:H:51:ALA:HA	2.49	0.42
1:A:106:VAL:HG11	1:A:214:ILE:HD11	2.02	0.42
1:A:1063:MET:HE3	1:A:1063:MET:HB3	1.81	0.42
2:B:555:ILE:HA	2:B:558:LEU:HD12	2.02	0.42
3:C:245:VAL:HG13	9:K:102:LYS:HD2	2.02	0.42
11:R:5:A:N3	11:R:5:A:H2'	2.35	0.42
1:A:814:PHE:CE1	2:B:514:LEU:HD21	2.55	0.41
1:A:867:ILE:HD13	1:A:1014:ALA:HB2	2.02	0.41
1:A:1171:GLN:O	1:A:1171:GLN:OE1	2.36	0.41
2:B:189:LEU:O	2:B:190:TYR:C	2.63	0.41
2:B:301:ILE:HA	2:B:379:GLY:O	2.20	0.41
2:B:304:ASP:OD1	2:B:306:ASN:HB2	2.20	0.41
2:B:365:THR:HG21	2:B:370:PHE:CG	2.55	0.41
2:B:778:MET:HE1	2:B:1094:ARG:NH1	2.35	0.41
2:B:846:ILE:HG23	2:B:974:PRO:HG2	2.01	0.41
2:B:983:ARG:O	2:B:984:HIS:CG	2.73	0.41
3:C:69:LEU:H	3:C:69:LEU:CD2	2.32	0.41
3:C:86:CYS:C	3:C:88:CYS:H	2.28	0.41
6:H:95:TYR:HD2	6:H:96:VAL:N	2.18	0.41
10:L:60:ARG:CG	10:L:61:THR:H	2.32	0.41
1:A:164:ARG:HB3	1:A:165:GLY:H	1.77	0.41
1:A:176:LYS:HA	1:A:181:LEU:CD2	2.50	0.41
1:A:567:LYS:HZ1	6:H:46:LEU:HB2	1.86	0.41
1:A:815:PHE:O	1:A:816:HIS:C	2.64	0.41
2:B:472:ALA:HB2	2:B:476:ARG:HD3	2.02	0.41
6:H:6:PHE:CZ	6:H:8:ASP:HB2	2.56	0.41
1:A:102:VAL:CG1	1:A:211:PHE:HE1	2.31	0.41
1:A:185:TRP:CE3	1:A:198:GLU:HG2	2.45	0.41
1:A:775:ILE:HG13	1:A:798:GLY:HA3	2.03	0.41
1:A:1369:ALA:O	1:A:1370:LEU:C	2.63	0.41
2:B:25:ILE:H	2:B:25:ILE:HG13	1.62	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:287:ARG:HG2	2:B:292:ILE:HD13	2.02	0.41
7:I:28:GLU:HB3	7:I:35:VAL:HG22	2.03	0.41
7:I:68:LEU:HB3	7:I:84:VAL:CG2	2.50	0.41
1:A:193:ASP:OD2	1:A:193:ASP:C	2.63	0.41
1:A:381:THR:O	1:A:383:TYR:N	2.53	0.41
1:A:878:ILE:HG22	1:A:879:GLU:N	2.36	0.41
1:A:1216:ILE:HG22	1:A:1220:PHE:HE1	1.85	0.41
1:A:1254:ALA:C	1:A:1256:GLU:H	2.29	0.41
2:B:188:ASP:HA	2:B:191:LYS:HE3	2.02	0.41
2:B:592:ASN:OD1	2:B:594:ALA:HB3	2.21	0.41
6:H:95:TYR:HB3	6:H:144:ILE:HB	2.02	0.41
9:K:50:LEU:HD11	9:K:75:ILE:HD13	2.02	0.41
9:K:82:ASP:HA	9:K:83:PRO:HD3	1.93	0.41
1:A:80:HIS:O	1:A:243:PRO:HG3	2.20	0.41
1:A:256:GLN:HG3	12:T:28:DT:O4	2.20	0.41
1:A:407:ARG:HG2	1:A:430:TRP:CZ3	2.56	0.41
1:A:901:LEU:H	1:A:926:GLN:HE21	1.68	0.41
1:A:1039:LYS:HE2	1:A:1043:ASP:OD2	2.21	0.41
2:B:20:ASP:O	2:B:20:ASP:CG	2.63	0.41
2:B:254:LEU:CD2	2:B:381:MET:HE1	2.50	0.41
2:B:260:GLY:O	2:B:267:ARG:HD3	2.21	0.41
2:B:294:ASP:C	2:B:296:GLU:H	2.29	0.41
2:B:482:VAL:O	2:B:483:LEU:C	2.64	0.41
11:R:9:G:C2	12:T:21:DC:O2	2.73	0.41
1:A:37:PHE:HA	1:A:38:PRO:HD3	1.83	0.41
1:A:501:LEU:HD23	1:A:501:LEU:HA	1.68	0.41
1:A:1345:ARG:HD2	1:A:1373:ASP:OD1	2.20	0.41
2:B:31:TRP:HA	2:B:34:ILE:HG13	2.02	0.41
2:B:463:THR:CG2	2:B:465:ASN:HD21	2.34	0.41
2:B:497:ARG:HG3	2:B:538:ASN:HD21	1.84	0.41
2:B:781:PHE:O	2:B:782:LEU:HG	2.20	0.41
3:C:101:LEU:HB3	3:C:155:LEU:HB2	2.03	0.41
3:C:247:GLY:O	3:C:248:ILE:C	2.63	0.41
5:F:84:TYR:CE1	5:F:152:ILE:HD12	2.55	0.41
7:I:34:TYR:CZ	7:I:36:GLU:HB3	2.55	0.41
1:A:187:LYS:CD	1:A:188:ASP:N	2.77	0.41
1:A:278:THR:O	1:A:282:ASN:HB2	2.20	0.41
1:A:384:ASN:O	1:A:385:ILE:C	2.63	0.41
1:A:399:HIS:HB3	1:A:400:PRO:HD3	2.02	0.41
1:A:483:ASP:HB3	2:B:837:ASP:HB3	2.01	0.41
1:A:1260:LEU:HD13	1:A:1260:LEU:C	2.46	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1280:GLU:O	1:A:1282:VAL:HG23	2.21	0.41
1:A:1398:MET:C	1:A:1400:CYS:H	2.27	0.41
2:B:212:LEU:HD23	2:B:212:LEU:HA	1.96	0.41
2:B:337:ARG:NH1	2:B:344:LYS:HZ3	2.19	0.41
2:B:360:PHE:HE2	2:B:374:LYS:HB3	1.85	0.41
2:B:492:LEU:HB3	2:B:751:VAL:HG21	2.02	0.41
2:B:721:LEU:HA	2:B:722:ASP:HA	1.78	0.41
2:B:868:MET:C	2:B:869:SER:HG	2.26	0.41
2:B:1120:GLU:CG	2:B:1121:GLY:N	2.81	0.41
3:C:148:ARG:N	3:C:151:GLN:OE1	2.53	0.41
3:C:182:PRO:CB	3:C:207:CYS:SG	3.06	0.41
1:A:507:VAL:CG1	1:A:521:MET:HE1	2.50	0.41
2:B:755:ILE:HD13	2:B:755:ILE:HA	1.62	0.41
2:B:757:PRO:HB3	2:B:1044:ALA:CB	2.50	0.41
6:H:118:PHE:O	6:H:120:GLY:N	2.53	0.41
1:A:261:ASP:HB3	1:A:322:VAL:HG12	2.03	0.41
1:A:446:ARG:NH1	1:A:478:TYR:O	2.54	0.41
1:A:642:CYS:O	1:A:645:LEU:HB3	2.21	0.41
1:A:1154:TYR:CE1	7:I:18:GLU:HG3	2.55	0.41
1:A:1256:GLU:O	1:A:1257:ASP:CB	2.68	0.41
2:B:34:ILE:O	2:B:37:PHE:N	2.49	0.41
2:B:129:PHE:HE2	2:B:166:PHE:HB2	1.84	0.41
2:B:361:LEU:N	2:B:362:PRO:HD3	2.35	0.41
2:B:488:TYR:O	2:B:490:SER:N	2.54	0.41
2:B:765:PRO:O	2:B:769:TYR:CD1	2.74	0.41
2:B:777:ALA:HB2	2:B:1093:GLN:HE21	1.86	0.41
2:B:808:ALA:O	2:B:812:LEU:HG	2.21	0.41
2:B:900:ALA:HA	2:B:901:PRO:HD3	1.92	0.41
2:B:980:PHE:CD1	2:B:990:ILE:HG13	2.55	0.41
3:C:238:ILE:O	3:C:239:PRO:C	2.63	0.41
1:A:513:SER:HA	1:A:514:PRO:HD3	1.93	0.41
1:A:590:ARG:HG3	1:A:590:ARG:HH11	1.85	0.41
1:A:1063:MET:SD	1:A:1436:ILE:HG23	2.61	0.41
1:A:1198:ASP:C	1:A:1200:ALA:H	2.29	0.41
2:B:273:LEU:HD11	2:B:285:ILE:HD12	2.03	0.41
2:B:492:LEU:HD23	2:B:492:LEU:HA	1.85	0.41
2:B:637:LEU:O	2:B:690:VAL:HA	2.20	0.41
2:B:817:LEU:N	2:B:818:PRO:HD3	2.35	0.41
2:B:976:ILE:O	2:B:990:ILE:O	2.39	0.41
2:B:1107:ALA:O	2:B:1108:ARG:CB	2.67	0.41
1:A:567:LYS:O	1:A:569:LYS:N	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:348:ARG:HG3	2:B:349:ILE:HD12	2.02	0.40
2:B:364:ILE:HG22	2:B:365:THR:HG22	2.03	0.40
2:B:579:ARG:HG3	2:B:623:GLU:HG2	2.02	0.40
2:B:864:LYS:HG3	2:B:872:GLU:CB	2.45	0.40
2:B:1120:GLU:O	2:B:1124:ARG:HD3	2.21	0.40
6:H:22:LYS:HD3	6:H:45:GLU:OE2	2.20	0.40
8:J:57:ILE:HD12	8:J:57:ILE:HA	1.77	0.40
9:K:44:ASN:HA	9:K:61:TYR:HE2	1.85	0.40
10:L:60:ARG:HG3	10:L:61:THR:N	2.35	0.40
1:A:269:ILE:HD11	1:A:300:VAL:HA	2.03	0.40
1:A:337:ARG:HG2	2:B:1132:GLU:CD	2.45	0.40
1:A:464:PRO:HB2	1:A:465:TYR:CD1	2.52	0.40
1:A:534:LEU:HA	1:A:539:THR:HG21	2.03	0.40
1:A:901:LEU:HD22	1:A:919:ILE:HG22	2.04	0.40
1:A:1155:ASP:HA	1:A:1156:PRO:HD3	1.79	0.40
1:A:1276:VAL:HG12	1:A:1277:GLU:O	2.21	0.40
2:B:42:GLY:O	2:B:43:LEU:HD23	2.22	0.40
2:B:168:GLY:N	2:B:450:ALA:HB1	2.32	0.40
2:B:910:VAL:HG12	2:B:911:ILE:N	2.36	0.40
2:B:915:THR:HB	2:B:934:LYS:HB3	2.04	0.40
7:I:75:CYS:SG	7:I:103:CYS:HB2	2.61	0.40
1:A:311:GLN:HA	1:A:312:PRO:HA	1.86	0.40
1:A:456:MET:HE3	1:A:507:VAL:HG22	2.02	0.40
1:A:545:GLN:O	1:A:549:MET:HG3	2.20	0.40
2:B:33:VAL:HG21	2:B:638:PHE:CZ	2.56	0.40
2:B:47:GLN:O	2:B:173:MET:HE1	2.20	0.40
2:B:1072:MET:HE2	2:B:1085:ILE:HG21	2.03	0.40
4:E:62:ALA:HB3	4:E:78:LEU:HB3	2.03	0.40
6:H:11:GLN:HE21	6:H:11:GLN:HB2	1.71	0.40
1:A:118:HIS:NE2	1:A:155:GLU:CD	2.79	0.40
1:A:230:ARG:HD3	1:A:232:GLU:OE2	2.21	0.40
1:A:512:VAL:HA	1:A:519:PRO:HA	2.02	0.40
1:A:909:ASP:OD2	1:A:910:PRO:HD2	2.21	0.40
1:A:1030:ARG:C	1:A:1032:LEU:N	2.79	0.40
2:B:785:TYR:CD1	2:B:785:TYR:C	3.00	0.40
2:B:1149:GLU:HG3	2:B:1153:GLU:HB2	2.03	0.40
7:I:59:VAL:HB	7:I:61:ASP:H	1.87	0.40
1:A:351:THR:HG21	1:A:466:SER:O	2.21	0.40
2:B:361:LEU:HD21	2:B:377:PHE:HD2	1.86	0.40
2:B:712:PRO:CD	2:B:713:ALA:H	2.33	0.40
2:B:827:ILE:CD1	2:B:1086:PHE:CD2	3.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1095:LEU:N	2:B:1095:LEU:HD23	2.35	0.40
4:E:205:SER:O	4:E:207:ARG:N	2.55	0.40
5:F:82:THR:O	5:F:136:ARG:NH1	2.48	0.40
6:H:105:GLU:OE1	6:H:115:TYR:OH	2.30	0.40
8:J:31:ASP:OD1	8:J:34:THR:OG1	2.40	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	1419/1733 (82%)	1089 (77%)	270 (19%)	60 (4%)	2	14
2	B	1145/1224 (94%)	896 (78%)	202 (18%)	47 (4%)	2	14
3	C	269/318 (85%)	198 (74%)	63 (23%)	8 (3%)	3	18
4	E	213/215 (99%)	175 (82%)	32 (15%)	6 (3%)	4	19
5	F	83/155 (54%)	68 (82%)	11 (13%)	4 (5%)	2	11
6	H	132/146 (90%)	100 (76%)	25 (19%)	7 (5%)	1	10
7	I	117/122 (96%)	85 (73%)	23 (20%)	9 (8%)	1	5
8	J	63/70 (90%)	52 (82%)	9 (14%)	2 (3%)	3	18
9	K	112/120 (93%)	96 (86%)	15 (13%)	1 (1%)	14	41
10	L	44/70 (63%)	29 (66%)	13 (30%)	2 (4%)	2	13
All	All	3597/4173 (86%)	2788 (78%)	663 (18%)	146 (4%)	2	14

All (146) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	57	ARG
1	A	120	GLU

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Mol	Chain	Res	Type
1	A	186	LYS
1	A	191	THR
1	A	193	ASP
1	A	194	ALA
1	A	424	ILE
1	A	1171	GLN
1	A	1254	ALA
1	A	1257	ASP
1	A	1270	ASN
2	B	439	ALA
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	869	SER
4	E	206	GLY
5	F	77	ASP
7	I	33	SER
7	I	47	GLU
7	I	79	HIS
7	I	106	CYS
1	A	78	PRO
1	A	161	LEU
1	A	258	GLY
1	A	307	ASP
1	A	846	GLU
1	A	958	VAL
1	A	1083	THR
1	A	1091	SER
1	A	1170	ILE
1	A	1173	HIS
1	A	1221	LYS
1	A	1437	GLY
2	B	21	GLU
2	B	65	GLU
2	B	531	GLN
2	B	575	PRO
2	B	831	SER
2	B	881	ASN

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Mol	Chain	Res	Type
3	C	125	MET
3	C	142	VAL
5	F	72	LYS
5	F	78	GLN
5	F	104	ASN
6	H	60	ALA
6	H	78	SER
6	H	81	PRO
6	H	119	GLY
7	I	9	ASP
7	I	11	ASN
7	I	116	ASN
8	J	6	ARG
8	J	10	CYS
9	K	70	ARG
10	L	47	ARG
1	A	55	ASP
1	A	154	SER
1	A	250	ILE
1	A	255	SER
1	A	311	GLN
1	A	567	LYS
1	A	1090	ALA
1	A	1156	PRO
1	A	1224	LEU
1	A	1390	ASN
1	A	1391	ARG
2	B	74	LEU
2	B	441	ASP
2	B	468	GLU
2	B	712	PRO
2	B	732	SER
2	B	830	TYR
2	B	943	SER
2	B	1017	ILE
2	B	1046	PRO
3	C	28	ALA
6	H	82	PRO
6	H	109	LYS
7	I	3	THR
7	I	107	SER
10	L	59	ALA

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Mol	Chain	Res	Type
1	A	66	LYS
1	A	189	ARG
1	A	418	SER
1	A	568	PRO
1	A	591	PHE
1	A	1190	PRO
2	B	76	GLN
2	B	79	THR
2	B	290	GLY
2	B	476	ARG
2	B	974	PRO
2	B	1214	PRO
3	C	214	ASN
4	E	76	GLY
4	E	86	PRO
4	E	124	VAL
6	H	75	ALA
1	A	149	GLU
1	A	169	ASN
1	A	308	ILE
1	A	417	TYR
1	A	599	SER
2	B	91	SER
2	B	294	ASP
2	B	484	ASN
2	B	647	GLY
2	B	676	VAL
2	B	792	MET
2	B	880	THR
2	B	1150	ARG
3	C	90	ASP
3	C	227	THR
4	E	38	PRO
4	E	101	GLN
1	A	332	LYS
1	A	972	HIS
1	A	1031	VAL
1	A	1388	GLY
2	B	70	ILE
2	B	489	SER
3	C	116	LYS
1	A	338	GLY

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Mol	Chain	Res	Type
1	A	392	VAL
2	B	168	GLY
2	B	731	VAL
3	C	182	PRO
1	A	756	ILE
1	A	364	VAL
1	A	396	PRO
1	A	639	PRO
1	A	1107	VAL
1	A	1429	ILE
2	B	292	ILE
2	B	976	ILE
1	A	35	ILE
1	A	56	PRO
1	A	667	GLY
2	B	410	GLY
2	B	479	VAL
2	B	555	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1248/1520 (82%)	1067 (86%)	181 (14%)	3	13
2	B	1000/1061 (94%)	860 (86%)	140 (14%)	3	13
3	C	238/274 (87%)	208 (87%)	30 (13%)	4	17
4	E	196/197 (100%)	183 (93%)	13 (7%)	15	40
5	F	74/137 (54%)	69 (93%)	5 (7%)	14	39
6	H	119/128 (93%)	113 (95%)	6 (5%)	22	48
7	I	113/116 (97%)	102 (90%)	11 (10%)	8	27
8	J	60/65 (92%)	50 (83%)	10 (17%)	2	9
9	K	99/102 (97%)	86 (87%)	13 (13%)	4	16
10	L	40/57 (70%)	35 (88%)	5 (12%)	4	17

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	3187/3657 (87%)	2773 (87%)	414 (13%)	4 16

All (414) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	LEU
1	A	23	SER
1	A	30	ILE
1	A	49	LYS
1	A	58	LEU
1	A	63	ARG
1	A	65	LEU
1	A	69	THR
1	A	84	ILE
1	A	93	VAL
1	A	108	MET
1	A	113	LEU
1	A	121	LEU
1	A	155	GLU
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	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	237	THR
1	A	239	LEU
1	A	250	ILE
1	A	266	LEU
1	A	270	LEU
1	A	271	LYS
1	A	306	ASN
1	A	308	ILE
1	A	313	GLN

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Mol	Chain	Res	Type
1	A	317	LYS
1	A	322	VAL
1	A	323	LYS
1	A	332	LYS
1	A	333	GLU
1	A	346	ASP
1	A	351	THR
1	A	373	THR
1	A	403	LYS
1	A	405	VAL
1	A	413	ILE
1	A	416	ARG
1	A	417	TYR
1	A	418	SER
1	A	419	LYS
1	A	424	ILE
1	A	442	VAL
1	A	443	LEU
1	A	445	ASN
1	A	450	LEU
1	A	452	LYS
1	A	460	VAL
1	A	463	ILE
1	A	465	TYR
1	A	466	SER
1	A	470	LEU
1	A	475	THR
1	A	486	GLU
1	A	516	SER
1	A	517	ASN
1	A	518	LYS
1	A	535	THR
1	A	545	GLN
1	A	550	LEU
1	A	565	ILE
1	A	576	GLN
1	A	595	THR
1	A	618	GLU
1	A	652	VAL
1	A	658	LEU
1	A	666	ILE
1	A	683	ILE

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Mol	Chain	Res	Type
1	A	687	LYS
1	A	688	LYS
1	A	691	LEU
1	A	732	LEU
1	A	740	LEU
1	A	756	ILE
1	A	758	ILE
1	A	764	CYS
1	A	765	VAL
1	A	770	VAL
1	A	771	GLU
1	A	783	THR
1	A	788	SER
1	A	803	SER
1	A	829	VAL
1	A	837	ILE
1	A	838	GLN
1	A	858	ASN
1	A	867	ILE
1	A	884	ASP
1	A	885	THR
1	A	889	SER
1	A	895	LYS
1	A	902	LEU
1	A	904	THR
1	A	908	LEU
1	A	919	ILE
1	A	920	LEU
1	A	923	LEU
1	A	929	LEU
1	A	961	ARG
1	A	964	ILE
1	A	969	GLN
1	A	970	THR
1	A	982	THR
1	A	988	LEU
1	A	998	LEU
1	A	999	VAL
1	A	1006	ILE
1	A	1017	LEU
1	A	1025	ARG
1	A	1031	VAL

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Mol	Chain	Res	Type
1	A	1033	GLN
1	A	1037	LEU
1	A	1039	LYS
1	A	1046	LEU
1	A	1049	ILE
1	A	1058	VAL
1	A	1067	LEU
1	A	1078	GLN
1	A	1079	MET
1	A	1084	PHE
1	A	1085	HIS
1	A	1089	VAL
1	A	1092	LYS
1	A	1113	THR
1	A	1116	LEU
1	A	1118	VAL
1	A	1146	VAL
1	A	1152	ILE
1	A	1169	ILE
1	A	1172	LEU
1	A	1174	PHE
1	A	1175	SER
1	A	1176	LEU
1	A	1177	LEU
1	A	1178	ASP
1	A	1179	GLU
1	A	1192	LEU
1	A	1222	ASN
1	A	1224	LEU
1	A	1227	ILE
1	A	1237	ILE
1	A	1240	CYS
1	A	1243	VAL
1	A	1246	LYS
1	A	1255	GLU
1	A	1256	GLU
1	A	1259	MET
1	A	1264	GLU
1	A	1267	MET
1	A	1283	VAL
1	A	1285	MET
1	A	1314	SER

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Mol	Chain	Res	Type
1	A	1322	ILE
1	A	1327	ILE
1	A	1329	THR
1	A	1333	ILE
1	A	1335	ILE
1	A	1341	ILE
1	A	1354	ASN
1	A	1355	VAL
1	A	1366	ARG
1	A	1385	THR
1	A	1393	ASN
1	A	1400	CYS
1	A	1403	GLU
1	A	1406	VAL
1	A	1407	GLU
1	A	1408	ILE
1	A	1428	VAL
1	A	1444	MET
2	B	25	ILE
2	B	26	THR
2	B	34	ILE
2	B	35	SER
2	B	44	VAL
2	B	63	ILE
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
2	B	89	GLU
2	B	90	ILE
2	B	98	THR
2	B	121	ASN
2	B	130	VAL
2	B	174	LEU
2	B	178	ASN
2	B	179	CYS
2	B	202	TYR

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Mol	Chain	Res	Type
2	B	206	ASN
2	B	213	ILE
2	B	223	VAL
2	B	244	LEU
2	B	246	LYS
2	B	268	THR
2	B	282	ILE
2	B	305	VAL
2	B	310	MET
2	B	315	LYS
2	B	317	CYS
2	B	327	ARG
2	B	336	ARG
2	B	337	ARG
2	B	341	LEU
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	438	GLU
2	B	440	HIS
2	B	444	MET
2	B	445	LYS
2	B	446	LEU
2	B	459	TYR
2	B	463	THR
2	B	466	TRP
2	B	470	LYS
2	B	474	SER
2	B	479	VAL
2	B	483	LEU
2	B	527	THR
2	B	542	MET
2	B	549	THR
2	B	570	VAL
2	B	582	VAL

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Mol	Chain	Res	Type
2	B	626	ILE
2	B	633	VAL
2	B	637	LEU
2	B	644	GLU
2	B	645	SER
2	B	658	ILE
2	B	678	GLU
2	B	694	ASP
2	B	701	ILE
2	B	710	LEU
2	B	711	GLU
2	B	755	ILE
2	B	762	ASN
2	B	764	SER
2	B	790	ASP
2	B	796	LEU
2	B	827	ILE
2	B	839	MET
2	B	844	SER
2	B	864	LYS
2	B	868	MET
2	B	869	SER
2	B	873	THR
2	B	878	GLN
2	B	886	LYS
2	B	899	ILE
2	B	906	SER
2	B	916	THR
2	B	941	LEU
2	B	943	SER
2	B	948	ILE
2	B	963	PHE
2	B	968	VAL
2	B	971	THR
2	B	973	ILE
2	B	975	GLN
2	B	979	LYS
2	B	989	THR
2	B	992	ILE
2	B	997	GLU
2	B	999	MET
2	B	1006	ILE

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Mol	Chain	Res	Type
2	B	1007	VAL
2	B	1012	ILE
2	B	1019	SER
2	B	1022	THR
2	B	1028	GLU
2	B	1048	THR
2	B	1050	ILE
2	B	1051	THR
2	B	1071	VAL
2	B	1082	MET
2	B	1084	GLN
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	1128	LEU
2	B	1132	GLU
2	B	1133	MET
2	B	1145	SER
2	B	1156	ASP
2	B	1159	ARG
2	B	1160	VAL
2	B	1165	ILE
2	B	1175	LEU
2	B	1190	ASP
2	B	1194	ILE
2	B	1196	ILE
2	B	1211	ASN
3	C	4	GLU
3	C	10	ILE
3	C	18	VAL
3	C	22	LEU
3	C	25	VAL
3	C	27	LEU
3	C	40	GLU
3	C	43	THR
3	C	46	ILE
3	C	57	VAL

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Mol	Chain	Res	Type
3	C	69	LEU
3	C	77	ILE
3	C	120	ILE
3	C	129	ILE
3	C	134	ILE
3	C	143	LEU
3	C	144	ILE
3	C	158	VAL
3	C	163	ILE
3	C	189	THR
3	C	195	GLN
3	C	197	SER
3	C	199	LYS
3	C	203	GLN
3	C	215	GLU
3	C	228	PHE
3	C	232	VAL
3	C	235	VAL
3	C	240	VAL
3	C	244	VAL
4	E	30	ILE
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	131	THR
4	E	134	THR
4	E	150	VAL
4	E	156	LEU
4	E	159	ASP
4	E	169	ARG
5	F	79	ARG
5	F	97	ARG
5	F	110	ASP
5	F	111	LEU
5	F	148	VAL
6	H	11	GLN
6	H	23	VAL
6	H	62	SER
6	H	94	ASP

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Mol	Chain	Res	Type
6	H	121	LEU
6	H	142	LEU
7	I	8	ARG
7	I	9	ASP
7	I	17	ARG
7	I	29	CYS
7	I	31	THR
7	I	59	VAL
7	I	75	CYS
7	I	83	ASN
7	I	95	THR
7	I	96	SER
7	I	104	LEU
8	J	3	VAL
8	J	5	VAL
8	J	7	CYS
8	J	12	LYS
8	J	13	VAL
8	J	29	GLU
8	J	31	ASP
8	J	34	THR
8	J	43	ARG
8	J	57	ILE
9	K	6	ARG
9	K	10	PHE
9	K	12	LEU
9	K	20	LYS
9	K	33	ILE
9	K	41	THR
9	K	42	LEU
9	K	101	LEU
9	K	102	LYS
9	K	106	GLU
9	K	107	THR
9	K	113	THR
9	K	114	LEU
10	L	31	CYS
10	L	49	LYS
10	L	55	ILE
10	L	61	THR
10	L	68	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (97)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	64	ASN
1	A	83	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	316	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	517	ASN
1	A	545	GLN
1	A	659	HIS
1	A	660	ASN
1	A	723	ASN
1	A	741	ASN
1	A	742	ASN
1	A	760	GLN
1	A	767	GLN
1	A	768	GLN
1	A	786	HIS
1	A	838	GLN
1	A	854	ASN
1	A	858	ASN
1	A	926	GLN
1	A	935	GLN
1	A	968	GLN
1	A	994	GLN
1	A	1033	GLN
1	A	1085	HIS
1	A	1173	HIS
1	A	1188	GLN
1	A	1218	GLN
1	A	1222	ASN
1	A	1278	ASN
1	A	1312	ASN

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Mol	Chain	Res	Type
1	A	1427	ASN
1	A	1432	GLN
2	B	103	ASN
2	B	206	ASN
2	B	215	GLN
2	B	236	HIS
2	B	366	GLN
2	B	395	GLN
2	B	443	ASN
2	B	465	ASN
2	B	494	HIS
2	B	515	HIS
2	B	516	ASN
2	B	518	HIS
2	B	538	ASN
2	B	648	HIS
2	B	657	HIS
2	B	706	GLN
2	B	744	HIS
2	B	761	HIS
2	B	762	ASN
2	B	767	ASN
2	B	794	ASN
2	B	822	ASN
2	B	835	GLN
2	B	842	ASN
2	B	878	GLN
2	B	975	GLN
2	B	984	HIS
2	B	986	GLN
2	B	1040	ASN
2	B	1084	GLN
2	B	1178	ASN
3	C	17	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

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Mol	Chain	Res	Type
3	C	271	ASN
4	E	104	ASN
4	E	143	ASN
4	E	174	GLN
4	E	179	GLN
6	H	11	GLN
6	H	131	ASN
7	I	79	HIS
7	I	83	ASN
8	J	64	ASN
9	K	65	HIS
9	K	76	GLN
10	L	66	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
11	R	11/13 (84%)	2 (18%)	0

All (2) RNA backbone outliers are listed below:

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

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	1429/1733 (82%)	0.12	21 (1%) 72 58	81, 135, 241, 393	0
2	B	1153/1224 (94%)	0.15	22 (1%) 66 51	80, 120, 251, 398	0
3	C	271/318 (85%)	0.02	3 (1%) 78 65	90, 114, 178, 337	0
4	E	215/215 (100%)	0.21	9 (4%) 40 29	111, 159, 272, 350	0
5	F	85/155 (54%)	-0.15	1 (1%) 76 64	110, 134, 173, 217	0
6	H	136/146 (93%)	0.30	5 (3%) 45 32	124, 172, 301, 360	0
7	I	119/122 (97%)	0.33	4 (3%) 48 35	111, 151, 193, 273	0
8	J	65/70 (92%)	-0.10	1 (1%) 72 58	87, 104, 152, 179	0
9	K	114/120 (95%)	-0.06	0 100 100	87, 119, 153, 172	0
10	L	46/70 (65%)	0.60	2 (4%) 40 29	107, 166, 257, 270	0
11	R	12/13 (92%)	-0.02	0 100 100	93, 123, 178, 190	0
12	T	28/28 (100%)	0.32	0 100 100	96, 205, 312, 314	0
13	N	14/14 (100%)	1.01	2 (14%) 6 7	280, 307, 312, 313	0
All	All	3687/4228 (87%)	0.14	70 (1%) 66 51	80, 131, 253, 398	0

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	882	THR	4.7
2	B	980	PHE	4.1
2	B	477	ALA	3.9
2	B	982	SER	3.6
13	N	1	DC	3.5
2	B	880	THR	3.5
1	A	844	ALA	3.5
10	L	32	ALA	3.4
7	I	105	SER	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	78	PRO	3.3
2	B	731	VAL	3.3
1	A	168	GLY	3.3
1	A	1267	MET	3.2
2	B	441	ASP	3.2
1	A	194	ALA	3.2
1	A	186	LYS	3.1
2	B	981	ALA	2.9
2	B	1211	ASN	2.9
1	A	195	ASP	2.8
1	A	192	GLY	2.8
4	E	93	MET	2.8
2	B	440	HIS	2.8
6	H	139	ASN	2.7
1	A	58	LEU	2.7
4	E	132	ILE	2.7
3	C	157	CYS	2.7
7	I	63	GLY	2.7
4	E	88	VAL	2.7
4	E	110	PHE	2.6
2	B	883	LEU	2.6
1	A	260	ASP	2.6
6	H	112	ILE	2.5
1	A	79	GLY	2.5
2	B	708	GLU	2.5
2	B	478	GLY	2.5
1	A	266	LEU	2.5
6	H	120	GLY	2.5
1	A	60	SER	2.5
2	B	383	ASN	2.4
1	A	193	ASP	2.4
7	I	56	ALA	2.4
2	B	132	VAL	2.4
4	E	124	VAL	2.4
8	J	65	PRO	2.3
1	A	250	ILE	2.3
2	B	84	ILE	2.3
5	F	71	GLU	2.3
4	E	16	PHE	2.3
7	I	82	GLU	2.3
1	A	1327	ILE	2.3
3	C	260	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
4	E	123	LEU	2.2
2	B	816	GLU	2.2
2	B	576	ASP	2.2
13	N	2	DT	2.2
1	A	386	ASP	2.2
1	A	973	ILE	2.2
6	H	105	GLU	2.2
4	E	86	PRO	2.2
2	B	906	SER	2.1
2	B	407	ASP	2.1
10	L	50	ASP	2.1
1	A	141	LEU	2.1
2	B	611	PRO	2.1
6	H	7	ASP	2.1
3	C	245	VAL	2.1
1	A	589	GLN	2.1
4	E	41	ASP	2.0
1	A	197	PRO	2.0
2	B	646	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
15	MG	A	1736	1/1	0.90	0.13	91,91,91,91	0
14	ZN	I	204	1/1	0.93	0.07	293,293,293,293	0
14	ZN	A	1735	1/1	0.97	0.06	145,145,145,145	0
14	ZN	A	1734	1/1	0.98	0.04	246,246,246,246	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
14	ZN	J	101	1/1	0.98	0.04	190,190,190,190	0
14	ZN	L	105	1/1	0.98	0.04	151,151,151,151	0
14	ZN	B	1307	1/1	0.98	0.03	160,160,160,160	0
14	ZN	C	319	1/1	0.99	0.02	135,135,135,135	0
14	ZN	I	203	1/1	0.99	0.04	147,147,147,147	0

6.5 Other polymers [i](#)

There are no such residues in this entry.