



# Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 02:59 am BST

PDB ID : 3GTJ  
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](mailto: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.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

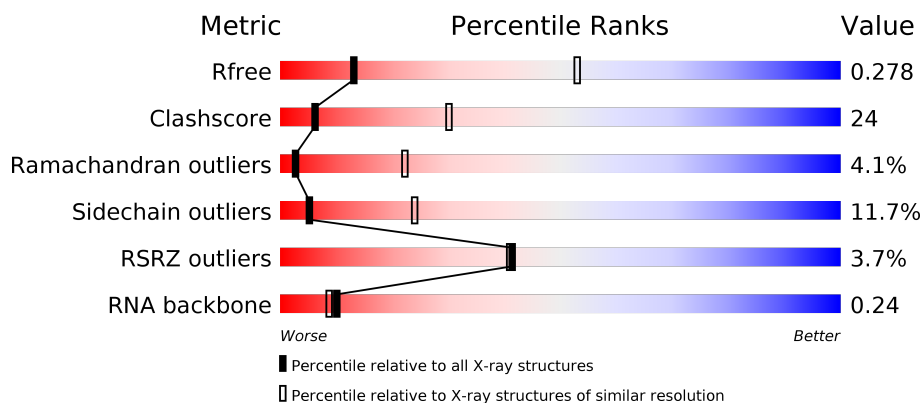
# 1 Overall quality at a glance

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))
$R_{free}$	130704	1486 (3.50-3.34)
Clashscore	141614	1572 (3.50-3.34)
Ramachandran outliers	138981	1534 (3.50-3.34)
Sidechain outliers	138945	1535 (3.50-3.34)
RSRZ outliers	127900	1395 (3.50-3.34)
RNA backbone	3102	1012 (3.88-2.96)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	<div> <div>3%</div> <div> <div></div> <div>45%</div> <div>30%</div> <div>7%</div> <div>18%</div> </div> </div>
2	B	1224	<div> <div>4%</div> <div> <div></div> <div>51%</div> <div>35%</div> <div>7%</div> <div>6%</div> </div> </div>
3	C	318	<div> <div>3%</div> <div> <div></div> <div>49%</div> <div>31%</div> <div>6%</div> <div>15%</div> </div> </div>
4	E	215	<div> <div>7%</div> <div> <div></div> <div>68%</div> <div>30%</div> <div></div> </div> </div>

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Mol	Chain	Length	Quality of chain
5	F	155	<div><div><div></div><div></div><div></div><div></div></div><div>%35%17%45%</div></div>
6	H	146	<div><div><div></div><div></div><div></div><div></div></div><div>5%55%32%5%7%</div></div>
7	I	122	<div><div><div></div><div></div><div></div><div></div></div><div>%52%35%10%..</div></div>
8	J	70	<div><div><div></div><div></div><div></div><div></div></div><div>4%50%33%10%7%</div></div>
9	K	120	<div><div><div></div><div></div><div></div><div></div></div><div>51%38%7%5%</div></div>
10	L	70	<div><div><div></div><div></div><div></div><div></div></div><div>3%46%11%9%34%</div></div>
11	R	13	<div><div><div></div><div></div><div></div><div></div></div><div>15%62%15%8%</div></div>
12	T	28	<div><div><div></div><div></div><div></div><div></div></div><div>18%36%36%29%</div></div>
13	N	14	<div><div><div></div><div></div><div></div><div></div></div><div>14%36%57%7%</div></div>

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

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

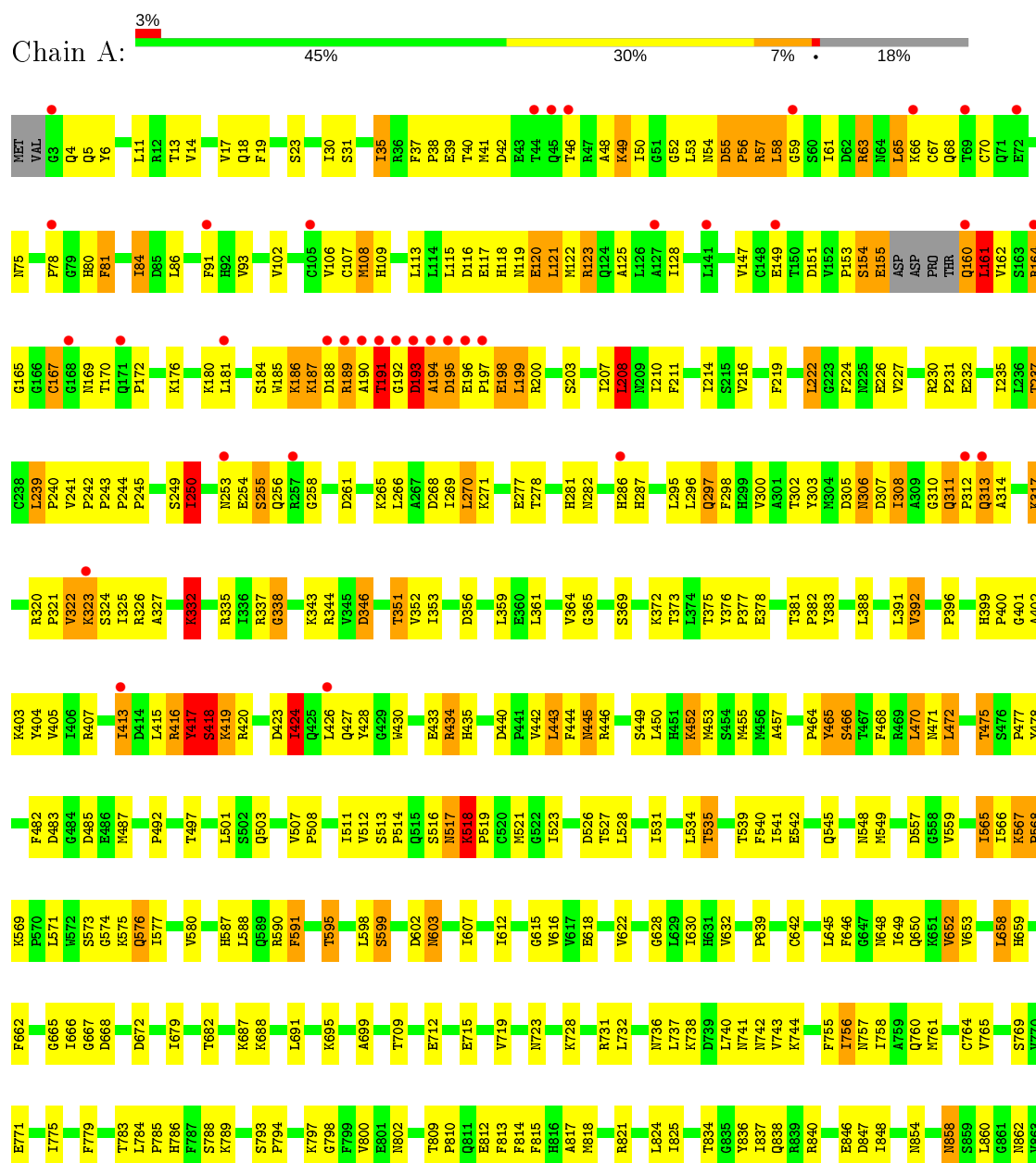
- Molecule 15 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

### 3 Residue-property plots [i](#)

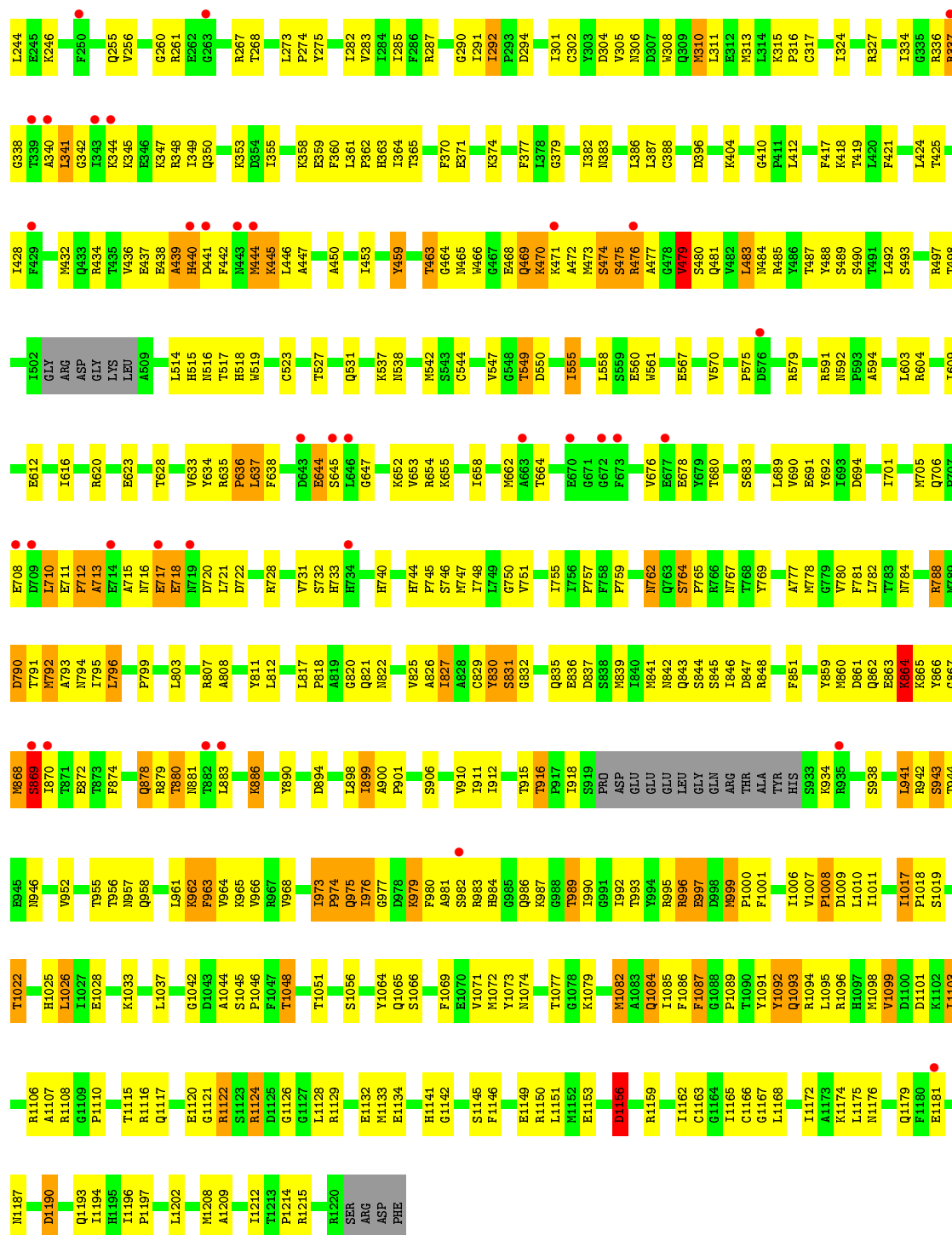
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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

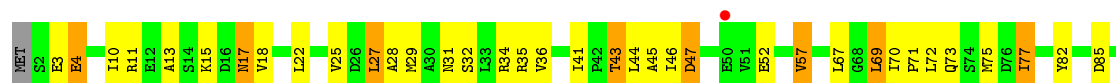


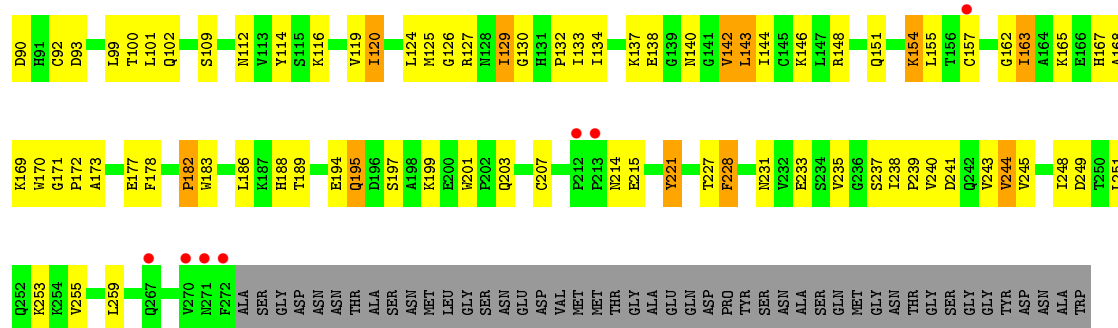




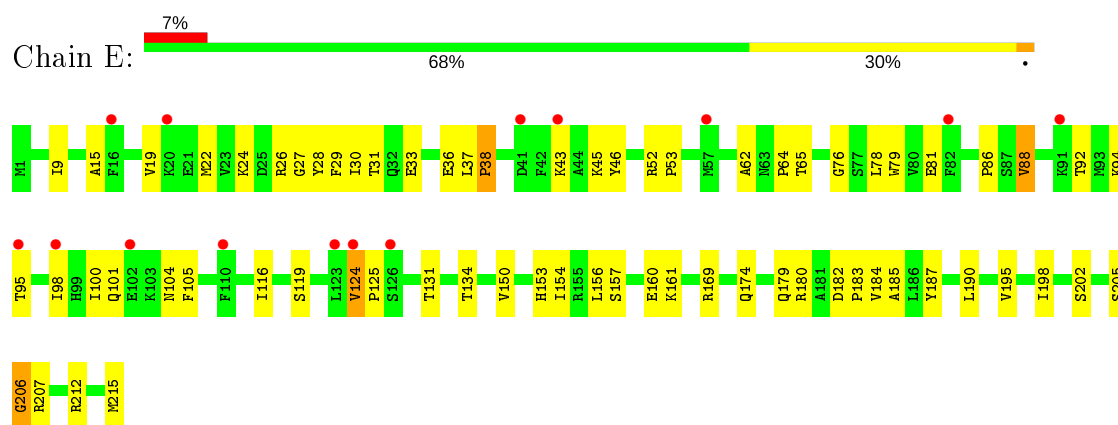


• Molecule 3: DNA-directed RNA polymerase II subunit RPB3

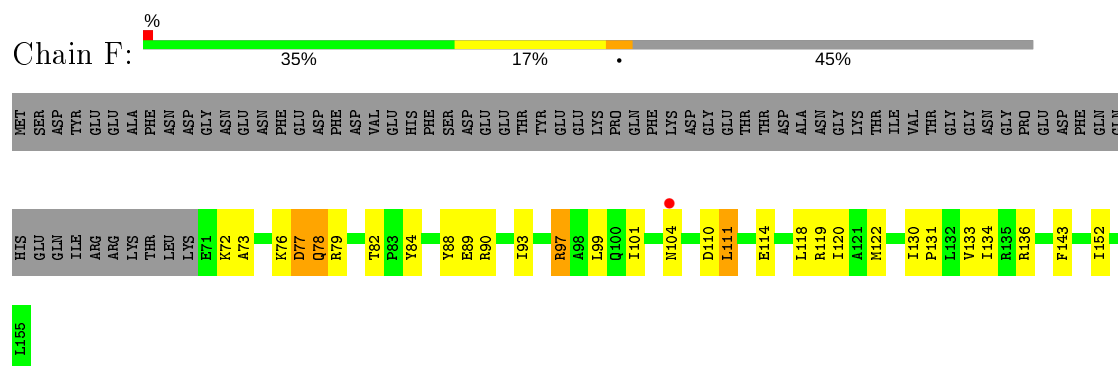




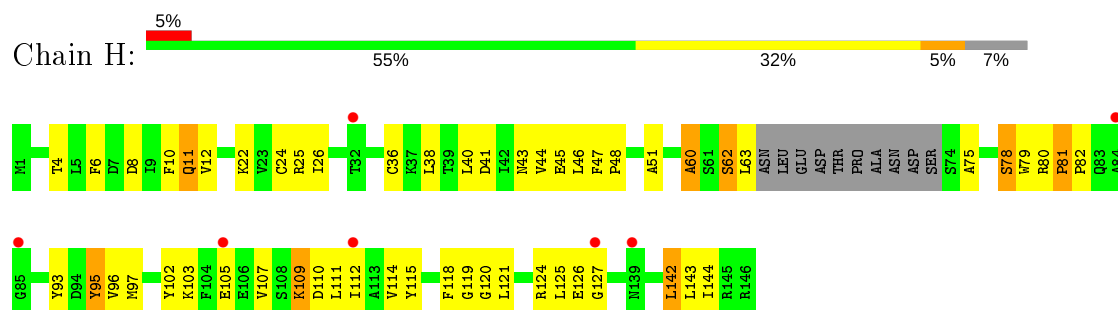
- Molecule 4: DNA-directed RNA polymerases I, II, and III subunit RPABC1



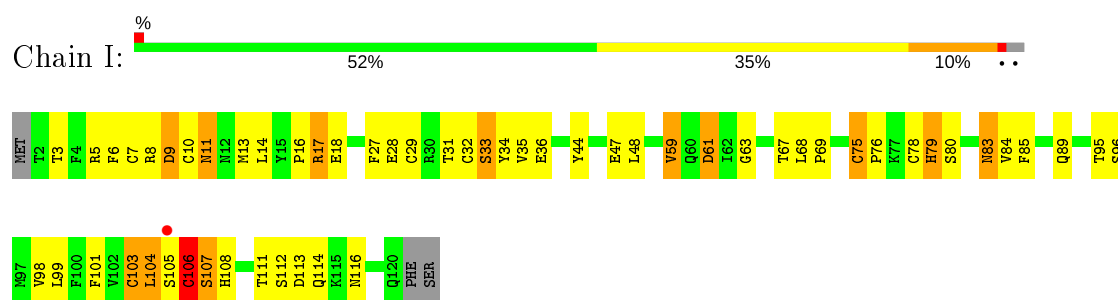
- Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC2



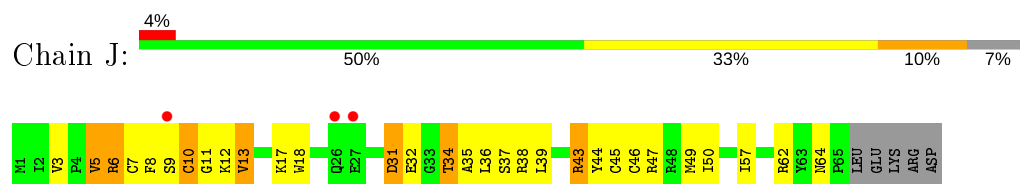
- Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC3



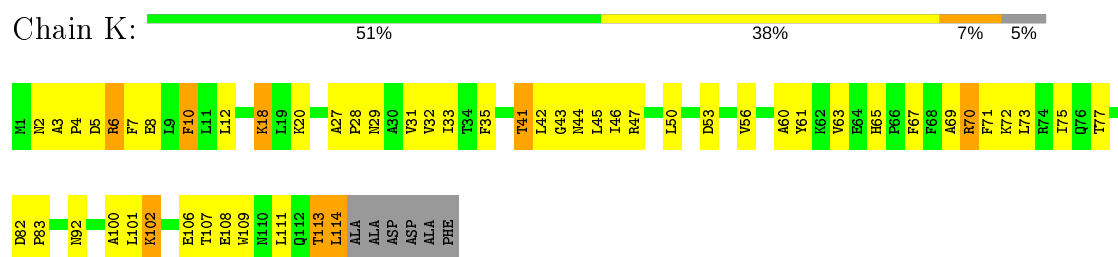
- Molecule 7: DNA-directed RNA polymerase II subunit RPB9



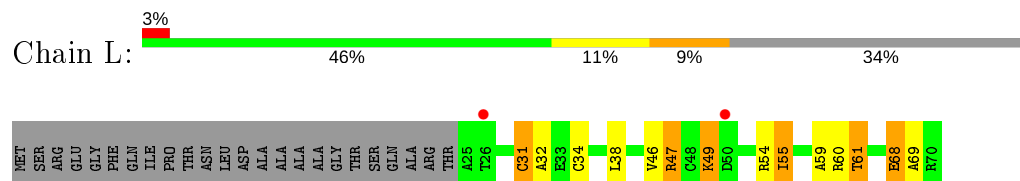
- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC5



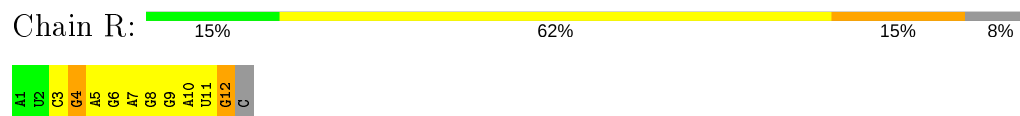
- Molecule 9: DNA-directed RNA polymerase II subunit RPB11



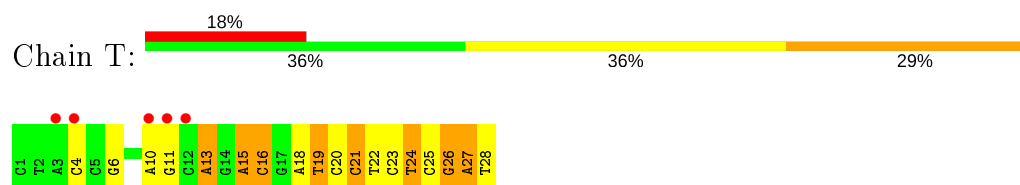
- Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC4



- Molecule 11: RNA (5'-R(\*AP\*UP\*CP\*GP\*AP\*GP\*AP\*GP\*GP\*AP\*UP\*GP\*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, $\alpha$ , $\beta$ , $\gamma$	170.92Å 225.50Å 195.93Å 90.00° 101.21° 90.00°	Depositor
Resolution (Å)	50.00 – 3.42 45.69 – 3.42	Depositor EDS
% Data completeness (in resolution range)	91.7 (50.00-3.42) 91.7 (45.69-3.42)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	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 (4.97%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	106.8	Xtriage
Anisotropy	0.267	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.25 , 77.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	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 <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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	0.73	1/11438 (0.0%)	0.77	11/15465 (0.1%)
2	B	0.80	5/9348 (0.1%)	0.80	5/12611 (0.0%)
3	C	0.92	1/2174 (0.0%)	0.82	3/2946 (0.1%)
4	E	0.79	1/1793 (0.1%)	0.70	1/2413 (0.0%)
5	F	0.65	0/696	0.71	0/940
6	H	0.66	0/1105	0.72	0/1495
7	I	0.80	1/989 (0.1%)	0.70	0/1331
8	J	0.93	2/541 (0.4%)	0.89	0/727
9	K	0.87	0/937	0.76	1/1265 (0.1%)
10	L	0.87	2/365 (0.5%)	0.86	0/485
11	R	0.74	0/292	1.18	0/455
12	T	1.29	2/634 (0.3%)	2.11	34/975 (3.5%)
13	N	1.21	1/317 (0.3%)	1.79	10/488 (2.0%)
All	All	0.80	16/30629 (0.1%)	0.86	65/41596 (0.2%)

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	T	23	DC	C1'-N1	6.70	1.57	1.49
13	N	2	DT	C1'-N1	5.91	1.56	1.49
8	J	17	LYS	CE-NZ	5.86	1.63	1.49
12	T	27	DA	N9-C4	5.85	1.41	1.37
1	A	1240	CYS	CB-SG	5.79	1.92	1.82
7	I	103	CYS	CB-SG	5.71	1.92	1.82
2	B	764	SER	CB-OG	5.69	1.49	1.42
10	L	68	GLU	CB-CG	5.46	1.62	1.52
10	L	68	GLU	CG-CD	5.31	1.59	1.51
3	C	138	GLU	CD-OE1	5.31	1.31	1.25
2	B	996	ARG	CZ-NH1	5.26	1.39	1.33
2	B	962	LYS	CE-NZ	5.20	1.62	1.49
8	J	13	VAL	CB-CG2	5.19	1.63	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	202	SER	CB-OG	5.16	1.49	1.42
2	B	847	ASP	CG-OD2	5.07	1.37	1.25
2	B	544	CYS	CB-SG	-5.04	1.73	1.81

All (65) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	T	16	DC	O4'-C4'-C3'	-15.04	96.98	106.00
12	T	27	DA	O4'-C4'-C3'	-10.64	99.61	106.00
12	T	22	DT	C4'-C3'-C2'	-9.48	94.57	103.10
12	T	15	DA	P-O3'-C3'	8.86	130.34	119.70
12	T	19	DT	C4-C5-C7	8.71	124.23	119.00
12	T	19	DT	C6-C5-C7	-8.62	117.73	122.90
12	T	23	DC	O4'-C1'-N1	8.25	113.78	108.00
12	T	16	DC	O4'-C1'-N1	8.16	113.71	108.00
12	T	22	DT	N3-C4-O4	7.96	124.68	119.90
12	T	22	DT	P-O3'-C3'	7.92	129.21	119.70
12	T	27	DA	O4'-C1'-N9	7.92	113.54	108.00
12	T	21	DC	C4'-C3'-C2'	-7.89	96.00	103.10
2	B	25	ILE	CB-CA-C	-7.82	95.96	111.60
12	T	21	DC	O4'-C4'-C3'	-7.67	101.40	106.00
12	T	16	DC	C4'-C3'-C2'	-7.42	96.42	103.10
12	T	20	DC	O4'-C4'-C3'	-7.34	101.56	104.50
13	N	3	DG	O4'-C1'-N9	7.17	113.02	108.00
13	N	10	DG	P-O3'-C3'	7.11	128.24	119.70
12	T	6	DG	P-O3'-C3'	6.91	127.99	119.70
12	T	24	DT	O4'-C1'-N1	6.85	112.79	108.00
12	T	23	DC	C6-N1-C2	-6.76	117.60	120.30
1	A	208	LEU	CA-CB-CG	6.75	130.84	115.30
1	A	936	LEU	CA-CB-CG	6.74	130.81	115.30
12	T	4	DC	O4'-C1'-N1	6.72	112.70	108.00
13	N	6	DT	O4'-C1'-N1	6.63	112.64	108.00
1	A	121	LEU	CA-CB-CG	6.61	130.49	115.30
13	N	1	DC	O4'-C1'-N1	6.55	112.59	108.00
1	A	117	GLU	N-CA-CB	6.46	122.23	110.60
2	B	74	LEU	CA-CB-CG	6.46	130.16	115.30
13	N	9	DC	O4'-C1'-N1	6.41	112.49	108.00
12	T	24	DT	N3-C4-O4	6.40	123.74	119.90
12	T	21	DC	P-O3'-C3'	6.37	127.34	119.70
1	A	116	ASP	CB-CA-C	-6.09	98.22	110.40
12	T	20	DC	C4'-C3'-C2'	-6.07	97.64	103.10
12	T	15	DA	C1'-O4'-C4'	-6.06	104.04	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	199	LEU	N-CA-CB	6.04	122.49	110.40
12	T	10	DA	O4'-C1'-N9	6.04	112.23	108.00
13	N	2	DT	C6-N1-C2	-5.88	118.36	121.30
9	K	114	LEU	CA-CB-CG	5.80	128.63	115.30
2	B	1156	ASP	N-CA-C	5.78	126.60	111.00
2	B	1026	LEU	CA-CB-CG	5.78	128.59	115.30
12	T	23	DC	C5-C6-N1	5.73	123.87	121.00
1	A	420	ARG	NE-CZ-NH2	-5.68	117.46	120.30
1	A	65	LEU	CA-CB-CG	5.60	128.19	115.30
13	N	5	DT	O4'-C1'-N1	5.57	111.90	108.00
13	N	2	DT	P-O3'-C3'	5.50	126.30	119.70
12	T	22	DT	C6-N1-C2	-5.44	118.58	121.30
13	N	13	DA	O4'-C1'-N9	5.43	111.80	108.00
12	T	26	DG	N3-C4-C5	-5.43	125.88	128.60
1	A	518	LYS	CB-CA-C	5.42	121.24	110.40
4	E	37	LEU	CA-CB-CG	5.42	127.76	115.30
2	B	1009	ASP	CB-CG-OD1	5.37	123.13	118.30
12	T	20	DC	P-O3'-C3'	5.34	126.11	119.70
3	C	183	TRP	N-CA-C	-5.27	96.76	111.00
12	T	27	DA	N1-C6-N6	-5.19	115.49	118.60
12	T	22	DT	C5-C4-O4	-5.18	121.27	124.90
3	C	47	ASP	CB-CG-OD2	5.17	122.95	118.30
12	T	27	DA	C2-N3-C4	5.14	113.17	110.60
1	A	472	LEU	CB-CG-CD1	-5.11	102.32	111.00
13	N	2	DT	O4'-C1'-N1	5.07	111.55	108.00
12	T	13	DA	P-O3'-C3'	5.06	125.78	119.70
12	T	11	DG	P-O3'-C3'	5.06	125.77	119.70
3	C	195	GLN	N-CA-C	5.04	124.62	111.00
12	T	26	DG	N3-C4-N9	5.03	129.02	126.00
1	A	426	LEU	CA-CB-CG	5.03	126.86	115.30

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	671	0
2	B	9168	0	9179	469	0
3	C	2135	0	2090	94	0
4	E	1757	0	1781	42	0
5	F	684	0	703	25	0
6	H	1087	0	1062	49	0
7	I	971	0	930	52	0
8	J	532	0	544	30	0
9	K	919	0	929	48	0
10	L	363	0	387	11	0
11	R	260	0	132	40	0
12	T	566	0	316	14	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	1	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	1450	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 24.

All (1450) 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
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
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:1169:ILE:CA	1:A:1170:ILE:HB	1.68	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1168:GLU:CA	1:A:1171:GLN:HB2	1.70	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
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:353:ILE:HD13	1:A:487:MET:HE2	1.34	1.10
11:R:4:G:H2'	11:R:5:A:H8	0.95	1.10
2:B:445:LYS:HA	2:B:446:LEU:HB3	1.24	1.10
1:A:1168:GLU:HA	1:A:1171:GLN:CB	1.82	1.10
1:A:1168:GLU:CB	1:A:1171:GLN:CB	2.30	1.10
1:A:1169:ILE:H	1:A:1170:ILE:C	1.55	1.09
1:A:58:LEU:O	1:A:58:LEU:HD22	1.50	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:1168:GLU:HB2	1:A:1171:GLN:HB3	1.07	1.06
1:A:55:ASP:H	1:A:56:PRO:CD	1.68	1.06
5:F:93:ILE:HD11	5:F:134:ILE:HD11	1.35	1.06
1:A:198:GLU:H	1:A:198:GLU:CD	1.59	1.06
1:A:1169:ILE:HG22	1:A:1170:ILE:HG12	1.38	1.05
1:A:1168:GLU:CB	1:A:1171:GLN:HB3	1.84	1.04
1:A:1092:LYS:HB3	1:A:1094:VAL:N	1.70	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: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
2:B:955:THR:HG22	2:B:956:THR:H	1.27	1.00
2:B:841:MET:HE3	2:B:980:PHE:CZ	1.96	1.00
2:B:980:PHE:CE1	2:B:990:ILE:HD11	1.97	0.99
1:A:1169:ILE:CB	1:A:1170:ILE:CB	2.30	0.98
1:A:313:GLN:HG2	1:A:314:ALA:CB	1.95	0.97
1:A:1246:LYS:O	1:A:1246:LYS:HD2	1.65	0.96
1:A:161:LEU:HD22	1:A:162:VAL:N	1.80	0.96
1:A:1169:ILE:HB	1:A:1170:ILE:HB	0.98	0.96
1:A:192:GLY:O	1:A:193:ASP:HB3	1.64	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:195:ASP:C	1:A:197:PRO:HD3	1.88	0.92
1:A:899:VAL:HB	1:A:929:LEU:HD11	1.51	0.92
3:C:167:HIS:HD2	3:C:169:LYS:H	1.15	0.92
1:A:1178:ASP:CB	1:A:1179:GLU:HA	1.98	0.92
1:A:40:THR:N	1:A:41:MET:HB2	1.83	0.92
2:B:341:LEU:H	2:B:341:LEU:HD22	1.35	0.91
1:A:485:ASP:OD2	11:R:10:A:H4'	1.70	0.91
1:A:445:ASN:HB3	1:A:455:MET:HG2	1.52	0.91
1:A:187:LYS:HZ2	1:A:188:ASP:H	1.15	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:HA	2:B:864:LYS:HE2	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:1173:HIS:NE2	1:A:1175:SER:HB3	1.88	0.89
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
2:B:841:MET:CE	2:B:980:PHE:CZ	2.56	0.88
1:A:310:GLY:H	1:A:311:GLN:HB3	1.37	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:351:THR:OG1	2:B:1103:ILE:HG12	1.73	0.87
1:A:470:LEU:HD21	1:A:487:MET:CE	2.05	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:58:LEU:C	1:A:58:LEU:HD22	1.96	0.84
1:A:566:ILE:HG23	1:A:566:ILE:O	1.77	0.84
1:A:160:GLN:CD	1:A:160:GLN:N	2.30	0.83
3:C:186:LEU:HB3	3:C:188:HIS:HD2	1.43	0.83
1:A:198:GLU:CD	1:A:198:GLU:N	2.30	0.83
1:A:666:ILE:HD11	2:B:1026:LEU:HB3	1.60	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:O	1:A:1170:ILE:HG22	1.78	0.83
1:A:1092:LYS:HB3	1:A:1093:LYS:C	1.99	0.82
1:A:55:ASP:N	1:A:56:PRO:CD	2.40	0.82
11:R:8:G:HO2'	11:R:9:G:H5'	1.43	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
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:CG2	1:A:1170:ILE:O	2.30	0.80
1:A:1085:HIS:CD2	1:A:1085:HIS:H	1.96	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1169:ILE:N	1:A:1170:ILE:C	2.36	0.79
1:A:1081:LEU:O	1:A:1083:THR:CB	2.30	0.79
1:A:310:GLY:H	1:A:311:GLN:CB	1.95	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:1178:ASP:CG	1:A:1179:GLU:HA	2.02	0.78
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
2:B:341:LEU:HB3	2:B:344:LYS:HE3	1.63	0.78
1:A:445:ASN:CB	1:A:455:MET:HG2	2.14	0.78
2:B:841:MET:HE3	2:B:980:PHE:CE1	2.18	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:NZ	1:A:187:LYS:HB2	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
1:A:1079:MET:HE1	1:A:1359:ASP:HB2	1.67	0.77
2:B:636:PRO:HB3	2:B:637:LEU:HA	1.65	0.77
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
1:A:470:LEU:HD21	1:A:487:MET:HE3	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
3:C:142:VAL:HG22	3:C:143:LEU:N	1.98	0.76
9:K:73:LEU:HD23	9:K:75:ILE:HD11	1.67	0.75
1:A:326:ARG:HG2	1:A:1406:VAL:HG21	1.68	0.75
1:A:187:LYS:O	1:A:189:ARG:HG3	1.85	0.75
1:A:1083:THR:CG2	1:A:1083:THR:O	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:1169:ILE:HB	1:A:1170:ILE:CG1	2.16	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
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
1:A:1083:THR:H	1:A:1084:PHE:CA	2.00	0.73
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:1167:GLU:O	1:A:1170:ILE:HG22	1.89	0.71
1:A:118:HIS:HE1	1:A:155:GLU:HG2	1.53	0.71
2:B:338:GLY:C	2:B:341:LEU:HD21	2.09	0.71
1:A:1402:PHE:CD2	1:A:1403:GLU:HB2	2.26	0.71
2:B:841:MET:HE1	2:B:980:PHE:CE2	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: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
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
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:N	2:B:341:LEU:HD22	2.07	0.70
1:A:185:TRP:HE3	1:A:198:GLU:HG2	1.56	0.70
1:A:470:LEU:HD21	1:A:487:MET:HE1	1.71	0.70
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
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:864:LYS:C	2:B:864:LYS:HD3	2.14	0.69
2:B:878:GLN:HG2	2:B:879:ARG:H	1.57	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:976:ILE:O	2:B:990:ILE:HB	1.92	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: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
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
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
1:A:53:LEU:HD23	1:A:53:LEU:C	2.13	0.67
2:B:636:PRO:CB	2:B:637:LEU:CA	2.71	0.67
1:A:53:LEU:CD2	1:A:54:ASN:N	2.57	0.67
1:A:401:GLY:O	1:A:435:HIS:CD2	2.48	0.67
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
11:R:8:G:C2'	11:R:9:G:H5'	2.25	0.67
1:A:187:LYS:HZ2	1:A:187:LYS:HB2	1.60	0.67
1:A:889:SER:HB2	1:A:892:ALA:H	1.60	0.67
3:C:182:PRO:HB3	3:C:207:CYS:SG	2.35	0.67
3:C:57:VAL:CG2	8:J:57:ILE:HD11	2.24	0.67
1:A:1084:PHE:CD2	1:A:1092:LYS:HG2	2.28	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
11:R:6:G:C2	11:R:7:A:C5	2.83	0.66
1:A:858:ASN:HD22	1:A:858:ASN:C	1.99	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:1117:GLN:HG2	2:B:1156:ASP:OD2	1.95	0.66
2:B:637:LEU:CD1	2:B:740:HIS:HB3	2.25	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:401:GLY:C	1:A:435:HIS:CD2	2.69	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: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:1167:GLU:O	1:A:1170:ILE:CG2	2.45	0.65
1:A:185:TRP:HH2	1:A:200:ARG:HD2	1.61	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:1168:GLU:HA	1:A:1170:ILE:O	1.97	0.65
1:A:1253:GLU:O	1:A:1254:ALA:C	2.34	0.65
1:A:189:ARG:NH2	1:A:196:GLU:O	2.30	0.65
2:B:862:GLN:HG2	2:B:963:PHE:HD1	1.62	0.65
1:A:1172:LEU:O	1:A:1174:PHE:N	2.30	0.65
1:A:765:VAL:HG22	1:A:800:VAL:HB	1.79	0.65
2:B:444:MET:CE	2:B:446:LEU:HD13	2.27	0.65
1:A:351:THR:HG23	1:A:352:VAL:N	2.11	0.65
2:B:445:LYS:HB3	2:B:447:ALA:H	1.61	0.65
2:B:65:GLU:CG	2:B:66:ASP:H	2.09	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:793:SER:HB2	1:A:794:PRO:HD2	1.77	0.64
1:A:482:PHE:O	2:B:989:THR:HG23	1.97	0.64
4:E:24:LYS:HB3	4:E:30:ILE:HD12	1.78	0.64
1:A:1444:MET:HB2	5:F:133:VAL:HG12	1.77	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:1082:ASN:N	1:A:1083:THR:HB	2.11	0.64
1:A:58:LEU:CD1	1:A:244:PRO:HD3	2.27	0.64
2:B:85:SER:N	2:B:86:ARG:HB3	2.11	0.64
1:A:1168:GLU:HG3	1:A:1168:GLU:O	1.96	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:517:ASN:O	1:A:518:LYS:HB3	1.96	0.64
1:A:56:PRO:O	1:A:58:LEU:N	2.30	0.64
1:A:738:LYS:NZ	3:C:194:GLU:HA	2.12	0.64
2:B:115:GLN:OE1	2:B:115:GLN:HA	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:163:ILE:HD13	9:K:10:PHE:CE1	2.32	0.64
3:C:133:ILE:HD11	3:C:237:SER:HA	1.79	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:CB	1:A:1093:LYS:C	2.66	0.63
2:B:444:MET:C	2:B:445:LYS:HG3	2.18	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
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
1:A:1246:LYS:C	1:A:1246:LYS:HD2	2.17	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:58:LEU:C	1:A:58:LEU:CD2	2.66	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:1077:THR:HG23	2:B:1079:LYS:H	1.62	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: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:1168:GLU:CG	1:A:1168:GLU:O	2.47	0.63
1:A:534:LEU:O	1:A:574:GLY:HA3	1.98	0.63
1:A:55:ASP:OD1	1:A:59:GLY:CA	2.33	0.63
2:B:341:LEU:CD2	2:B:341:LEU:H	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:438:GLU:O	2:B:439:ALA:C	2.37	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:338:GLY:C	2:B:341:LEU:CD2	2.68	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: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
2:B:841:MET:HE3	2:B:990:ILE:HD11	1.82	0.62
1:A:503:GLN:HE22	5:F:90:ARG:HH21	1.48	0.62
2:B:66:ASP:O	2:B:66:ASP:CG	2.38	0.62
1:A:731:ARG:HG3	1:A:755:PHE:CZ	2.35	0.62
1:A:310:GLY:CA	1:A:311:GLN:CB	2.71	0.61
2:B:459:TYR:C	2:B:459:TYR:CD2	2.74	0.61
1:A:1253:GLU:HG2	1:A:1253:GLU:O	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:1172:ILE:HG22	2:B:1174:LYS:HG3	1.83	0.61
2:B:190:TYR:CE1	8:J:62:ARG:HG2	2.35	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
1:A:320:ARG:HA	1:A:320:ARG:HE	1.65	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:CD	2:B:864:LYS:O	2.30	0.60
1:A:1179:GLU:HG3	1:A:1179:GLU:O	2.01	0.60
1:A:419:LYS:HZ3	1:A:419:LYS:HB3	1.66	0.60
1:A:466:SER:O	2:B:1103:ILE:HD11	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1081:LEU:C	1:A:1083:THR:OG1	2.40	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
7:I:83:ASN:C	7:I:83:ASN:HD22	2.06	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
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:1118:VAL:HG23	1:A:1306:LEU:HB2	1.83	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
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:1178:ASP:CB	1:A:1179:GLU:CA	2.77	0.59
1:A:324:SER:OG	1:A:325:ILE:N	2.36	0.59
1:A:413:ILE:HD12	1:A:413:ILE:N	2.18	0.59
1:A:119:ASN:O	1:A:120:GLU:O	2.21	0.59
1:A:58:LEU:HG	1:A:80:HIS:HB2	1.84	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1170:ILE:O	1:A:1171:GLN:HB2	2.02	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
2:B:440:HIS:C	2:B:442:PHE:H	2.07	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
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:1223:ASP:O	1:A:1224:LEU:HB3	2.03	0.58
1:A:53:LEU:CD2	1:A:54:ASN:HB3	2.33	0.58
2:B:652:LYS:HB3	2:B:689:LEU:HD23	1.85	0.58
3:C:142:VAL:CG2	3:C:143:LEU:H	2.05	0.58
3:C:27:LEU:HD12	3:C:228:PHE:HE2	1.69	0.58
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:575:LYS:NZ	1:A:615:GLY:O	2.33	0.57
1:A:848:ILE:HD13	1:A:858:ASN:HB3	1.86	0.57
2:B:839:MET:HE3	2:B:1010:LEU:HD12	1.86	0.57
1:A:356:ASP:OD2	9:K:65:HIS:HE1	1.87	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:459:TYR:C	2:B:459:TYR:HD2	2.08	0.57
2:B:628:THR:O	2:B:628:THR:HG22	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:1178:ASP:OD2	1:A:1179:GLU:HA	2.04	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
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:1085:HIS:CD2	1:A:1085:HIS:N	2.71	0.57
1:A:1089:VAL:HG13	1:A:1089:VAL:O	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:527:THR:HG21	1:A:650:GLN:HG2	1.86	0.57
1:A:587:HIS:HE2	1:A:969:GLN:HG2	1.68	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:1246:LYS:C	1:A:1246:LYS:CD	2.73	0.57
1:A:1015:VAL:HG12	1:A:1019:CYS:SG	2.44	0.57
1:A:900:ASP:HA	1:A:926:GLN:HE22	1.70	0.57
2:B:274:PRO:HB2	2:B:359:GLU:HB3	1.87	0.57
2:B:716:ASN:O	2:B:717:GLU:HB2	2.04	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
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
2:B:778:MET:HE2	2:B:1094:ARG:HD3	1.85	0.56
2:B:1168:LEU:HD13	2:B:1208:MET:HE3	1.87	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:1072:ILE:O	1:A:1075:PRO:HD2	2.05	0.56
1:A:902:LEU:HG	1:A:926:GLN:HG3	1.87	0.56
2:B:980:PHE:CE1	2:B:990:ILE:CG1	2.89	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:O	1:A:35:ILE:HG22	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1081:LEU:C	1:A:1083:THR:CB	2.74	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:1001:PHE:HE1	3:C:178:PHE:HB3	1.71	0.56
1:A:1167:GLU:C	1:A:1170:ILE:HG22	2.26	0.56
1:A:1169:ILE:N	1:A:1170:ILE:HG22	2.21	0.56
1:A:419:LYS:HZ2	1:A:419:LYS:HB3	1.69	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
2:B:65:GLU:HG2	2:B:66:ASP:N	2.21	0.56
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
1:A:1192:LEU:HG	1:A:1193:LEU:N	2.21	0.55
1:A:343:LYS:HZ1	2:B:1197:PRO:HB3	1.69	0.55
2:B:102:VAL:HG12	2:B:112:LEU:HB2	1.88	0.55
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
2:B:221:ASN:OD1	2:B:242:SER:HA	2.06	0.55
2:B:516:ASN:ND2	2:B:516:ASN:H	2.04	0.55
1:A:1017:LEU:HB2	4:E:206:GLY:H	1.70	0.55
6:H:107:VAL:O	6:H:109:LYS:HG3	2.06	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: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:1169:ILE:H	1:A:1170:ILE:CG2	2.20	0.55
1:A:540:PHE:HB3	1:A:571:LEU:HD23	1.88	0.55
1:A:31:SER:HB2	1:A:81:PHE:O	2.07	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:1134:ILE:O	1:A:1138:ILE:HG12	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
1:A:901:LEU:N	1:A:926:GLN:HE21	2.05	0.55
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:1219:THR:HG21	1:A:1271:ILE:HD11	1.90	0.54
1:A:836:TYR:CE2	1:A:840:ARG:HD2	2.42	0.54
2:B:65:GLU:CG	2:B:66:ASP:N	2.69	0.54
1:A:824:LEU:O	11:R:12:G:N2	2.38	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:1084:GLN:HG2	3:C:201:TRP:CZ2	2.42	0.54
1:A:1081:LEU:C	1:A:1083:THR:HB	2.27	0.54
1:A:1092:LYS:HG3	1:A:1094:VAL:O	2.08	0.54
1:A:198:GLU:OE2	1:A:198:GLU:N	2.39	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
2:B:843:GLN:HG2	2:B:993:THR:CB	2.35	0.54
8:J:9:SER:OG	8:J:45:CYS:HB2	2.07	0.54
3:C:3:GLU:HG2	9:K:100:ALA:HB1	1.90	0.54
1:A:351:THR:HG22	1:A:352:VAL:O	2.08	0.54
3:C:27:LEU:HD12	3:C:228:PHE:CE2	2.41	0.54
1:A:369:SER:HB2	9:K:2:ASN:OD1	2.08	0.54
1:A:567:LYS:HZ1	6:H:46:LEU:HB2	1.73	0.54
3:C:69:LEU:H	3:C:69:LEU:HD23	1.73	0.54
1:A:1169:ILE:CG2	1:A:1170:ILE:CB	2.86	0.54
1:A:1172:LEU:O	1:A:1173:HIS:C	2.45	0.54
1:A:151:ASP:HB2	1:A:162:VAL:O	2.08	0.54
2:B:1084:GLN:CD	2:B:1084:GLN:H	2.11	0.54
12:T:13:DA:H61	13:N:2:DT:C7	2.20	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1163:CYS:HB3	2:B:1167:GLY:H	1.72	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
6:H:95:TYR:HD2	6:H:95:TYR:C	2.10	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:769:SER:OG	1:A:1085:HIS:CE1	2.60	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:1319:VAL:HG12	1:A:1322:ILE:HG23	1.90	0.53
1:A:351:THR:HG23	1:A:352:VAL:H	1.72	0.53
3:C:52:GLU:HB3	3:C:154:LYS:HB3	1.89	0.53
1:A:1084:PHE:CD1	1:A:1084:PHE:N	2.74	0.53
1:A:1259:MET:O	1:A:1262:LYS:N	2.40	0.53
1:A:871:ASP:OD1	1:A:1366:ARG:NH2	2.41	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:143:LEU:C	3:C:143:LEU:HD12	2.29	0.53
6:H:93:TYR:CD1	6:H:143:LEU:HD23	2.42	0.53
3:C:165:LYS:O	9:K:6:ARG:NH1	2.40	0.53
1:A:907:THR:HG22	1:A:908:LEU:N	2.22	0.53
1:A:1079:MET:CE	1:A:1359:ASP:CB	2.78	0.53
1:A:53:LEU:HD23	1:A:54:ASN:CA	2.38	0.53
1:A:630:ILE:HD12	1:A:630:ILE:N	2.23	0.53
1:A:1220:PHE:O	1:A:1221:LYS:HB2	2.09	0.53
1:A:658:LEU:HG	1:A:659:HIS:CD2	2.44	0.53
2:B:560:GLU:O	2:B:561:TRP:CD1	2.62	0.53
6:H:95:TYR:CD2	6:H:95:TYR:C	2.81	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:302:THR:HG23	1:A:306:ASN:HB3	1.91	0.53
1:A:53:LEU:HD23	1:A:54:ASN:CB	2.38	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:J:10:CYS:SG	8:J:46:CYS:SG	3.07	0.53
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
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
2:B:338:GLY:H	2:B:341:LEU:HD21	1.73	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
3:C:29:MET:HE2	9:K:45:LEU:HD11	1.90	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
2:B:842:ASN:HD22	2:B:845:SER:HB3	1.73	0.52
6:H:36:CYS:HA	6:H:126:GLU:O	2.09	0.52
6:H:26:ILE:HG22	6:H:40:LEU:O	2.09	0.52
1:A:1082:ASN:HA	1:A:1083:THR:HB	0.66	0.52
1:A:265:LYS:HA	1:A:268:ASP:HB2	1.91	0.52
7:I:80:SER:HB3	7:I:105:SER:HB2	1.91	0.52
1:A:388:LEU:HA	1:A:391:LEU:HD12	1.91	0.52
1:A:343:LYS:HE2	2:B:1151:LEU:HD23	1.91	0.52
2:B:273:LEU:HD21	2:B:360:PHE:CD1	2.36	0.52
5:F:82:THR:HG22	5:F:84:TYR:H	1.75	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:548:ASN:OD1	9:K:60:ALA:HB1	2.09	0.52
1:A:1281:ARG:O	1:A:1281:ARG:HG3	2.09	0.52
2:B:1168:LEU:HD13	2:B:1208:MET:CE	2.40	0.52
2:B:712:PRO:O	2:B:713:ALA:HB2	2.10	0.52
2:B:85:SER:CA	2:B:86:ARG:HB3	2.40	0.52
1:A:890:ASP:OD2	1:A:1296:GLY:HA2	2.09	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
2:B:434:ARG:HA	2:B:437:GLU:HG3	1.92	0.52
2:B:879:ARG:CZ	2:B:879:ARG:HA	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:259:LEU:HD21	9:K:92:ASN:OD1	2.10	0.52
3:C:69:LEU:N	3:C:69:LEU:CD2	2.73	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
1:A:645:LEU:O	1:A:646:PHE:C	2.48	0.51
2:B:428:ILE:O	2:B:432:MET:HG3	2.10	0.51
2:B:444:MET:O	2:B:445:LYS:HG3	2.10	0.51
2:B:464:GLY:HA3	2:B:479:VAL:O	2.10	0.51
2:B:487:THR:HG22	2:B:488:TYR:N	2.24	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
2:B:132:VAL:HG21	2:B:445:LYS:HZ1	1.75	0.51
2:B:616:ILE:N	2:B:616:ILE:HD12	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
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:CD2	9:K:10:PHE:N	2.78	0.51
1:A:172:PRO:HD3	1:A:185:TRP:HE1	1.75	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:1181:GLU:HA	2:B:1187:ASN:O	2.10	0.51
2:B:341:LEU:HB3	2:B:344:LYS:CE	2.36	0.51
5:F:73:ALA:HB2	5:F:143:PHE:CZ	2.46	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
1:A:662:PHE:HB3	2:B:829:CYS:SG	2.51	0.51
3:C:47:ASP:HA	10:L:69:ALA:CB	2.34	0.51
4:E:179:GLN:O	4:E:182:ASP:HB2	2.11	0.51
4:E:9:ILE:HD12	4:E:53:PRO:HG3	1.93	0.51
8:J:3:VAL:HG21	8:J:18:TRP:CB	2.40	0.51
1:A:255:SER:HA	1:A:256:GLN:C	2.31	0.51
1:A:56:PRO:C	1:A:58:LEU:N	2.63	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
2:B:1174:LYS:HB2	2:B:1179:GLN:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:886:LYS:HB2	2:B:890:TYR:OH	2.11	0.51
11:R:6:G:C2	11:R:7:A:C8	2.98	0.51
2:B:87:LYS:NZ	2:B:436:VAL:HG11	2.26	0.50
1:A:738:LYS:HZ1	3:C:194:GLU:HA	1.75	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
1:A:161:LEU:HD22	1:A:161:LEU:C	2.28	0.50
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:OE1	1:A:160:GLN:N	2.43	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
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:964:VAL:HG12	2:B:965:LYS:N	2.26	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:1429:ILE:O	1:A:1429:ILE:HG22	2.12	0.50
2:B:1142:GLY:HA3	5:F:88:TYR:HE2	1.77	0.50
2:B:717:GLU:O	2:B:718:GLU:C	2.50	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
1:A:338:GLY:HA2	2:B:1129:ARG:HH22	1.76	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:1146:VAL:O	1:A:1197:LEU:HD23	2.12	0.50
1:A:125:ALA:O	1:A:128:ILE:HG22	2.12	0.50
1:A:194:ALA:C	1:A:195:ASP:OD2	2.50	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
2:B:115:GLN:HG2	2:B:193:LYS:HB2	1.94	0.50
2:B:20:ASP:N	2:B:655:LYS:HZ3	2.10	0.50
3:C:124:LEU:C	3:C:126:GLY:N	2.65	0.50
5:F:76:LYS:O	5:F:77:ASP:O	2.30	0.50
1:A:567:LYS:HE2	6:H:95:TYR:CZ	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:715:GLU:O	1:A:719:VAL:HG23	2.12	0.50
1:A:1410:PHE:HD2	2:B:1212:ILE:HD11	1.77	0.50
1:A:1167:GLU:O	1:A:1170:ILE:O	2.30	0.49
1:A:482:PHE:CE1	2:B:836:GLU:HB2	2.47	0.49
1:A:531:ILE:O	1:A:531:ILE:HG12	2.12	0.49
1:A:668:ASP:OD2	1:A:742:ASN:HB2	2.12	0.49
2:B:1149:GLU:C	2:B:1151:LEU:H	2.15	0.49
2:B:308:TRP:O	2:B:311:LEU:N	2.45	0.49
2:B:71:LEU:HG	2:B:72:GLU:HB2	1.93	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
2:B:868:MET:C	2:B:869:SER:OG	2.51	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:1227:ILE:HG22	1:A:1228:TRP:H	1.77	0.49
1:A:719:VAL:O	1:A:723:ASN:ND2	2.45	0.49
3:C:241:ASP:HB3	9:K:109:TRP:CZ2	2.47	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:1255:GLU:O	1:A:1255:GLU:HG3	2.10	0.49
1:A:1364:ASN:OD1	1:A:1366:ARG:HD2	2.13	0.49
2:B:807:ARG:HG2	2:B:1045:SER:OG	2.12	0.49
2:B:340:ALA:O	2:B:342:GLY:N	2.44	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:1131:ALA:HA	1:A:1134:ILE:HD12	1.94	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:39:GLU:HB3	1:A:41:MET:CB	2.41	0.49
2:B:981:ALA:C	2:B:1092:TYR:CE2	2.86	0.49
1:A:413:ILE:CD1	1:A:413:ILE:N	2.75	0.49
1:A:465:TYR:CD1	1:A:465:TYR:N	2.81	0.49
1:A:590:ARG:O	1:A:591:PHE:HB2	2.13	0.49
2:B:784:ASN:CG	2:B:788:ARG:HD2	2.32	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
8:J:8:PHE:CD1	8:J:49:MET:HE1	2.48	0.49
12:T:26:DG:H21	12:T:27:DA:H1'	1.78	0.49
1:A:1081:LEU:O	1:A:1083:THR:CG2	2.60	0.49
1:A:188:ASP:C	1:A:189:ARG:CG	2.80	0.49
6:H:4:THR:HA	6:H:60:ALA:CB	2.43	0.49
1:A:1406:VAL:HG12	1:A:1410:PHE:CE1	2.48	0.49
1:A:523:ILE:HG23	1:A:527:THR:OG1	2.13	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
9:K:6:ARG:C	9:K:8:GLU:H	2.16	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
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
1:A:1017:LEU:HB2	4:E:205:SER:HA	1.95	0.48
5:F:133:VAL:O	5:F:133:VAL:HG13	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:185:TRP:O	1:A:186:LYS:CG	2.61	0.48
1:A:18:GLN:O	2:B:1215:ARG:HG2	2.13	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
1:A:1030:ARG:C	1:A:1032:LEU:H	2.16	0.48
1:A:1287:TYR:CD2	1:A:1305:VAL:HG21	2.48	0.48
1:A:351:THR:HG22	1:A:352:VAL:N	2.28	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:1057:VAL:HG12	1:A:1058:VAL:O	2.12	0.48
1:A:1089:VAL:CG1	1:A:1089:VAL:O	2.61	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
3:C:35:ARG:NH1	9:K:41:THR:OG1	2.47	0.48
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
1:A:591:PHE:HA	1:A:595:THR:HG21	1.95	0.48
2:B:1175:LEU:HD23	2:B:1176:ASN:N	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:64:CYS:SG	2:B:65:GLU:N	2.86	0.48
1:A:738:LYS:HZ3	3:C:194:GLU:HA	1.78	0.48
8:J:43:ARG:NH1	8:J:43:ARG:HB3	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
3:C:167:HIS:CD2	3:C:168:ALA:N	2.81	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:820:GLY:N	2:B:1091:TYR:OH	2.47	0.48
2:B:337:ARG:NH1	2:B:344:LYS:NZ	2.62	0.48
2:B:35:SER:HB3	2:B:811:TYR:CE2	2.49	0.48
1:A:1119:TYR:HD1	1:A:1326:ARG:HB3	1.79	0.48
2:B:519:TRP:HZ2	2:B:705:MET:HE1	1.78	0.48
2:B:717:GLU:O	2:B:720:ASP:N	2.47	0.48
2:B:793:ALA:C	2:B:794:ASN:HD22	2.17	0.48
2:B:868:MET:O	2:B:869:SER:OG	2.30	0.48
1:A:1376:THR:HG22	4:E:212:ARG:HH22	1.78	0.48
9:K:65:HIS:CD2	9:K:67:PHE:HB2	2.43	0.48
1:A:417:TYR:HB2	1:A:418:SER:H	1.52	0.48
1:A:402:ALA:HA	1:A:435:HIS:HD2	1.79	0.48
1:A:900:ASP:HA	1:A:926:GLN:NE2	2.28	0.48
2:B:25:ILE:HD11	2:B:653:VAL:HB	1.95	0.48
1:A:1188:GLN:O	1:A:1244:ARG:HD3	2.14	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
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
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:1243:VAL:HG13	1:A:1244:ARG:HB2	1.95	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
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:153:PRO:C	1:A:155:GLU:H	2.17	0.47
1:A:541:ILE:HD13	1:A:549:MET:HE3	1.95	0.47
1:A:598:LEU:HB3	6:H:25:ARG:HH12	1.78	0.47
1:A:6:TYR:O	2:B:1175:LEU:HD21	2.14	0.47
2:B:567:GLU:CD	2:B:567:GLU:H	2.17	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HH11	2:B:485:ARG:HG2	1.79	0.47
2:B:865:LYS:HG2	2:B:867:GLY:C	2.34	0.47
3:C:238:ILE:HG22	3:C:239:PRO:O	2.14	0.47
1:A:184:SER:HB2	1:A:199:LEU:HD23	1.97	0.47
1:A:53:LEU:CD2	1:A:54:ASN:CB	2.91	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:1103:ILE:O	2:B:1122:ARG:NH1	2.47	0.47
2:B:438:GLU:HG2	2:B:440:HIS:CD2	2.49	0.47
1:A:67:CYS:O	1:A:70:CYS:HB2	2.14	0.47
6:H:142:LEU:HD12	6:H:143:LEU:N	2.29	0.47
1:A:4:GLN:O	1:A:5:GLN:HG3	2.14	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
2:B:69:LEU:H	2:B:90:ILE:HG22	1.79	0.47
4:E:27:GLY:O	4:E:65:THR:HG22	2.15	0.47
11:R:6:G:N1	11:R:7:A:C5	2.83	0.47
1:A:1253:GLU:O	1:A:1255:GLU:HG2	2.14	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:91:PHE:H	1:A:297:GLN:NE2	2.10	0.47
2:B:1082:MET:HA	3:C:189:THR:HA	1.97	0.47
2:B:999:MET:HG2	2:B:1007:VAL:HG13	1.95	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
2:B:445:LYS:HA	2:B:447:ALA:H	1.79	0.47
1:A:254:GLU:HG3	2:B:918:ILE:HG21	1.97	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
1:A:1407:GLU:H	1:A:1407:GLU:CD	2.18	0.47
9:K:18:LYS:O	9:K:18:LYS:HD3	2.14	0.47
11:R:5:A:N3	11:R:6:G:C8	2.83	0.47
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:56:PRO:C	1:A:58:LEU:H	2.18	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:1245:PRO:O	1:A:1246:LYS:CG	2.61	0.46
1:A:13:THR:HG22	1:A:14:VAL:N	2.30	0.46
3:C:29:MET:HE3	3:C:29:MET:HB2	1.86	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
3:C:15:LYS:HZ2	9:K:114:LEU:HD13	1.79	0.46
6:H:47:PHE:HB3	6:H:95:TYR:CD1	2.51	0.46
1:A:1144:LYS:HD2	1:A:1269:GLU:HG2	1.97	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:75:ASN:HA	2:B:1116:ARG:HH22	1.79	0.46
2:B:31:TRP:CZ3	2:B:34:ILE:HD12	2.49	0.46
2:B:31:TRP:O	2:B:34:ILE:N	2.48	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:841:MET:CE	2:B:980:PHE:CE2	2.87	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:1098:VAL:N	1:A:1099:PRO:CD	2.79	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
1:A:873:MET:HG2	1:A:957:PRO:HG3	1.97	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
6:H:41:ASP:HB2	6:H:121:LEU:HB3	1.96	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
1:A:61:ILE:O	1:A:63:ARG:NH2	2.49	0.46
1:A:649:ILE:O	1:A:653:VAL:HG23	2.16	0.46
3:C:93:ASP:O	3:C:127:ARG:NH2	2.48	0.46
4:E:153:HIS:O	4:E:154:ILE:HD13	2.15	0.46
4:E:45:LYS:HD3	4:E:46:TYR:HE1	1.81	0.46
7:I:106:CYS:O	7:I:107:SER:HB2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:361:LEU:HD21	2:B:377:PHE:CD2	2.51	0.46
2:B:794:ASN:HD22	2:B:794:ASN:N	2.14	0.46
2:B:122:LEU:HD22	2:B:958:GLN:HG3	1.97	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: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
1:A:757:ASN:O	1:A:761:MET:HG3	2.15	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
2:B:440:HIS:C	2:B:442:PHE:N	2.68	0.46
2:B:547:VAL:HG12	2:B:612:GLU:OE2	2.16	0.46
3:C:127:ARG:HG3	3:C:129:ILE:HG22	1.98	0.46
3:C:114:TYR:CD2	3:C:140:ASN:HB3	2.51	0.46
8:J:44:TYR:C	8:J:44:TYR:CD1	2.89	0.46
2:B:658:ILE:HA	2:B:658:ILE:HD12	1.87	0.46
4:E:45:LYS:HD3	4:E:46:TYR:CE1	2.51	0.46
2:B:488:TYR:C	2:B:490:SER:H	2.19	0.45
11:R:7:A:C2	11:R:8:G:C5	3.04	0.45
1:A:1168:GLU:CA	1:A:1170:ILE:HG22	2.47	0.45
1:A:1236:LEU:C	1:A:1237:ILE:HG13	2.35	0.45
1:A:286:HIS:HB3	1:A:287:HIS:CB	2.43	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: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
3:C:46:ILE:HG23	3:C:157:CYS:HB3	1.97	0.45
1:A:862:ASN:OD1	4:E:174:GLN:HA	2.16	0.45
1:A:1081:LEU:C	1:A:1083:THR:HG1	2.18	0.45
1:A:1168:GLU:HB3	1:A:1171:GLN:HG3	1.98	0.45
1:A:1449:SER:HA	1:A:1450:LEU:C	2.37	0.45
1:A:298:PHE:HE1	1:A:313:GLN:HG3	1.80	0.45
1:A:557:ASP:OD1	1:A:559:VAL:HB	2.17	0.45
2:B:438:GLU:CG	2:B:440:HIS:CD2	2.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:444:MET:HE3	2:B:446:LEU:HD13	1.96	0.45
6:H:142:LEU:HD12	6:H:142:LEU:C	2.37	0.45
1:A:1116:LEU:HB2	1:A:1308:THR:HB	1.98	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
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:1098:VAL:N	1:A:1099:PRO:HD2	2.31	0.45
1:A:365:GLY:O	1:A:468:PHE:HA	2.17	0.45
1:A:526:ASP:HB2	2:B:835:GLN:CD	2.37	0.45
1:A:775:ILE:HB	1:A:797:LYS:C	2.36	0.45
1:A:815:PHE:O	1:A:818:MET:N	2.50	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:1392:SER:O	1:A:1393:ASN:C	2.54	0.45
1:A:19:PHE:O	1:A:1416:ALA:HA	2.17	0.45
1:A:219:PHE:O	1:A:222:LEU:HD12	2.17	0.45
1:A:37:PHE:HB2	1:A:52:GLY:HA3	1.99	0.45
2:B:839:MET:CE	2:B:1010:LEU:HD12	2.46	0.45
2:B:662:MET:C	2:B:664:THR:H	2.19	0.45
5:F:130:ILE:HA	5:F:131:PRO:HD3	1.79	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
1:A:86:LEU:HB2	1:A:237:THR:O	2.16	0.45
1:A:921:GLY:O	1:A:922:ASP:HB3	2.17	0.45
2:B:344:LYS:HG3	2:B:348:ARG:HB3	1.98	0.45
2:B:386:LEU:C	2:B:388:CYS:H	2.19	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:1082:ASN:N	1:A:1083:THR:CB	2.76	0.45
1:A:189:ARG:CZ	1:A:196:GLU:O	2.64	0.45
1:A:249:SER:C	1:A:250:ILE:HG13	2.36	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
2:B:757:PRO:HB3	2:B:1044:ALA:HB1	1.97	0.45
2:B:48:LEU:HD23	2:B:173:MET:SD	2.57	0.45
2:B:282:ILE:HD12	2:B:283:VAL:N	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:63:ILE:HD12	2:B:63:ILE:HA	1.65	0.45
4:E:205:SER:O	4:E:206:GLY:C	2.56	0.45
1:A:1152:ILE:HB	7:I:44:TYR:HB3	1.98	0.45
2:B:620:ARG:NH1	7:I:68:LEU:HD21	2.32	0.45
1:A:1017:LEU:HD12	4:E:206:GLY:H	1.82	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:558:LEU:C	2:B:560:GLU:H	2.19	0.44
2:B:71:LEU:H	2:B:88:TYR:HA	1.82	0.44
9:K:108:GLU:O	9:K:111:LEU:HB2	2.17	0.44
9:K:35:PHE:HD1	9:K:35:PHE:H	1.65	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:492:PRO:HB3	1:A:497:THR:CG2	2.46	0.44
1:A:847:ASP:HB3	1:A:1424:VAL:HG23	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:70:ILE:HB	2:B:71:LEU:HA	1.99	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:999:MET:HG2	2:B:1008:PRO:HD2	2.00	0.44
2:B:235:SER:OG	2:B:236:HIS:HD2	2.01	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
9:K:82:ASP:OD1	9:K:83:PRO:HD2	2.17	0.44
1:A:1017:LEU:HD12	4:E:206:GLY:N	2.32	0.44
1:A:873:MET:C	1:A:1058:VAL:HG23	2.37	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
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
2:B:973:ILE:CG2	2:B:974:PRO:HD2	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:173:ALA:O	3:C:233:GLU:O	2.35	0.44
3:C:70:ILE:HA	3:C:71:PRO:HD3	1.83	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:17:ARG:NH1	7:I:17:ARG:HB2	2.31	0.44
7:I:5:ARG:HG3	7:I:6:PHE:N	2.33	0.44
9:K:56:VAL:HA	9:K:77:THR:HG22	1.99	0.44
1:A:1092:LYS:CG	1:A:1094:VAL:O	2.66	0.44
1:A:115:LEU:HD12	1:A:122:MET:CE	2.48	0.44
1:A:1443:VAL:C	1:A:1444:MET:HG2	2.38	0.44
1:A:188:ASP:C	1:A:189:ARG:HG3	2.38	0.44
1:A:198:GLU:O	1:A:198:GLU:OE1	2.35	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:877:HIS:O	1:A:878:ILE:HG13	2.17	0.44
1:A:956:LEU:HA	1:A:956:LEU:HD23	1.61	0.44
2:B:826:ALA:O	2:B:1011:ILE:HA	2.17	0.44
1:A:497:THR:HG23	2:B:1146:PHE:HD1	1.82	0.44
7:I:84:VAL:HG22	7:I:85:PHE:N	2.33	0.44
1:A:1195:LEU:HB2	1:A:1238:ILE:HB	1.99	0.44
1:A:305:ASP:OD1	1:A:306:ASN:N	2.51	0.44
1:A:37:PHE:HB3	1:A:39:GLU:OE1	2.18	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:112:ASN:ND2	3:C:146:LYS:HD3	2.33	0.44
4:E:29:PHE:C	4:E:30:ILE:HG13	2.38	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
1:A:1079:MET:HE3	1:A:1359:ASP:HB2	1.91	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
2:B:863:GLU:CB	2:B:864:LYS:HB2	2.36	0.44
2:B:73:GLN:HG3	2:B:86:ARG:HG3	1.98	0.44
6:H:78:SER:O	6:H:79:TRP:C	2.56	0.44
7:I:75:CYS:HB2	7:I:78:CYS:SG	2.57	0.44
7:I:75:CYS:SG	7:I:78:CYS:SG	3.16	0.44
11:R:8:G:C2'	11:R:9:G:C5'	2.96	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1064:VAL:O	1:A:1064:VAL:HG12	2.18	0.44
2:B:121:ASN:HD22	2:B:121:ASN:N	2.16	0.44
2:B:794:ASN:C	2:B:795:ILE:HD12	2.38	0.44
2:B:995:ARG:HB3	2:B:997:GLU:OE2	2.17	0.44
5:F:133:VAL:CG1	5:F:133:VAL:O	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
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:1098:MET:O	2:B:1099:VAL:C	2.55	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
8:J:50:ILE:HD13	8:J:50:ILE:HA	1.74	0.43
9:K:7:PHE:CD1	9:K:7:PHE:C	2.91	0.43
1:A:942:PHE:C	1:A:942:PHE:CD2	2.90	0.43
2:B:1033:LYS:HA	2:B:1089:PRO:HG2	2.00	0.43
2:B:745:PRO:C	2:B:747:MET:N	2.70	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:1269:GLU:O	1:A:1270:ASN:CB	2.66	0.43
1:A:185:TRP:O	1:A:186:LYS:HB2	2.18	0.43
2:B:386:LEU:C	2:B:388:CYS:N	2.71	0.43
2:B:745:PRO:O	2:B:748:ILE:HG12	2.19	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:HE3	3:C:137:LYS:HB3	1.82	0.43
5:F:77:ASP:O	5:F:78:GLN:O	2.37	0.43
1:A:1147:THR:HB	7:I:48:LEU:HD12	2.01	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:46:THR:C	1:A:48:ALA:H	2.21	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:31:TRP:O	2:B:32:ALA:C	2.57	0.43
2:B:471:LYS:HA	2:B:472:ALA:HA	1.67	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
2:B:792:MET:HE1	12:T:24:DT:OP1	2.18	0.43
1:A:193:ASP:OD2	1:A:193:ASP:O	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
1:A:1171:GLN:O	1:A:1171:GLN:CD	2.57	0.43
1:A:877:HIS:C	1:A:878:ILE:HG13	2.38	0.43
2:B:1101:ASP:HA	2:B:1122:ARG:HH22	1.84	0.43
2:B:26:THR:HG22	2:B:708:GLU:OE1	2.18	0.43
8:J:11:GLY:O	8:J:12:LYS:C	2.56	0.43
1:A:1447:GLU:C	1:A:1449:SER:H	2.22	0.43
1:A:913:LEU:HG	1:A:915:SER:H	1.83	0.43
2:B:803:LEU:O	2:B:1042:GLY:HA3	2.18	0.43
2:B:473:MET:HA	2:B:474:SER:HA	1.59	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:1172:LEU:O	1:A:1172:LEU:HG	2.19	0.43
1:A:49:LYS:CB	1:A:55:ASP:OD2	2.58	0.43
1:A:540:PHE:CB	1:A:571:LEU:HD23	2.49	0.43
1:A:58:LEU:O	1:A:58:LEU:CG	2.65	0.43
2:B:469:GLN:O	2:B:470:LYS:HB2	2.19	0.43
1:A:1158:PRO:HG3	1:A:1188:GLN:HE21	1.84	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:HA	1:A:919:ILE:HD13	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
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:1166:ASP:HB3	1:A:1169:ILE:HD13	2.00	0.42
2:B:1056:SER:CB	2:B:1066:SER:O	2.62	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1092:LYS:HD3	1:A:1092:LYS:HA	1.29	0.42
1:A:1172:LEU:C	1:A:1174:PHE:N	2.72	0.42
1:A:207:ILE:O	1:A:210:ILE:HB	2.19	0.42
1:A:511:ILE:HG12	1:A:521:MET:CE	2.49	0.42
1:A:883:LEU:O	1:A:885:THR:N	2.42	0.42
2:B:324:ILE:HG22	2:B:324:ILE:O	2.19	0.42
2:B:942:ARG:HA	2:B:942:ARG:HD3	1.85	0.42
9:K:31:VAL:HG12	9:K:32:VAL:N	2.34	0.42
9:K:53:ASP:HB3	9:K:56:VAL:HG23	2.01	0.42
1:A:464:PRO:HD2	9:K:67:PHE:CD1	2.54	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
3:C:167:HIS:C	3:C:167:HIS:CD2	2.91	0.42
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:1329:THR:HG23	1:A:1331:SER:H	1.84	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
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
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: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
1:A:1436:ILE:O	1:A:1437:GLY:C	2.56	0.42
1:A:344:ARG:NH1	2:B:1129:ARG:HB2	2.35	0.42
1:A:1319:VAL:O	1:A:1322:ILE:CD1	2.68	0.42
1:A:1428:VAL:C	1:A:1430:LEU:H	2.23	0.42
1:A:668:ASP:HB3	1:A:743:VAL:CG2	2.42	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
1:A:1437:GLY:HA3	5:F:88:TYR:CD2	2.54	0.42
12:T:27:DA:N3	12:T:27:DA:H2'	2.34	0.42
1:A:286:HIS:CB	1:A:287:HIS:HB2	2.44	0.42
2:B:195:CYS:HA	2:B:196:PRO:HD3	1.93	0.42
2:B:232:SER:C	2:B:261:ARG:HH21	2.22	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:67:SER:HB2	2:B:92:PHE:HD1	1.85	0.42
3:C:171:GLY:HA2	3:C:172:PRO:HD3	1.66	0.42
1:A:963:ILE:HD12	1:A:1049:ILE:HG13	2.01	0.42
1:A:193:ASP:O	1:A:194:ALA:HB2	2.18	0.42
2:B:778:MET:HE1	2:B:1094:ARG:HD3	2.00	0.42
7:I:106:CYS:SG	7:I:107:SER:N	2.92	0.42
1:A:464:PRO:HD2	9:K:67:PHE:HD1	1.85	0.42
1:A:1212:VAL:O	1:A:1216:ILE:HG13	2.20	0.42
1:A:1254:ALA:C	1:A:1256:GLU:N	2.72	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
2:B:744:HIS:HA	2:B:745:PRO:HD3	1.91	0.42
6:H:12:VAL:CG1	6:H:51:ALA:HA	2.49	0.42
1:A:1044:TRP:O	1:A:1045:VAL:C	2.58	0.42
1:A:106:VAL:HG11	1:A:214:ILE:HD11	2.02	0.42
2:B:555:ILE:HA	2:B:558:LEU:HD12	2.02	0.42
7:I:11:ASN:O	7:I:11:ASN:CG	2.58	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:867:ILE:HD13	1:A:1014:ALA:HB2	2.02	0.41
1:A:1171:GLN:OE1	1:A:1171:GLN:O	2.36	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
1:A:814:PHE:CE1	2:B:514:LEU:HD21	2.55	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
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
2:B:472:ALA:HB2	2:B:476:ARG:HD3	2.02	0.41
3:C:75:MET:C	3:C:77:ILE:H	2.23	0.41
6:H:6:PHE:CZ	6:H:8:ASP:HB2	2.56	0.41
1:A:185:TRP:CE3	1:A:198:GLU:HG2	2.45	0.41
1:A:102:VAL:CG1	1:A:211:PHE:HE1	2.31	0.41
1:A:775:ILE:HG13	1:A:798:GLY:HA3	2.03	0.41
2:B:25:ILE:H	2:B:25:ILE:HG13	1.62	0.41
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:I:68:LEU:HB3	7:I:84:VAL:CG2	2.50	0.41
1:A:1216:ILE:HG22	1:A:1220:PHE:HE1	1.85	0.41
1:A:381:THR:O	1:A:383:TYR:N	2.53	0.41
1:A:423:ASP:CG	1:A:424:ILE:H	2.24	0.41
1:A:878:ILE:HG22	1:A:879:GLU:N	2.36	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:1039:LYS:HE2	1:A:1043:ASP:OD2	2.21	0.41
1:A:80:HIS:O	1:A:243:PRO:HG3	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
2:B:260:GLY:O	2:B:267:ARG:HD3	2.21	0.41
11:R:9:G:C2	12:T:21:DC:O2	2.73	0.41
1:A:256:GLN:HG3	12:T:28:DT:O4	2.20	0.41
1:A:1345:ARG:HD2	1:A:1373:ASP:OD1	2.20	0.41
1:A:37:PHE:HA	1:A:38:PRO:HD3	1.83	0.41
1:A:501:LEU:HA	1:A:501:LEU:HD23	1.68	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
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:1280:GLU:O	1:A:1282:VAL:HG23	2.21	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: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
2:B:1120:GLU:CG	2:B:1121:GLY:N	2.81	0.41
2:B:212:LEU:HD23	2:B:212:LEU:HA	1.96	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:715:ALA:HB3	2:B:716:ASN:C	2.41	0.41
2:B:721:LEU:HA	2:B:722:ASP:HA	1.78	0.41
3:C:148:ARG:N	3:C:151:GLN:OE1	2.53	0.41
3:C:15:LYS:HZ2	9:K:114:LEU:HD22	1.85	0.41
3:C:182:PRO:CB	3:C:207:CYS:SG	3.06	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1259:MET:HE2	1:A:1259:MET:HB2	1.88	0.41
2:B:755:ILE:HA	2:B:755:ILE:HD13	1.62	0.41
2:B:757:PRO:HB3	2:B:1044:ALA:CB	2.50	0.41
3:C:172:PRO:C	3:C:235:VAL:HG23	2.41	0.41
6:H:118:PHE:O	6:H:120:GLY:N	2.53	0.41
1:A:115:LEU:HD12	1:A:122:MET:HE3	2.03	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
2:B:777:ALA:HB2	2:B:1093:GLN:HE21	1.86	0.41
2:B:361:LEU:N	2:B:362:PRO:HD3	2.35	0.41
2:B:808:ALA:O	2:B:812:LEU:HG	2.21	0.41
2:B:980:PHE:CD1	2:B:990:ILE:HG13	2.55	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
1:A:1272:THR:C	1:A:1273:LEU:HD12	2.41	0.41
1:A:1344:GLY:O	1:A:1345:ARG:C	2.58	0.41
1:A:642:CYS:O	1:A:645:LEU:HB3	2.21	0.41
1:A:858:ASN:ND2	1:A:858:ASN:C	2.68	0.41
2:B:1072:MET:HE2	2:B:1085:ILE:HG21	2.03	0.41
2:B:129:PHE:HE2	2:B:166:PHE:HB2	1.84	0.41
2:B:34:ILE:O	2:B:37:PHE:N	2.49	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:900:ALA:HA	2:B:901:PRO:HD3	1.92	0.41
1:A:1063:MET:SD	1:A:1436:ILE:HG23	2.61	0.41
1:A:513:SER:HA	1:A:514:PRO:HD3	1.93	0.41
1:A:53:LEU:C	1:A:53:LEU:CD2	2.83	0.41
1:A:590:ARG:HH11	1:A:590:ARG:HG3	1.85	0.41
1:A:812:GLU:O	1:A:813:PHE:C	2.59	0.41
2:B:1107:ALA:O	2:B:1108:ARG:CB	2.67	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
11:R:7:A:HO2'	11:R:8:G:H5'	1.79	0.41
1:A:1364:ASN:O	1:A:1365:TYR:C	2.58	0.40
1:A:190:ALA:C	1:A:191:THR:OG1	2.59	0.40
1:A:381:THR:C	1:A:383:TYR:N	2.74	0.40
1:A:567:LYS:O	1:A:569:LYS:N	2.54	0.40
2:B:1120:GLU:O	2:B:1124:ARG:HD3	2.21	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
6:H:22:LYS:HD3	6:H:45:GLU:OE2	2.20	0.40
8:J:57:ILE:HA	8:J:57:ILE:HD12	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: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
1:A:269:ILE:HD11	1:A:300:VAL:HA	2.03	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
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: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
4:E:62:ALA:HB3	4:E:78:LEU:HB3	2.03	0.40
6:H:11:GLN:HB2	6:H:11:GLN:HE21	1.71	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:889:SER:C	1:A:891:ALA:N	2.73	0.40
1:A:909:ASP:OD2	1:A:910:PRO:HD2	2.21	0.40
1:A:917:SER:C	1:A:919:ILE:H	2.23	0.40
2:B:1149:GLU:HG3	2:B:1153:GLU:HB2	2.03	0.40
2:B:745:PRO:C	2:B:747:MET:H	2.23	0.40
7:I:59:VAL:HB	7:I:61:ASP:H	1.87	0.40
7:I:83:ASN:ND2	7:I:83:ASN:C	2.72	0.40
1:A:351:THR:HG21	1:A:466:SER:O	2.21	0.40
1:A:56:PRO:O	1:A:57:ARG:C	2.59	0.40
2:B:1095:LEU:N	2:B:1095:LEU:HD23	2.35	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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%)	3	22
2	B	1145/1224 (94%)	896 (78%)	202 (18%)	47 (4%)	3	22
3	C	269/318 (85%)	198 (74%)	63 (23%)	8 (3%)	4	28
4	E	213/215 (99%)	175 (82%)	32 (15%)	6 (3%)	5	30
5	F	83/155 (54%)	68 (82%)	11 (13%)	4 (5%)	2	18
6	H	132/146 (90%)	100 (76%)	25 (19%)	7 (5%)	2	16
7	I	117/122 (96%)	85 (73%)	23 (20%)	9 (8%)	1	9
8	J	63/70 (90%)	52 (82%)	9 (14%)	2 (3%)	4	27
9	K	112/120 (93%)	96 (86%)	15 (13%)	1 (1%)	17	53
10	L	44/70 (63%)	29 (66%)	13 (30%)	2 (4%)	2	20
All	All	3597/4173 (86%)	2788 (78%)	663 (18%)	146 (4%)	3	22

All (146) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	57	ARG
1	A	120	GLU
1	A	186	LYS
1	A	191	THR
1	A	193	ASP
1	A	194	ALA

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Mol	Chain	Res	Type
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
3	C	125	MET
3	C	142	VAL
5	F	72	LYS
5	F	78	GLN

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Mol	Chain	Res	Type
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
1	A	66	LYS
1	A	189	ARG
1	A	418	SER
1	A	568	PRO

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Mol	Chain	Res	Type
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
1	A	392	VAL
2	B	168	GLY
2	B	731	VAL
3	C	182	PRO

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Mol	Chain	Res	Type
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%)	1088 (87%)	160 (13%)	4	20
2	B	1000/1061 (94%)	875 (88%)	125 (12%)	4	21
3	C	238/274 (87%)	208 (87%)	30 (13%)	4	21
4	E	196/197 (100%)	184 (94%)	12 (6%)	18	51
5	F	74/137 (54%)	70 (95%)	4 (5%)	22	55
6	H	119/128 (93%)	115 (97%)	4 (3%)	37	68
7	I	113/116 (97%)	99 (88%)	14 (12%)	4	21
8	J	60/65 (92%)	54 (90%)	6 (10%)	7	31
9	K	99/102 (97%)	86 (87%)	13 (13%)	4	20
10	L	40/57 (70%)	35 (88%)	5 (12%)	4	21
All	All	3187/3657 (87%)	2814 (88%)	373 (12%)	5	24

All (373) 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	81	PHE
1	A	84	ILE
1	A	93	VAL
1	A	108	MET
1	A	113	LEU
1	A	121	LEU
1	A	123	ARG
1	A	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	193	ASP
1	A	195	ASP
1	A	198	GLU
1	A	208	LEU
1	A	216	VAL
1	A	222	LEU
1	A	226	GLU
1	A	227	VAL
1	A	237	THR
1	A	239	LEU
1	A	250	ILE
1	A	266	LEU
1	A	270	LEU
1	A	271	LYS
1	A	297	GLN
1	A	306	ASN
1	A	308	ILE
1	A	313	GLN
1	A	317	LYS
1	A	322	VAL
1	A	323	LYS

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Mol	Chain	Res	Type
1	A	332	LYS
1	A	346	ASP
1	A	351	THR
1	A	373	THR
1	A	403	LYS
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	427	GLN
1	A	434	ARG
1	A	440	ASP
1	A	442	VAL
1	A	443	LEU
1	A	445	ASN
1	A	450	LEU
1	A	452	LYS
1	A	465	TYR
1	A	466	SER
1	A	470	LEU
1	A	475	THR
1	A	516	SER
1	A	517	ASN
1	A	518	LYS
1	A	535	THR
1	A	565	ILE
1	A	576	GLN
1	A	595	THR
1	A	603	ASN
1	A	618	GLU
1	A	652	VAL
1	A	658	LEU
1	A	687	LYS
1	A	688	LYS
1	A	732	LEU
1	A	740	LEU
1	A	758	ILE
1	A	764	CYS
1	A	771	GLU
1	A	783	THR

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Mol	Chain	Res	Type
1	A	788	SER
1	A	837	ILE
1	A	838	GLN
1	A	854	ASN
1	A	858	ASN
1	A	867	ILE
1	A	884	ASP
1	A	885	THR
1	A	889	SER
1	A	895	LYS
1	A	902	LEU
1	A	904	THR
1	A	908	LEU
1	A	920	LEU
1	A	923	LEU
1	A	929	LEU
1	A	949	ASP
1	A	961	ARG
1	A	969	GLN
1	A	982	THR
1	A	988	LEU
1	A	1006	ILE
1	A	1017	LEU
1	A	1025	ARG
1	A	1033	GLN
1	A	1035	TYR
1	A	1039	LYS
1	A	1046	LEU
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	1112	LYS
1	A	1113	THR
1	A	1118	VAL
1	A	1146	VAL
1	A	1169	ILE
1	A	1172	LEU

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Mol	Chain	Res	Type
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	1237	ILE
1	A	1243	VAL
1	A	1246	LYS
1	A	1256	GLU
1	A	1258	HIS
1	A	1259	MET
1	A	1264	GLU
1	A	1267	MET
1	A	1285	MET
1	A	1314	SER
1	A	1322	ILE
1	A	1327	ILE
1	A	1329	THR
1	A	1333	ILE
1	A	1334	ASP
1	A	1336	MET
1	A	1354	ASN
1	A	1366	ARG
1	A	1385	THR
1	A	1391	ARG
1	A	1393	ASN
1	A	1400	CYS
1	A	1403	GLU
1	A	1444	MET
2	B	26	THR
2	B	35	SER
2	B	39	ARG
2	B	44	VAL
2	B	46	GLN
2	B	63	ILE
2	B	66	ASP
2	B	67	SER
2	B	68	THR

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Mol	Chain	Res	Type
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	120	ARG
2	B	121	ASN
2	B	130	VAL
2	B	164	LYS
2	B	174	LEU
2	B	179	CYS
2	B	202	TYR
2	B	206	ASN
2	B	223	VAL
2	B	244	LEU
2	B	246	LYS
2	B	268	THR
2	B	305	VAL
2	B	310	MET
2	B	317	CYS
2	B	327	ARG
2	B	336	ARG
2	B	337	ARG
2	B	341	LEU
2	B	355	ILE
2	B	371	GLU
2	B	396	ASP
2	B	404	LYS
2	B	412	LEU
2	B	419	THR
2	B	424	LEU
2	B	425	THR
2	B	440	HIS
2	B	444	MET
2	B	445	LYS
2	B	459	TYR
2	B	463	THR
2	B	466	TRP

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Mol	Chain	Res	Type
2	B	469	GLN
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	604	ARG
2	B	633	VAL
2	B	637	LEU
2	B	644	GLU
2	B	645	SER
2	B	678	GLU
2	B	694	ASP
2	B	701	ILE
2	B	710	LEU
2	B	711	GLU
2	B	762	ASN
2	B	764	SER
2	B	788	ARG
2	B	790	ASP
2	B	796	LEU
2	B	827	ILE
2	B	844	SER
2	B	864	LYS
2	B	868	MET
2	B	869	SER
2	B	878	GLN
2	B	883	LEU
2	B	886	LYS
2	B	894	ASP
2	B	899	ILE
2	B	916	THR
2	B	941	LEU
2	B	943	SER
2	B	963	PHE
2	B	968	VAL
2	B	973	ILE
2	B	975	GLN
2	B	979	LYS

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Mol	Chain	Res	Type
2	B	989	THR
2	B	992	ILE
2	B	997	GLU
2	B	999	MET
2	B	1006	ILE
2	B	1008	PRO
2	B	1019	SER
2	B	1022	THR
2	B	1028	GLU
2	B	1048	THR
2	B	1051	THR
2	B	1071	VAL
2	B	1082	MET
2	B	1084	GLN
2	B	1087	PHE
2	B	1092	TYR
2	B	1093	GLN
2	B	1096	ARG
2	B	1099	VAL
2	B	1103	ILE
2	B	1115	THR
2	B	1122	ARG
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	1165	ILE
2	B	1190	ASP
2	B	1194	ILE
2	B	1196	ILE
3	C	4	GLU
3	C	10	ILE
3	C	11	ARG
3	C	17	ASN
3	C	18	VAL
3	C	22	LEU
3	C	25	VAL
3	C	27	LEU
3	C	34	ARG
3	C	43	THR

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Mol	Chain	Res	Type
3	C	57	VAL
3	C	69	LEU
3	C	77	ILE
3	C	92	CYS
3	C	109	SER
3	C	120	ILE
3	C	129	ILE
3	C	134	ILE
3	C	143	LEU
3	C	154	LYS
3	C	163	ILE
3	C	195	GLN
3	C	197	SER
3	C	199	LYS
3	C	203	GLN
3	C	215	GLU
3	C	221	TYR
3	C	228	PHE
3	C	240	VAL
3	C	244	VAL
4	E	31	THR
4	E	33	GLU
4	E	43	LYS
4	E	88	VAL
4	E	92	THR
4	E	95	THR
4	E	104	ASN
4	E	131	THR
4	E	134	THR
4	E	150	VAL
4	E	156	LEU
4	E	169	ARG
5	F	79	ARG
5	F	97	ARG
5	F	110	ASP
5	F	111	LEU
6	H	11	GLN
6	H	62	SER
6	H	95	TYR
6	H	142	LEU
7	I	8	ARG
7	I	9	ASP

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Mol	Chain	Res	Type
7	I	13	MET
7	I	17	ARG
7	I	29	CYS
7	I	31	THR
7	I	59	VAL
7	I	61	ASP
7	I	75	CYS
7	I	83	ASN
7	I	95	THR
7	I	96	SER
7	I	104	LEU
7	I	106	CYS
8	J	5	VAL
8	J	7	CYS
8	J	13	VAL
8	J	31	ASP
8	J	34	THR
8	J	43	ARG
9	K	5	ASP
9	K	6	ARG
9	K	10	PHE
9	K	12	LEU
9	K	18	LYS
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	107	THR
9	K	113	THR
10	L	31	CYS
10	L	49	LYS
10	L	55	ILE
10	L	61	THR
10	L	68	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (83) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	64	ASN
1	A	83	HIS

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Mol	Chain	Res	Type
1	A	92	HIS
1	A	119	ASN
1	A	171	GLN
1	A	253	ASN
1	A	273	ASN
1	A	281	HIS
1	A	306	ASN
1	A	311	GLN
1	A	399	HIS
1	A	435	HIS
1	A	445	ASN
1	A	471	ASN
1	A	493	GLN
1	A	503	GLN
1	A	545	GLN
1	A	659	HIS
1	A	660	ASN
1	A	723	ASN
1	A	741	ASN
1	A	742	ASN
1	A	768	GLN
1	A	786	HIS
1	A	858	ASN
1	A	877	HIS
1	A	926	GLN
1	A	968	GLN
1	A	994	GLN
1	A	1033	GLN
1	A	1085	HIS
1	A	1173	HIS
1	A	1188	GLN
1	A	1222	ASN
1	A	1278	ASN
1	A	1427	ASN
1	A	1432	GLN
2	B	121	ASN
2	B	215	GLN
2	B	236	HIS
2	B	366	GLN
2	B	395	GLN
2	B	440	HIS
2	B	465	ASN

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Mol	Chain	Res	Type
2	B	494	HIS
2	B	515	HIS
2	B	516	ASN
2	B	518	HIS
2	B	538	ASN
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	862	GLN
2	B	975	GLN
2	B	984	HIS
2	B	986	GLN
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
4	E	8	ASN
4	E	104	ASN
6	H	11	GLN
6	H	35	GLN
6	H	137	GLN
7	I	60	GLN
7	I	79	HIS
7	I	83	ASN
7	I	89	GLN
8	J	64	ASN
9	K	65	HIS

### 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 [i](#)

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	1429/1733 (82%)	0.12	49 (3%) 45 44	81, 135, 241, 393	0
2	B	1153/1224 (94%)	0.17	43 (3%) 41 41	80, 120, 251, 398	0
3	C	271/318 (85%)	-0.02	8 (2%) 50 49	90, 114, 178, 337	0
4	E	215/215 (100%)	0.11	14 (6%) 18 21	111, 159, 272, 350	0
5	F	85/155 (54%)	-0.14	1 (1%) 79 77	110, 134, 173, 217	0
6	H	136/146 (93%)	0.21	7 (5%) 28 28	124, 172, 301, 361	0
7	I	119/122 (97%)	0.05	1 (0%) 86 84	111, 151, 193, 273	0
8	J	65/70 (92%)	-0.04	3 (4%) 32 32	87, 104, 152, 179	0
9	K	114/120 (95%)	-0.14	0 100 100	87, 119, 153, 172	0
10	L	46/70 (65%)	0.24	2 (4%) 35 35	107, 166, 257, 270	0
11	R	12/13 (92%)	-0.21	0 100 100	93, 123, 178, 190	0
12	T	28/28 (100%)	0.52	5 (17%) 1 2	96, 205, 312, 314	0
13	N	14/14 (100%)	0.68	2 (14%) 2 4	280, 307, 312, 313	0
All	All	3687/4228 (87%)	0.11	135 (3%) 41 41	80, 131, 253, 398	0

All (135) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	44	THR	9.4
2	B	882	THR	8.4
1	A	45	GLN	6.7
2	B	88	TYR	5.8
1	A	168	GLY	5.5
2	B	869	SER	5.2
13	N	1	DC	5.0
2	B	476	ARG	4.8
4	E	123	LEU	4.7

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	B	339	THR	4.5
12	T	3	DA	4.5
1	A	66	LYS	4.5
1	A	46	THR	4.4
2	B	441	ASP	4.4
1	A	253	ASN	4.4
1	A	1267	MET	4.2
2	B	883	LEU	4.2
1	A	1123	GLY	4.1
3	C	270	VAL	4.0
2	B	83	ASN	4.0
1	A	191	THR	3.9
2	B	870	ILE	3.9
3	C	271	ASN	3.9
1	A	1083	THR	3.8
2	B	719	ASN	3.8
1	A	72	GLU	3.8
4	E	16	PHE	3.8
2	B	708	GLU	3.7
2	B	471	LYS	3.7
2	B	85	SER	3.7
1	A	190	ALA	3.6
6	H	139	ASN	3.5
1	A	69	THR	3.5
4	E	126	SER	3.5
1	A	312	PRO	3.5
6	H	112	ILE	3.5
4	E	110	PHE	3.4
1	A	1232	ASN	3.4
2	B	250	PHE	3.4
1	A	141	LEU	3.4
12	T	11	DG	3.3
7	I	105	SER	3.3
2	B	440	HIS	3.3
1	A	192	GLY	3.3
4	E	102	GLU	3.3
6	H	84	ALA	3.3
10	L	50	ASP	3.2
2	B	709	ASP	3.2
1	A	127	ALA	3.2
10	L	26	THR	3.1
1	A	171	GLN	3.0

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Mol	Chain	Res	Type	RSRZ
6	H	32	THR	3.0
2	B	672	GLY	3.0
1	A	1080	THR	3.0
1	A	1085	HIS	3.0
2	B	677	GLU	2.9
12	T	10	DA	2.9
2	B	646	LEU	2.9
1	A	195	ASP	2.9
1	A	194	ALA	2.8
1	A	426	LEU	2.8
2	B	106	ASP	2.8
2	B	1181	GLU	2.8
1	A	197	PRO	2.8
3	C	212	PRO	2.8
4	E	95	THR	2.8
2	B	340	ALA	2.8
1	A	105	CYS	2.7
1	A	286	HIS	2.7
13	N	8	DT	2.7
1	A	78	PRO	2.7
2	B	663	ALA	2.6
2	B	645	SER	2.6
1	A	1167	GLU	2.6
1	A	164	ARG	2.6
2	B	576	ASP	2.6
12	T	12	DC	2.6
2	B	429	PHE	2.5
2	B	670	GLU	2.5
4	E	57	MET	2.5
12	T	4	DC	2.5
1	A	181	LEU	2.5
2	B	443	ASN	2.5
3	C	213	PRO	2.5
1	A	149	GLU	2.5
2	B	78	THR	2.4
1	A	91	PHE	2.4
4	E	91	LYS	2.4
1	A	189	ARG	2.4
1	A	1451	VAL	2.4
4	E	20	LYS	2.4
3	C	267	GLN	2.4
2	B	643	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
2	B	75	ALA	2.4
2	B	717	GLU	2.4
1	A	193	ASP	2.3
3	C	50	GLU	2.3
8	J	26	GLN	2.3
1	A	188	ASP	2.3
3	C	157	CYS	2.3
1	A	1192	LEU	2.3
2	B	337	ARG	2.3
2	B	91	SER	2.3
1	A	59	GLY	2.3
6	H	127	GLY	2.3
1	A	257	ARG	2.2
2	B	344	LYS	2.2
1	A	323	LYS	2.2
1	A	1150	SER	2.2
2	B	935	ARG	2.2
2	B	982	SER	2.2
2	B	673	PHE	2.2
8	J	9	SER	2.2
4	E	43	LYS	2.2
2	B	444	MET	2.2
8	J	27	GLU	2.2
6	H	85	GLY	2.2
1	A	413	ILE	2.1
1	A	3	GLY	2.1
1	A	1299	VAL	2.1
2	B	343	ILE	2.1
6	H	105	GLU	2.1
4	E	41	ASP	2.1
1	A	160	GLN	2.1
1	A	313	GLN	2.1
4	E	82	PHE	2.1
5	F	104	ASN	2.1
2	B	734	HIS	2.1
1	A	1179	GLU	2.1
4	E	98	ILE	2.1
3	C	272	PHE	2.0
2	B	714	GLU	2.0
1	A	196	GLU	2.0
2	B	263	GLY	2.0
4	E	124	VAL	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
14	ZN	J	101	1/1	0.93	0.21	190,190,190,190	0
14	ZN	B	1307	1/1	0.93	0.12	160,160,160,160	0
15	MG	A	1736	1/1	0.94	0.14	91,91,91,91	0
14	ZN	A	1734	1/1	0.94	0.05	246,246,246,246	0
14	ZN	I	203	1/1	0.95	0.15	147,147,147,147	0
14	ZN	L	105	1/1	0.95	0.08	151,151,151,151	0
14	ZN	A	1735	1/1	0.95	0.11	145,145,145,145	0
14	ZN	I	204	1/1	0.98	0.17	293,293,293,293	0
14	ZN	C	319	1/1	0.99	0.08	135,135,135,135	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.