



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 24, 2018 – 05:43 AM EST

PDB ID : 1PV4  
Title : X-ray crystal structure of the Rho transcription termination factor in complex with single stranded DNA  
Authors : Skordalakes, E.; Berger, J.M.  
Deposited on : 2003-06-26  
Resolution : 3.00 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

<http://wwpdb.org/validation/2016/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)	:	1.9-1692
EDS	:	rb-20030736
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20030736

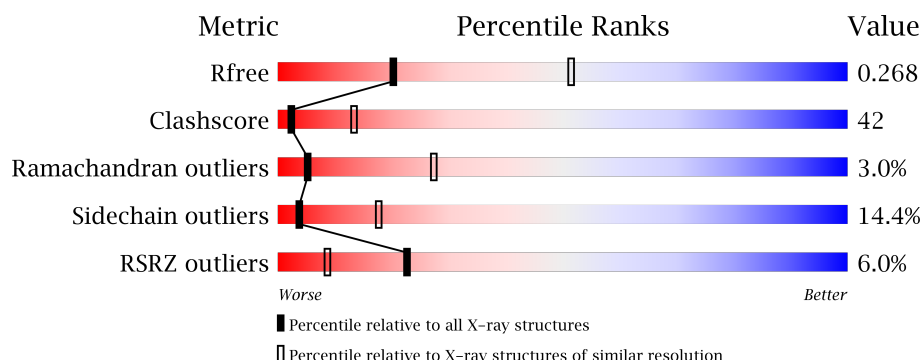
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 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))
$R_{free}$	100719	1692 (3.00-3.00)
Clashscore	112137	2037 (3.00-3.00)
Ramachandran outliers	110173	1973 (3.00-3.00)
Sidechain outliers	110143	1976 (3.00-3.00)
RSRZ outliers	101464	1716 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . 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	G	2	<div> <div>100%</div> <div>50%</div> </div>
1	H	2	<div> <div>50%</div> <div>50%</div> </div>
1	J	2	<div> <div>100%</div> <div>50%</div> </div>
1	K	2	<div> <div>50%</div> <div>50%</div> </div>
1	L	2	<div> <div>100%</div> <div>100%</div> </div>

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Mol	Chain	Length	Quality of chain
2	A	419	<div><div></div><div>9%</div><div>42%</div><div>47%</div><div>8%</div><div>• •</div></div>
2	B	419	<div><div></div><div>7%</div><div>37%</div><div>39%</div><div>8%</div><div>15%</div></div>
2	C	419	<div><div></div><div>2%</div><div>40%</div><div>45%</div><div>12%</div><div>• •</div></div>
2	D	419	<div><div></div><div>5%</div><div>41%</div><div>44%</div><div>11%</div><div>• •</div></div>
2	E	419	<div><div></div><div>3%</div><div>38%</div><div>47%</div><div>11%</div><div>• •</div></div>
2	F	419	<div><div></div><div>7%</div><div>39%</div><div>49%</div><div>8%</div><div>• •</div></div>



## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 19077 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 DNA chain called 5'-D(P\*CP\*C)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	G	2	Total	C	N	O	P	0	0	0
			38	18	6	12	2			
1	H	2	Total	C	N	O	P	0	0	0
			38	18	6	12	2			
1	J	2	Total	C	N	O	P	0	0	0
			38	18	6	12	2			
1	K	2	Total	C	N	O	P	0	0	0
			38	18	6	12	2			
1	L	2	Total	C	N	O	P	0	0	0
			38	18	6	12	2			

- Molecule 2 is a protein called Transcription termination factor rho.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	A	408	Total	C	N	O	S	Se	0	0	0
			3208	2025	562	604	1	16			
2	B	358	Total	C	N	O	S	Se	0	0	0
			2813	1776	494	529	1	13			
2	C	408	Total	C	N	O	S	Se	0	0	0
			3208	2025	562	604	1	16			
2	D	408	Total	C	N	O	S	Se	0	0	0
			3208	2025	562	604	1	16			
2	E	407	Total	C	N	O	S	Se	0	0	0
			3201	2020	561	603	1	16			
2	F	408	Total	C	N	O	S	Se	0	0	0
			3208	2025	562	604	1	16			

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	MODIFIED RESIDUE	UNP P0AG30
A	21	MSE	MET	MODIFIED RESIDUE	UNP P0AG30
A	29	MSE	MET	MODIFIED RESIDUE	UNP P0AG30

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Chain	Residue	Modelled	Actual	Comment	Reference
A	147	MSE	MET	MODIFIED RESIDUE	UNP P0AG30
A	186	MSE	MET	MODIFIED RESIDUE	UNP P0AG30
A	205	MSE	MET	MODIFIED RESIDUE	UNP P0AG30
A	219	MSE	MET	MODIFIED RESIDUE	UNP P0AG30
A	245	MSE	MET	MODIFIED RESIDUE	UNP P0AG30
A	327	MSE	MET	MODIFIED RESIDUE	UNP P0AG30
A	341	MSE	MET	MODIFIED RESIDUE	UNP P0AG30
A	380	MSE	MET	MODIFIED RESIDUE	UNP P0AG30
A	390	MSE	MET	MODIFIED RESIDUE	UNP P0AG30
A	396	MSE	MET	MODIFIED RESIDUE	UNP P0AG30
A	405	MSE	MET	MODIFIED RESIDUE	UNP P0AG30
A	415	MSE	MET	MODIFIED RESIDUE	UNP P0AG30
A	416	MSE	MET	MODIFIED RESIDUE	UNP P0AG30
B	1	MSE	MET	MODIFIED RESIDUE	UNP P0AG30
B	21	MSE	MET	MODIFIED RESIDUE	UNP P0AG30
B	29	MSE	MET	MODIFIED RESIDUE	UNP P0AG30
B	147	MSE	MET	MODIFIED RESIDUE	UNP P0AG30
B	186	MSE	MET	MODIFIED RESIDUE	UNP P0AG30
B	205	MSE	MET	MODIFIED RESIDUE	UNP P0AG30
B	219	MSE	MET	MODIFIED RESIDUE	UNP P0AG30
B	245	MSE	MET	MODIFIED RESIDUE	UNP P0AG30
B	327	MSE	MET	MODIFIED RESIDUE	UNP P0AG30
B	341	MSE	MET	MODIFIED RESIDUE	UNP P0AG30
B	380	MSE	MET	MODIFIED RESIDUE	UNP P0AG30
B	390	MSE	MET	MODIFIED RESIDUE	UNP P0AG30
B	396	MSE	MET	MODIFIED RESIDUE	UNP P0AG30
B	405	MSE	MET	MODIFIED RESIDUE	UNP P0AG30
B	415	MSE	MET	MODIFIED RESIDUE	UNP P0AG30
B	416	MSE	MET	MODIFIED RESIDUE	UNP P0AG30
C	1	MSE	MET	MODIFIED RESIDUE	UNP P0AG30
C	21	MSE	MET	MODIFIED RESIDUE	UNP P0AG30
C	29	MSE	MET	MODIFIED RESIDUE	UNP P0AG30
C	147	MSE	MET	MODIFIED RESIDUE	UNP P0AG30
C	186	MSE	MET	MODIFIED RESIDUE	UNP P0AG30
C	205	MSE	MET	MODIFIED RESIDUE	UNP P0AG30
C	219	MSE	MET	MODIFIED RESIDUE	UNP P0AG30
C	245	MSE	MET	MODIFIED RESIDUE	UNP P0AG30
C	327	MSE	MET	MODIFIED RESIDUE	UNP P0AG30
C	341	MSE	MET	MODIFIED RESIDUE	UNP P0AG30
C	380	MSE	MET	MODIFIED RESIDUE	UNP P0AG30
C	390	MSE	MET	MODIFIED RESIDUE	UNP P0AG30
C	396	MSE	MET	MODIFIED RESIDUE	UNP P0AG30

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Chain	Residue	Modelled	Actual	Comment	Reference
C	405	MSE	MET	MODIFIED RESIDUE	UNP P0AG30
C	415	MSE	MET	MODIFIED RESIDUE	UNP P0AG30
C	416	MSE	MET	MODIFIED RESIDUE	UNP P0AG30
D	1	MSE	MET	MODIFIED RESIDUE	UNP P0AG30
D	21	MSE	MET	MODIFIED RESIDUE	UNP P0AG30
D	29	MSE	MET	MODIFIED RESIDUE	UNP P0AG30
D	147	MSE	MET	MODIFIED RESIDUE	UNP P0AG30
D	186	MSE	MET	MODIFIED RESIDUE	UNP P0AG30
D	205	MSE	MET	MODIFIED RESIDUE	UNP P0AG30
D	219	MSE	MET	MODIFIED RESIDUE	UNP P0AG30
D	245	MSE	MET	MODIFIED RESIDUE	UNP P0AG30
D	327	MSE	MET	MODIFIED RESIDUE	UNP P0AG30
D	341	MSE	MET	MODIFIED RESIDUE	UNP P0AG30
D	380	MSE	MET	MODIFIED RESIDUE	UNP P0AG30
D	390	MSE	MET	MODIFIED RESIDUE	UNP P0AG30
D	396	MSE	MET	MODIFIED RESIDUE	UNP P0AG30
D	405	MSE	MET	MODIFIED RESIDUE	UNP P0AG30
D	415	MSE	MET	MODIFIED RESIDUE	UNP P0AG30
D	416	MSE	MET	MODIFIED RESIDUE	UNP P0AG30
E	1	MSE	MET	MODIFIED RESIDUE	UNP P0AG30
E	21	MSE	MET	MODIFIED RESIDUE	UNP P0AG30
E	29	MSE	MET	MODIFIED RESIDUE	UNP P0AG30
E	147	MSE	MET	MODIFIED RESIDUE	UNP P0AG30
E	186	MSE	MET	MODIFIED RESIDUE	UNP P0AG30
E	205	MSE	MET	MODIFIED RESIDUE	UNP P0AG30
E	219	MSE	MET	MODIFIED RESIDUE	UNP P0AG30
E	245	MSE	MET	MODIFIED RESIDUE	UNP P0AG30
E	327	MSE	MET	MODIFIED RESIDUE	UNP P0AG30
E	341	MSE	MET	MODIFIED RESIDUE	UNP P0AG30
E	380	MSE	MET	MODIFIED RESIDUE	UNP P0AG30
E	390	MSE	MET	MODIFIED RESIDUE	UNP P0AG30
E	396	MSE	MET	MODIFIED RESIDUE	UNP P0AG30
E	405	MSE	MET	MODIFIED RESIDUE	UNP P0AG30
E	415	MSE	MET	MODIFIED RESIDUE	UNP P0AG30
E	416	MSE	MET	MODIFIED RESIDUE	UNP P0AG30
F	1	MSE	MET	MODIFIED RESIDUE	UNP P0AG30
F	21	MSE	MET	MODIFIED RESIDUE	UNP P0AG30
F	29	MSE	MET	MODIFIED RESIDUE	UNP P0AG30
F	147	MSE	MET	MODIFIED RESIDUE	UNP P0AG30
F	186	MSE	MET	MODIFIED RESIDUE	UNP P0AG30
F	205	MSE	MET	MODIFIED RESIDUE	UNP P0AG30
F	219	MSE	MET	MODIFIED RESIDUE	UNP P0AG30

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Chain	Residue	Modelled	Actual	Comment	Reference
F	245	MSE	MET	MODIFIED RESIDUE	UNP P0AG30
F	327	MSE	MET	MODIFIED RESIDUE	UNP P0AG30
F	341	MSE	MET	MODIFIED RESIDUE	UNP P0AG30
F	380	MSE	MET	MODIFIED RESIDUE	UNP P0AG30
F	390	MSE	MET	MODIFIED RESIDUE	UNP P0AG30
F	396	MSE	MET	MODIFIED RESIDUE	UNP P0AG30
F	405	MSE	MET	MODIFIED RESIDUE	UNP P0AG30
F	415	MSE	MET	MODIFIED RESIDUE	UNP P0AG30
F	416	MSE	MET	MODIFIED RESIDUE	UNP P0AG30

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	G	1	Total O 1 1	0	0
3	J	1	Total O 1 1	0	0
3	A	3	Total O 3 3	0	0
3	B	2	Total O 2 2	0	0
3	C	7	Total O 7 7	0	0
3	D	7	Total O 7 7	0	0
3	E	14	Total O 14 14	0	0
3	F	6	Total O 6 6	0	0

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

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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: 5'-D(P\*CP\*C)-3'

Chain G:  100%



- Molecule 1: 5'-D(P\*CP\*C)-3'

Chain H:  50% 50%



- Molecule 1: 5'-D(P\*CP\*C)-3'

Chain J:  100% 50% 50%



- Molecule 1: 5'-D(P\*CP\*C)-3'

Chain K:  50% 50%




- Molecule 1: 5'-D(P\*CP\*C)-3'

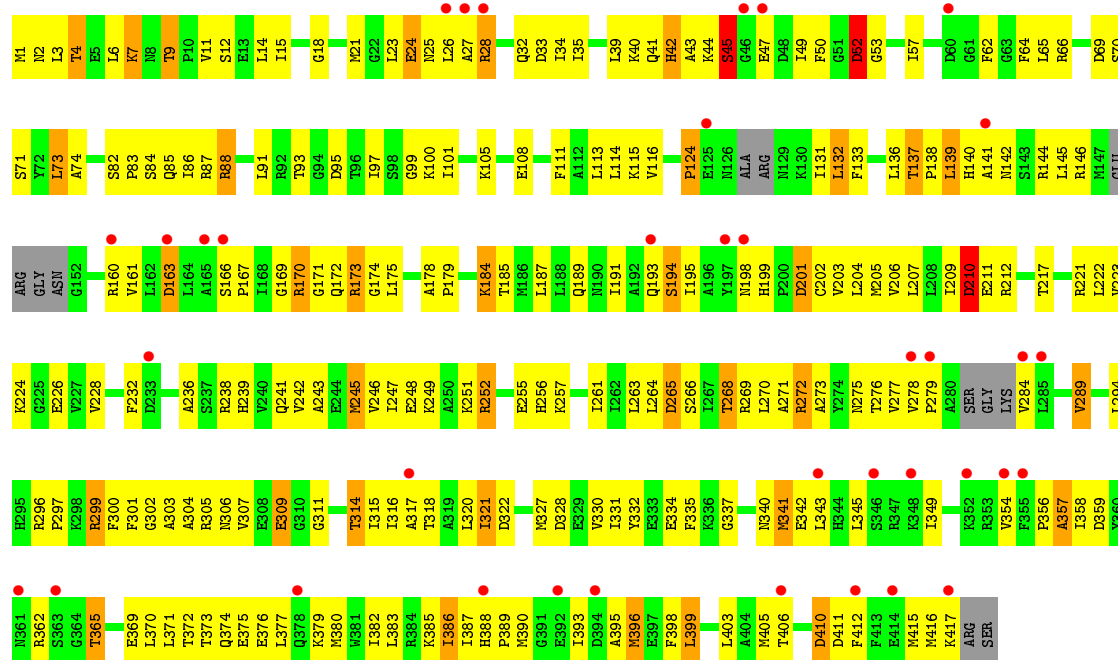
Chain L:  100% 100%



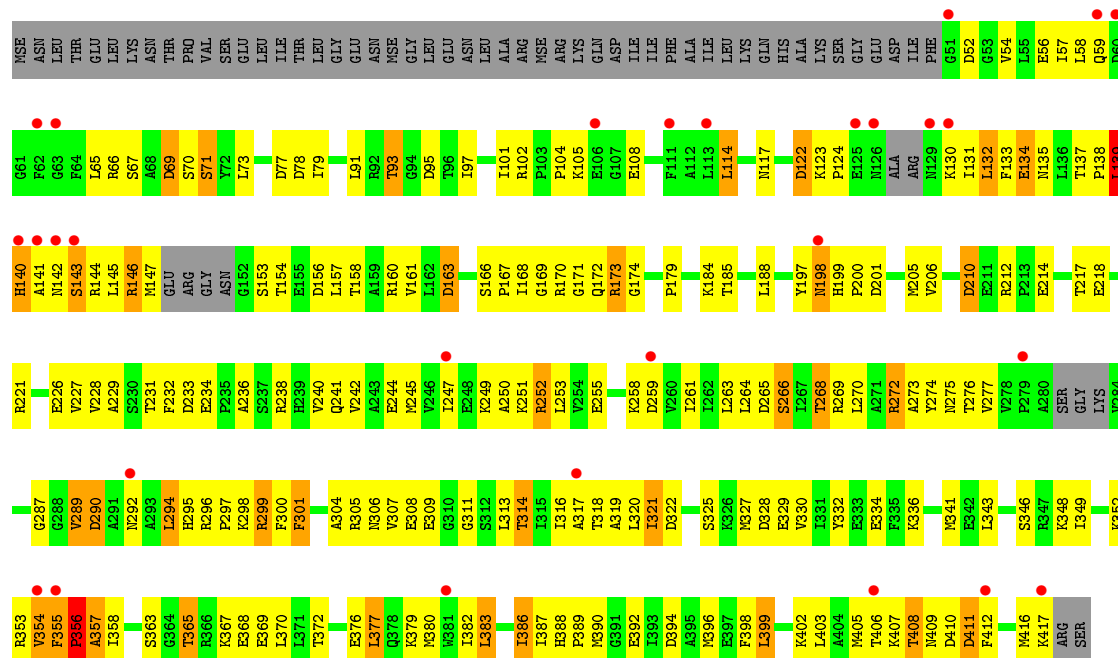
- Molecule 2: Transcription termination factor rho

Chain A:  9% 42% 47% 8%

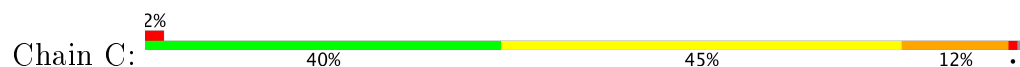


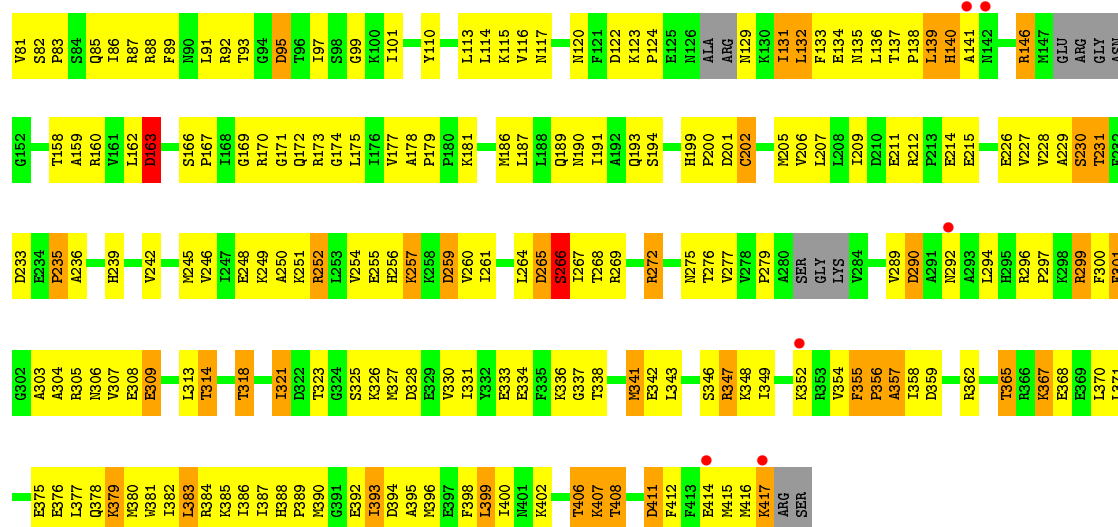


• Molecule 2: Transcription termination factor rho

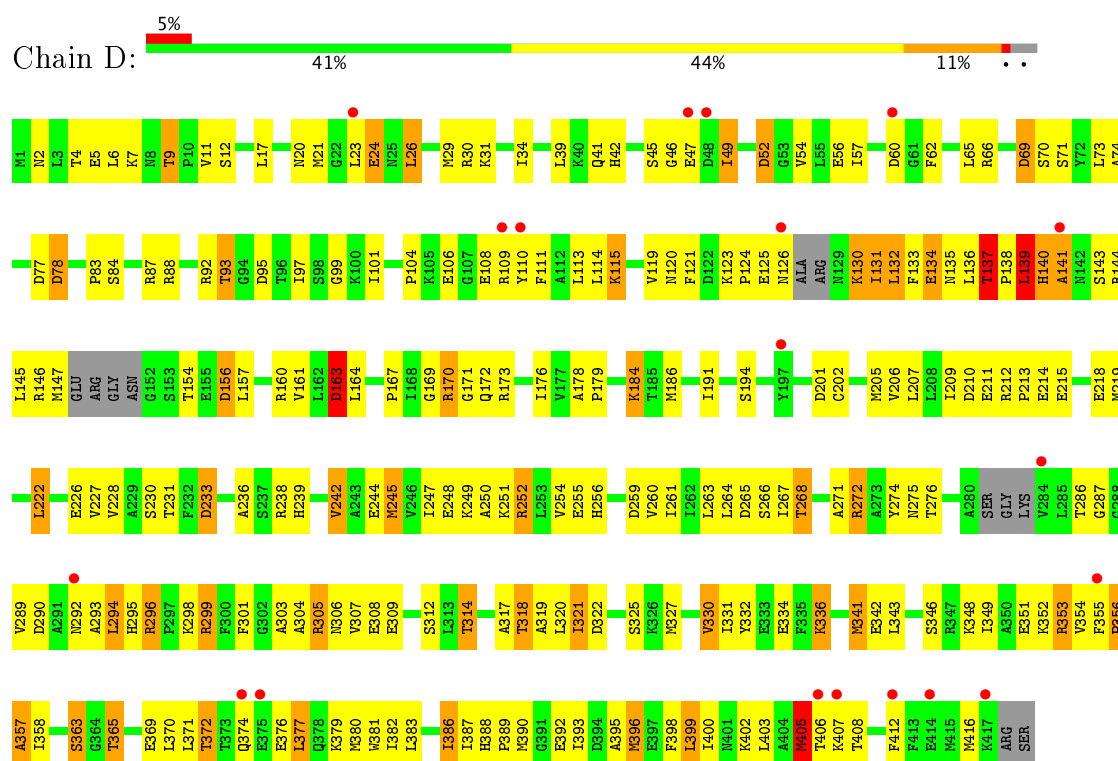


• Molecule 2: Transcription termination factor rho

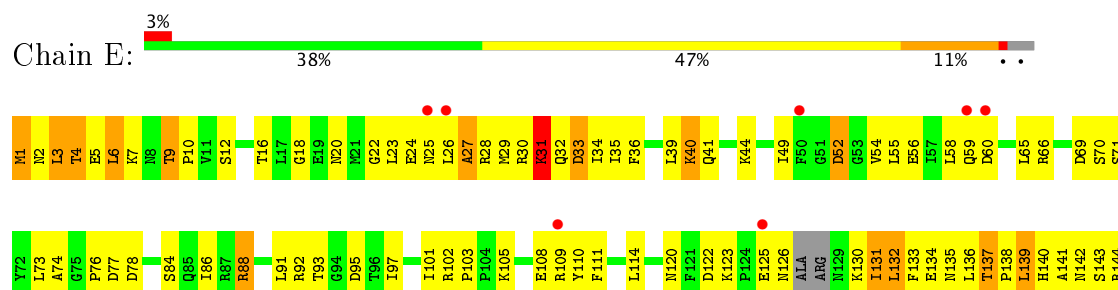


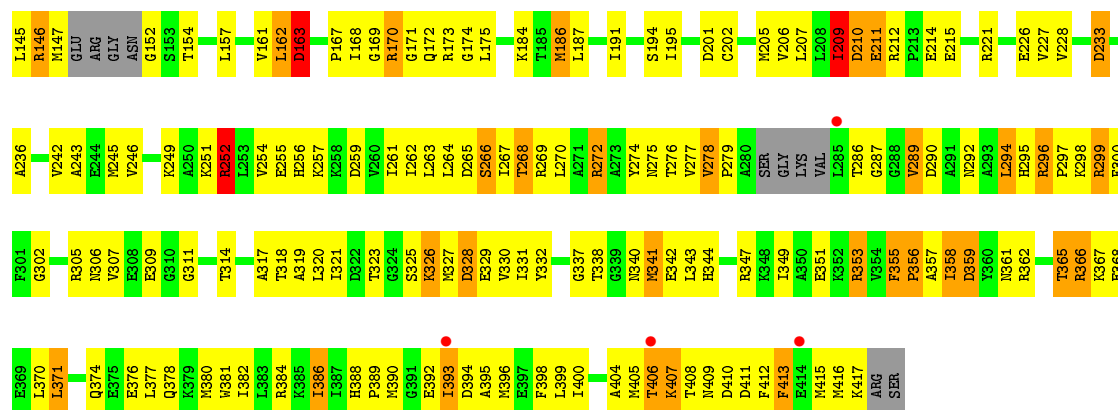


• Molecule 2: Transcription termination factor rho

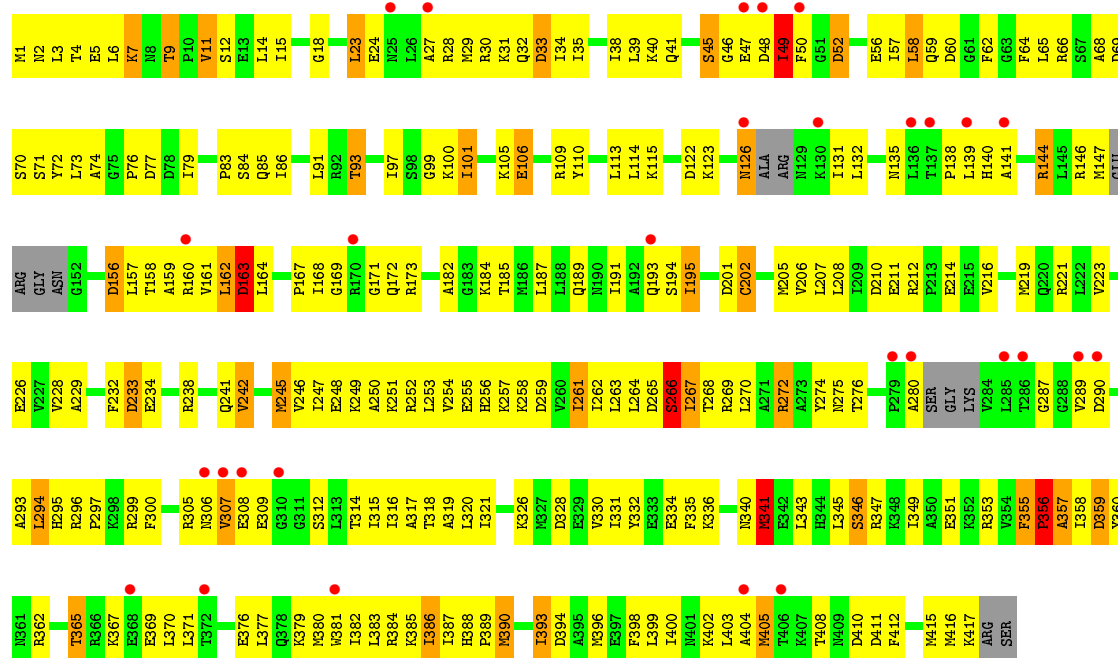


• Molecule 2: Transcription termination factor rho





• Molecule 2: Transcription termination factor rho



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	118.56 Å   204.33 Å   147.37 Å 90.00°   95.86°   90.00°	Depositor
Resolution (Å)	20.00 – 3.00 29.89 – 2.90	Depositor EDS
% Data completeness (in resolution range)	97.9 (20.00-3.00) 96.6 (29.89-2.90)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.05	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.97 (at 2.90 Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, $R_{free}$	0.270   ,   0.296 0.243   ,   0.268	Depositor DCC
$R_{free}$ test set	3379 reflections (5.28%)	DCC
Wilson B-factor (Å <sup>2</sup> )	86.7	Xtriage
Anisotropy	0.162	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 102.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	19077	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.08% 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 ⓘ

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	G	0.67	0/41	1.16	0/60
1	H	0.89	0/41	1.34	1/60 (1.7%)
1	J	0.99	0/41	1.58	1/60 (1.7%)
1	K	0.95	0/41	1.59	1/60 (1.7%)
1	L	0.93	0/41	1.79	3/60 (5.0%)
2	A	0.57	0/3238	0.77	9/4334 (0.2%)
2	B	0.57	0/2841	0.80	13/3805 (0.3%)
2	C	0.76	0/3238	0.88	11/4334 (0.3%)
2	D	0.74	0/3238	0.90	11/4334 (0.3%)
2	E	0.70	0/3231	0.89	11/4324 (0.3%)
2	F	0.60	0/3238	0.80	11/4334 (0.3%)
All	All	0.67	0/19229	0.85	72/25765 (0.3%)

There are no bond length outliers.

All (72) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	233	ASP	CB-CG-OD2	10.35	127.61	118.30
2	E	163	ASP	CB-CG-OD2	7.97	125.47	118.30
2	D	233	ASP	CB-CG-OD1	-7.79	111.29	118.30
2	D	77	ASP	CB-CG-OD2	7.54	125.08	118.30
2	A	265	ASP	CB-CG-OD2	7.30	124.87	118.30
1	L	3	DC	P-O3'-C3'	7.21	128.35	119.70
2	D	95	ASP	CB-CG-OD2	6.79	124.41	118.30
2	E	328	ASP	CB-CG-OD2	6.67	124.31	118.30
1	J	3	DC	P-O3'-C3'	6.55	127.56	119.70
2	E	52	ASP	CB-CG-OD2	6.42	124.07	118.30
2	D	52	ASP	CB-CG-OD2	6.34	124.00	118.30
2	C	328	ASP	CB-CG-OD2	6.28	123.95	118.30
2	B	69	ASP	CB-CG-OD2	6.23	123.91	118.30
2	F	163	ASP	CB-CG-OD2	6.20	123.88	118.30
2	C	201	ASP	CB-CG-OD2	6.13	123.82	118.30
2	C	33	ASP	CB-CG-OD2	6.13	123.81	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	210	ASP	CB-CG-OD2	6.12	123.81	118.30
2	E	201	ASP	CB-CG-OD2	6.04	123.74	118.30
2	D	201	ASP	CB-CG-OD2	6.00	123.70	118.30
2	C	52	ASP	CB-CG-OD2	5.98	123.68	118.30
2	A	201	ASP	CB-CG-OD2	5.96	123.66	118.30
2	A	328	ASP	CB-CG-OD2	5.94	123.65	118.30
2	B	328	ASP	CB-CG-OD2	5.93	123.63	118.30
2	F	52	ASP	CB-CG-OD2	5.92	123.62	118.30
2	A	69	ASP	CB-CG-OD2	5.86	123.58	118.30
2	D	78	ASP	CB-CG-OD2	5.79	123.51	118.30
2	B	201	ASP	CB-CG-OD2	5.78	123.50	118.30
1	H	3	DC	P-O3'-C3'	5.75	126.60	119.70
2	D	69	ASP	CB-CG-OD2	5.75	123.47	118.30
2	C	95	ASP	CB-CG-OD2	5.74	123.47	118.30
2	F	259	ASP	CB-CG-OD2	5.74	123.47	118.30
2	B	163	ASP	CB-CG-OD2	5.67	123.40	118.30
2	E	233	ASP	CB-CG-OD2	5.66	123.40	118.30
2	A	52	ASP	CB-CG-OD2	5.66	123.39	118.30
1	L	4	DC	C1'-O4'-C4'	-5.66	104.44	110.10
2	D	259	ASP	CB-CG-OD2	5.64	123.37	118.30
2	F	410	ASP	CB-CG-OD2	5.61	123.35	118.30
2	E	210	ASP	CB-CG-OD2	5.61	123.34	118.30
2	C	259	ASP	CB-CG-OD2	5.47	123.22	118.30
2	B	173	ARG	NE-CZ-NH2	-5.46	117.57	120.30
2	B	173	ARG	NE-CZ-NH1	5.45	123.03	120.30
2	F	233	ASP	CB-CG-OD2	5.43	123.19	118.30
2	F	201	ASP	CB-CG-OD2	5.42	123.18	118.30
1	K	3	DC	P-O3'-C3'	5.39	126.17	119.70
2	D	163	ASP	CB-CG-OD2	5.33	123.10	118.30
2	B	95	ASP	CB-CG-OD2	5.33	123.09	118.30
2	F	328	ASP	CB-CG-OD2	5.32	123.09	118.30
2	F	156	ASP	CB-CG-OD2	5.32	123.08	118.30
2	A	163	ASP	CB-CG-OD2	5.30	123.08	118.30
2	C	69	ASP	CB-CG-OD2	5.30	123.07	118.30
2	B	78	ASP	CB-CG-OD2	5.29	123.06	118.30
2	A	95	ASP	CB-CG-OD2	5.26	123.04	118.30
2	E	252	ARG	NE-CZ-NH1	-5.26	117.67	120.30
2	C	163	ASP	CB-CG-OD2	5.21	122.98	118.30
2	D	156	ASP	CB-CG-OD2	5.20	122.98	118.30
2	B	410	ASP	CB-CG-OD2	5.20	122.98	118.30
2	E	33	ASP	CB-CG-OD2	5.20	122.98	118.30
2	E	122	ASP	CB-CG-OD2	5.18	122.97	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	359	ASP	CB-CG-OD2	5.18	122.96	118.30
2	F	69	ASP	CB-CG-OD2	5.15	122.94	118.30
2	B	77	ASP	CB-CG-OD2	5.14	122.93	118.30
2	E	60	ASP	CB-CG-OD2	5.13	122.92	118.30
2	F	33	ASP	CB-CG-OD2	5.11	122.90	118.30
2	C	48	ASP	CB-CG-OD2	5.10	122.89	118.30
2	A	210	ASP	CB-CG-OD2	5.10	122.89	118.30
2	E	265	ASP	CB-CG-OD2	5.07	122.86	118.30
2	B	122	ASP	CB-CG-OD2	5.06	122.85	118.30
2	B	411	ASP	CB-CG-OD2	5.02	122.82	118.30
2	F	77	ASP	CB-CG-OD2	5.02	122.82	118.30
2	C	265	ASP	CB-CG-OD2	5.01	122.81	118.30
2	A	410	ASP	CB-CG-OD2	5.01	122.81	118.30
1	L	4	DC	O4'-C1'-N1	5.00	111.50	108.00

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	38	0	23	2	0
1	H	38	0	23	3	0
1	J	38	0	23	5	0
1	K	38	0	23	5	0
1	L	38	0	23	8	0
2	A	3208	0	3284	278	0
2	B	2813	0	2870	229	0
2	C	3208	0	3284	308	0
2	D	3208	0	3284	273	0
2	E	3201	0	3275	308	0
2	F	3208	0	3284	259	0
3	A	3	0	0	2	0
3	B	2	0	0	2	0
3	C	7	0	0	1	0
3	D	7	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	14	0	0	6	0
3	F	6	0	0	3	0
3	G	1	0	0	0	0
3	J	1	0	0	0	0
All	All	19077	0	19396	1597	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 42.

All (1597) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:355:PHE:HB3	2:F:356:PRO:CD	1.59	1.33
2:C:379:LYS:HG2	2:C:412:PHE:CD2	1.72	1.23
2:C:177:VAL:CG1	2:C:321:ILE:HD12	1.69	1.22
2:A:265:ASP:O	2:A:318:THR:HB	1.36	1.22
2:C:141:ALA:CB	2:C:370:LEU:HB2	1.72	1.19
2:E:152:GLY:HA2	2:E:407:LYS:HE3	1.20	1.17
2:E:356:PRO:HB2	2:E:396:MSE:HE2	1.28	1.14
2:E:141:ALA:CB	2:E:370:LEU:HB2	1.76	1.14
2:C:141:ALA:HA	2:C:371:LEU:CD2	1.79	1.13
2:C:141:ALA:HB3	2:C:370:LEU:CB	1.77	1.12
2:C:341:MSE:HE3	2:C:342:GLU:HA	1.26	1.11
2:E:272:ARG:HG3	2:E:272:ARG:HH11	1.06	1.11
2:C:412:PHE:CZ	2:C:416:MSE:SE	2.54	1.11
2:E:341:MSE:HE3	2:E:342:GLU:HA	1.26	1.10
2:B:390:MSE:HE1	2:B:398:PHE:HB2	1.11	1.10
2:A:272:ARG:HG3	2:A:272:ARG:HH11	1.04	1.09
2:B:272:ARG:HH11	2:B:272:ARG:HG3	0.95	1.09
2:D:390:MSE:HE3	2:D:395:ALA:HA	1.28	1.09
2:C:141:ALA:CB	2:C:370:LEU:CB	2.30	1.08
2:A:372:THR:HG23	2:A:376:GLU:HB3	1.34	1.07
2:C:177:VAL:HG13	2:C:321:ILE:CD1	1.84	1.07
2:A:226:GLU:OE2	2:A:249:LYS:HE2	1.53	1.07
2:C:390:MSE:HE1	2:C:398:PHE:HB2	1.34	1.05
2:F:390:MSE:HE1	2:F:398:PHE:CG	1.90	1.05
2:A:390:MSE:HE2	2:A:395:ALA:HA	1.38	1.04
2:C:141:ALA:HA	2:C:371:LEU:HD21	1.38	1.04
2:F:355:PHE:HB3	2:F:356:PRO:HD3	1.36	1.04
2:E:141:ALA:HB1	2:E:370:LEU:HB2	1.03	1.03
2:D:161:VAL:HG21	2:D:396:MSE:HE1	1.39	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:3:DC:H4'	1:H:4:DC:O5'	1.58	1.02
2:C:272:ARG:HH11	2:C:272:ARG:HG3	1.16	1.02
2:D:268:THR:HG21	2:D:320:LEU:H	1.24	1.02
2:C:356:PRO:O	2:C:358:ILE:HG13	1.60	1.02
2:E:341:MSE:C	2:E:341:MSE:HE3	1.81	1.01
2:C:83:PRO:O	2:C:87:ARG:HG3	1.59	1.01
2:D:341:MSE:CE	2:D:342:GLU:HA	1.90	1.01
2:E:341:MSE:HE3	2:E:342:GLU:CA	1.89	1.01
2:C:177:VAL:CG1	2:C:321:ILE:CD1	2.39	1.01
2:C:379:LYS:HZ2	2:C:412:PHE:HB2	1.26	1.01
2:D:289:VAL:HG11	2:D:330:VAL:HG11	1.41	1.01
2:F:202:CYS:SG	2:F:261:ILE:HD11	2.00	1.00
2:F:343:LEU:HD11	2:F:358:ILE:HD13	1.42	1.00
2:C:23:LEU:HD21	2:C:41:GLN:HG3	1.42	1.00
2:B:390:MSE:HE1	2:B:398:PHE:CB	1.90	1.00
2:A:245:MSE:CE	2:A:245:MSE:HA	1.91	1.00
2:E:169:GLY:H	2:E:172:GLN:HG2	1.27	1.00
2:C:141:ALA:HB3	2:C:370:LEU:HB3	1.40	1.00
2:C:79:ILE:HD13	2:C:101:ILE:HG21	1.39	1.00
2:E:140:HIS:CB	2:E:306:ASN:HB2	1.92	1.00
2:C:289:VAL:HG11	2:C:330:VAL:HG11	1.44	0.99
2:A:141:ALA:O	2:A:370:LEU:HB3	1.61	0.99
2:C:341:MSE:HE3	2:C:342:GLU:CA	1.93	0.98
2:F:355:PHE:CB	2:F:356:PRO:CD	2.40	0.97
2:E:141:ALA:HB1	2:E:370:LEU:CB	1.95	0.97
2:F:359:ASP:O	2:F:359:ASP:OD1	1.81	0.97
2:B:272:ARG:NH1	2:B:272:ARG:HG3	1.70	0.96
2:D:160:ARG:HD2	2:D:408:THR:CG2	1.95	0.96
2:A:1:MSE:HG3	2:A:2:ASN:H	1.31	0.96
2:A:4:THR:HG21	2:A:52:ASP:OD2	1.65	0.96
2:F:49:ILE:HG22	2:F:101:ILE:HD11	1.47	0.96
2:C:2:ASN:OD1	2:C:4:THR:HG22	1.67	0.95
2:D:341:MSE:HE3	2:D:342:GLU:CA	1.96	0.95
2:D:341:MSE:CE	2:D:342:GLU:CA	2.44	0.95
2:B:272:ARG:HH11	2:B:272:ARG:CG	1.78	0.95
2:D:131:ILE:HG21	2:D:133:PHE:HD2	1.32	0.95
2:C:177:VAL:HG13	2:C:321:ILE:HD12	0.97	0.95
2:A:341:MSE:HE3	2:A:341:MSE:O	1.66	0.94
2:D:131:ILE:CG2	2:D:133:PHE:HD2	1.80	0.94
2:D:236:ALA:HA	2:D:239:HIS:HD2	1.31	0.94
2:C:272:ARG:HD3	2:C:327:MSE:SE	2.17	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:379:LYS:NZ	2:C:412:PHE:HB2	1.83	0.94
2:E:141:ALA:HB3	2:E:370:LEU:CD1	1.98	0.94
2:B:269:ARG:HH11	2:B:272:ARG:NH1	1.65	0.93
2:E:396:MSE:O	2:E:400:ILE:HG13	1.68	0.93
2:F:169:GLY:H	2:F:172:GLN:HG3	1.32	0.93
2:B:140:HIS:HA	2:B:306:ASN:HB3	1.50	0.93
2:A:140:HIS:CB	2:A:306:ASN:HB3	1.99	0.92
2:A:272:ARG:CG	2:A:272:ARG:HH11	1.81	0.92
2:C:205:MSE:HE3	2:C:226:GLU:OE1	1.69	0.92
2:C:171:GLY:H	2:C:314:THR:CG2	1.82	0.92
2:D:167:PRO:O	2:D:365:THR:HG21	1.70	0.92
2:D:341:MSE:C	2:D:341:MSE:HE2	1.89	0.92
2:C:341:MSE:O	2:C:341:MSE:CE	2.18	0.92
2:C:356:PRO:HD2	2:C:400:ILE:HD11	1.52	0.92
2:E:272:ARG:HG3	2:E:272:ARG:NH1	1.80	0.91
2:B:269:ARG:HH11	2:B:272:ARG:HH12	0.98	0.91
2:E:132:LEU:HD22	2:E:251:LYS:HD3	1.48	0.91
2:A:161:VAL:HG11	2:A:396:MSE:HE1	1.51	0.91
2:A:132:LEU:HD22	2:A:251:LYS:HD3	1.51	0.91
2:F:4:THR:HB	2:F:52:ASP:OD1	1.70	0.91
2:E:23:LEU:HD21	2:E:41:GLN:HG3	1.52	0.91
2:E:141:ALA:CB	2:E:370:LEU:CB	2.48	0.90
2:B:321:ILE:HD11	2:B:332:TYR:CG	2.07	0.90
2:D:169:GLY:H	2:D:172:GLN:CG	1.84	0.90
2:C:269:ARG:HH11	2:C:272:ARG:HH12	1.17	0.90
2:F:390:MSE:HE2	2:F:398:PHE:HB2	1.53	0.90
2:F:141:ALA:HB1	2:F:370:LEU:HB2	1.52	0.90
2:C:379:LYS:HZ2	2:C:412:PHE:CB	1.84	0.89
2:D:169:GLY:H	2:D:172:GLN:HG2	1.36	0.89
2:D:238:ARG:O	2:D:242:VAL:HG23	1.73	0.89
2:E:356:PRO:CB	2:E:396:MSE:HE2	2.03	0.89
2:A:272:ARG:NH1	2:A:272:ARG:HG3	1.82	0.89
2:B:261:ILE:HG12	2:B:314:THR:CG2	2.02	0.89
2:E:169:GLY:H	2:E:172:GLN:CG	1.85	0.89
2:C:412:PHE:HZ	2:C:416:MSE:SE	2.06	0.88
2:D:131:ILE:HG22	2:D:133:PHE:H	1.38	0.88
2:B:269:ARG:NH1	2:B:272:ARG:HH12	1.71	0.88
2:E:275:ASN:ND2	2:E:327:MSE:HE1	1.89	0.88
2:A:140:HIS:HA	2:A:306:ASN:HD22	1.39	0.88
2:B:131:ILE:CG2	2:B:133:PHE:HD2	1.85	0.88
2:E:139:LEU:HD22	2:E:367:LYS:HD2	1.56	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:139:LEU:HD13	2:E:214:GLU:HG3	1.55	0.88
2:F:135:ASN:HB3	2:F:307:VAL:HG22	1.56	0.88
2:C:160:ARG:HG2	2:C:408:THR:HG23	1.55	0.88
2:A:372:THR:CG2	2:A:376:GLU:HB3	2.03	0.88
2:E:390:MSE:HE1	2:E:398:PHE:HB2	1.52	0.88
2:F:355:PHE:HB3	2:F:356:PRO:HD2	1.53	0.88
2:A:405:MSE:SE	2:A:415:MSE:CE	2.72	0.88
2:D:133:PHE:HB3	3:E:430:HOH:O	1.74	0.87
2:A:131:ILE:HG22	2:A:133:PHE:HD2	1.39	0.87
2:D:321:ILE:HD11	2:D:332:TYR:CD2	2.09	0.87
2:D:4:THR:HB	2:D:52:ASP:OD1	1.74	0.87
2:E:136:LEU:HD12	2:F:221:ARG:NH2	1.89	0.87
2:B:275:ASN:HD22	2:B:327:MSE:HE1	1.36	0.87
2:D:137:THR:HG22	2:D:305:ARG:HB2	1.56	0.87
2:C:416:MSE:O	2:C:417:LYS:HB2	1.72	0.87
2:F:141:ALA:HB1	2:F:370:LEU:CB	2.05	0.87
2:D:136:LEU:O	2:D:138:PRO:HD3	1.74	0.86
2:A:385:LYS:HE2	2:B:353:ARG:HH12	1.40	0.86
2:C:294:LEU:CD1	2:C:334:GLU:HG3	2.05	0.86
2:C:379:LYS:HG2	2:C:412:PHE:CE2	2.10	0.86
2:A:144:ARG:HH11	2:A:146:ARG:HE	1.20	0.85
2:B:261:ILE:HG12	2:B:314:THR:HG23	1.57	0.85
2:C:167:PRO:HD2	2:C:365:THR:HG23	1.57	0.85
2:B:268:THR:HG21	2:B:320:LEU:H	1.40	0.85
2:C:341:MSE:O	2:C:341:MSE:HE2	1.77	0.85
2:E:205:MSE:HE3	2:E:226:GLU:OE1	1.76	0.85
2:F:207:LEU:HD11	2:F:242:VAL:CG1	2.07	0.85
2:E:132:LEU:HA	2:E:135:ASN:ND2	1.91	0.85
2:E:341:MSE:CE	2:E:341:MSE:O	2.24	0.85
2:E:152:GLY:CA	2:E:407:LYS:HE3	2.04	0.85
2:C:272:ARG:CD	2:C:327:MSE:SE	2.75	0.85
2:D:341:MSE:O	2:D:341:MSE:HE2	1.75	0.85
2:A:376:GLU:O	2:A:380:MSE:HG3	1.75	0.84
2:E:152:GLY:HA2	2:E:407:LYS:CE	2.04	0.84
2:C:390:MSE:HE1	2:C:398:PHE:CB	2.06	0.84
2:D:341:MSE:HE3	2:D:342:GLU:C	1.98	0.84
2:A:275:ASN:HD22	2:A:327:MSE:HE3	1.42	0.84
2:B:141:ALA:HB1	2:B:370:LEU:HB2	1.59	0.84
2:D:387:ILE:HG23	2:D:390:MSE:HE2	1.59	0.84
2:A:49:ILE:HG22	2:A:101:ILE:HG12	1.57	0.84
2:E:381:TRP:CZ3	2:F:353:ARG:HD3	2.12	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:144:ARG:HG3	2:A:145:LEU:N	1.92	0.84
2:B:174:GLY:HA3	2:B:341:MSE:HE3	1.59	0.84
2:E:366:ARG:HH11	2:E:366:ARG:HG3	1.41	0.84
2:A:169:GLY:H	2:A:172:GLN:CG	1.90	0.84
2:A:24:GLU:O	2:A:26:LEU:HD23	1.77	0.84
2:F:169:GLY:N	2:F:172:GLN:HG3	1.91	0.84
2:A:140:HIS:CB	2:A:306:ASN:CB	2.56	0.83
2:A:416:MSE:O	2:A:417:LYS:HB2	1.79	0.83
2:C:141:ALA:HA	2:C:371:LEU:HD23	1.58	0.83
2:E:359:ASP:O	2:E:359:ASP:OD1	1.97	0.83
2:A:341:MSE:HE3	2:A:341:MSE:C	1.98	0.83
2:D:405:MSE:O	2:D:406:THR:HG23	1.77	0.83
2:E:341:MSE:O	2:E:341:MSE:HE3	1.77	0.83
2:E:174:GLY:CA	2:E:341:MSE:HE2	2.08	0.83
2:C:379:LYS:CG	2:C:412:PHE:CD2	2.60	0.83
2:E:139:LEU:CD2	2:E:367:LYS:HG3	2.08	0.83
2:D:54:VAL:HG21	2:D:249:LYS:HD2	1.60	0.83
2:A:261:ILE:HG12	2:A:314:THR:HG23	1.61	0.82
2:C:379:LYS:HG2	2:C:412:PHE:CG	2.14	0.82
2:E:341:MSE:CE	2:E:342:GLU:HA	2.07	0.82
2:D:135:ASN:HB3	2:D:307:VAL:HG13	1.62	0.82
2:D:336:LYS:HD2	3:D:425:HOH:O	1.79	0.82
2:F:56:GLU:HG3	2:F:245:MSE:HE1	1.60	0.82
2:E:341:MSE:CE	2:E:341:MSE:C	2.47	0.82
2:F:168:ILE:HG12	2:F:341:MSE:HE3	1.61	0.82
2:A:66:ARG:HH11	2:A:66:ARG:HG2	1.44	0.82
2:C:29:MSE:HG3	2:C:34:ILE:HG13	1.62	0.82
2:D:154:THR:O	2:D:157:LEU:HB2	1.79	0.82
2:A:245:MSE:HE3	2:A:245:MSE:HA	1.62	0.82
2:C:341:MSE:C	2:C:341:MSE:HE3	2.00	0.82
2:A:294:LEU:HD13	2:A:334:GLU:HG3	1.61	0.82
2:A:405:MSE:O	2:A:406:THR:HG23	1.79	0.82
2:A:236:ALA:HA	2:A:239:HIS:HD2	1.45	0.82
2:B:416:MSE:O	2:B:417:LYS:HB2	1.78	0.82
2:C:23:LEU:HD21	2:C:41:GLN:CG	2.08	0.82
2:E:416:MSE:O	2:E:417:LYS:HB2	1.78	0.82
2:B:228:VAL:CG1	2:B:242:VAL:HG13	2.09	0.82
2:C:140:HIS:CB	2:C:306:ASN:HB2	2.09	0.81
2:C:355:PHE:HB2	2:C:356:PRO:HD3	1.61	0.81
2:E:407:LYS:HE2	3:E:428:HOH:O	1.80	0.81
2:B:132:LEU:HD22	2:B:251:LYS:HD3	1.60	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:147:MSE:HE1	2:D:191:ILE:HG23	1.63	0.81
2:E:386:ILE:HD11	2:E:398:PHE:CE2	2.15	0.81
2:C:171:GLY:H	2:C:314:THR:HG22	1.44	0.81
2:B:205:MSE:HE3	2:B:226:GLU:OE1	1.81	0.81
2:E:341:MSE:HE3	2:E:342:GLU:N	1.94	0.81
1:J:3:DC:H4'	1:J:4:DC:O5'	1.80	0.80
2:E:411:ASP:OD1	2:E:412:PHE:N	2.14	0.80
2:A:266:SER:HA	2:A:318:THR:O	1.79	0.80
2:C:23:LEU:CD2	2:C:41:GLN:HG3	2.12	0.80
2:E:356:PRO:HB2	2:E:396:MSE:CE	2.10	0.80
2:B:355:PHE:HB3	2:B:356:PRO:HD3	1.63	0.80
2:B:272:ARG:HD2	2:B:327:MSE:SE	2.31	0.80
2:E:141:ALA:HB3	2:E:370:LEU:HD12	1.63	0.80
2:A:174:GLY:HA2	2:A:341:MSE:HE2	1.63	0.80
2:E:209:ILE:HG22	2:E:210:ASP:N	1.97	0.79
2:F:390:MSE:CE	2:F:398:PHE:HB2	2.13	0.79
2:C:381:TRP:HB3	2:D:353:ARG:NH2	1.98	0.79
2:F:169:GLY:H	2:F:172:GLN:CG	1.95	0.79
2:C:79:ILE:CD1	2:C:101:ILE:HG21	2.13	0.79
2:B:140:HIS:CA	2:B:306:ASN:HB3	2.12	0.79
2:A:100:LYS:HD2	2:A:115:LYS:HD2	1.65	0.79
2:E:173:ARG:HH21	2:F:212:ARG:HD2	1.46	0.79
2:A:144:ARG:NH1	2:A:146:ARG:HE	1.79	0.78
2:E:5:GLU:O	2:E:9:THR:HG22	1.83	0.78
2:D:268:THR:HG21	2:D:320:LEU:N	1.99	0.78
2:D:289:VAL:CG1	2:D:330:VAL:HG11	2.13	0.78
2:B:140:HIS:HA	2:B:306:ASN:CB	2.12	0.78
2:D:236:ALA:HA	2:D:239:HIS:CD2	2.18	0.78
2:D:268:THR:CG2	2:D:320:LEU:H	1.97	0.78
2:D:261:ILE:HG12	2:D:314:THR:HG23	1.66	0.78
2:E:411:ASP:O	2:E:415:MSE:HG2	1.84	0.78
2:D:251:LYS:O	2:D:255:GLU:HG3	1.84	0.78
2:B:336:LYS:HE3	2:C:323:THR:O	1.84	0.77
2:D:160:ARG:HD2	2:D:408:THR:HG21	1.65	0.77
2:D:356:PRO:HB2	2:D:396:MSE:HE2	1.66	0.77
2:B:289:VAL:HG11	2:B:330:VAL:HG11	1.65	0.77
2:B:355:PHE:HB3	2:B:356:PRO:CD	2.15	0.77
2:C:272:ARG:HG3	2:C:272:ARG:NH1	1.86	0.77
2:E:141:ALA:CB	2:E:370:LEU:HD12	2.14	0.77
2:B:316:ILE:HD12	2:B:341:MSE:CE	2.15	0.77
2:A:49:ILE:HG22	2:A:101:ILE:CG1	2.15	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:341:MSE:C	2:C:341:MSE:CE	2.54	0.77
2:B:251:LYS:O	2:B:255:GLU:HG3	1.83	0.76
2:E:206:VAL:HB	2:E:227:VAL:HG22	1.65	0.76
2:B:275:ASN:ND2	2:B:327:MSE:HE1	2.00	0.76
2:D:17:LEU:HD23	2:D:17:LEU:O	1.84	0.76
2:E:272:ARG:HE	2:E:327:MSE:SE	2.18	0.76
2:A:390:MSE:HE1	2:A:398:PHE:HB3	1.66	0.76
2:B:355:PHE:CB	2:B:356:PRO:CD	2.64	0.76
2:B:131:ILE:HD11	2:C:28:ARG:O	1.86	0.76
2:F:355:PHE:CB	2:F:356:PRO:HD2	2.11	0.76
2:D:341:MSE:HE2	2:D:342:GLU:HA	1.66	0.76
2:E:174:GLY:HA2	2:E:341:MSE:HE2	1.67	0.75
2:F:146:ARG:O	2:F:147:MSE:HG3	1.86	0.75
2:C:160:ARG:HG2	2:C:408:THR:CG2	2.15	0.75
2:C:92:ARG:CZ	2:C:131:ILE:HD11	2.17	0.75
2:A:275:ASN:HD22	2:A:327:MSE:CE	1.98	0.75
2:C:139:LEU:O	2:C:140:HIS:CB	2.34	0.75
2:C:29:MSE:HG3	2:C:34:ILE:CG1	2.17	0.75
2:C:91:LEU:HD13	2:C:97:ILE:HD11	1.68	0.75
2:C:341:MSE:O	2:C:341:MSE:HE3	1.84	0.75
2:C:141:ALA:HB1	2:C:370:LEU:CB	2.15	0.75
2:D:294:LEU:O	2:D:298:LYS:HG3	1.87	0.75
2:C:415:MSE:O	2:C:415:MSE:HG2	1.85	0.75
2:C:341:MSE:CE	2:C:342:GLU:HA	2.14	0.74
2:F:252:ARG:HD3	2:F:255:GLU:OE1	1.87	0.74
2:E:275:ASN:HD22	2:E:327:MSE:HE1	1.49	0.74
2:F:60:ASP:HB2	2:F:62:PHE:CE2	2.22	0.74
2:A:245:MSE:HA	2:A:245:MSE:HE2	1.67	0.74
2:B:131:ILE:HG21	2:B:133:PHE:HD2	1.52	0.74
2:E:136:LEU:HD12	2:F:221:ARG:HH21	1.51	0.74
2:E:137:THR:CG2	2:E:305:ARG:HD3	2.18	0.74
2:D:346:SER:HB3	2:D:349:ILE:HG13	1.70	0.73
2:E:321:ILE:HD11	2:E:332:TYR:CD2	2.24	0.73
2:B:268:THR:CG2	2:B:320:LEU:H	2.02	0.73
2:F:268:THR:HG21	2:F:320:LEU:H	1.53	0.73
2:B:295:HIS:NE2	2:C:235:PRO:HD3	2.03	0.73
2:C:4:THR:CG2	2:C:5:GLU:N	2.52	0.73
2:D:143:SER:OG	2:D:170:ARG:HD2	1.89	0.73
2:D:275:ASN:HD21	2:D:289:VAL:HA	1.54	0.73
2:E:186:MSE:HE2	2:E:355:PHE:CD2	2.24	0.73
2:B:131:ILE:CG2	2:B:133:PHE:CD2	2.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:386:ILE:HD11	2:E:398:PHE:HE2	1.53	0.73
2:C:122:ASP:OD1	2:C:123:LYS:N	2.22	0.72
2:A:372:THR:HG23	2:A:376:GLU:CB	2.15	0.72
1:G:3:DC:H4'	1:G:4:DC:O5'	1.88	0.72
2:B:388:HIS:HB3	2:B:389:PRO:HD3	1.69	0.72
2:E:170:ARG:NH1	2:E:202:CYS:SG	2.62	0.72
2:E:390:MSE:HE1	2:E:398:PHE:CB	2.19	0.72
2:F:382:ILE:O	2:F:386:ILE:HG23	1.88	0.72
2:A:271:ALA:HB3	2:A:331:ILE:HD13	1.70	0.72
2:D:144:ARG:HD3	2:D:146:ARG:HH21	1.53	0.72
2:F:272:ARG:HH11	2:F:272:ARG:CB	2.02	0.72
2:A:161:VAL:HG12	2:A:358:ILE:HD12	1.71	0.72
2:A:356:PRO:HB2	2:A:396:MSE:HE3	1.69	0.72
2:D:131:ILE:CG2	2:D:133:PHE:CD2	2.69	0.72
2:E:131:ILE:HG23	2:E:133:PHE:H	1.55	0.72
2:E:137:THR:HG23	2:E:305:ARG:HD3	1.72	0.72
2:A:261:ILE:HG12	2:A:314:THR:CG2	2.20	0.72
2:C:160:ARG:HE	2:C:408:THR:HG23	1.55	0.72
2:D:24:GLU:O	2:D:26:LEU:CD2	2.38	0.72
2:D:161:VAL:CG2	2:D:396:MSE:HE1	2.19	0.72
2:F:157:LEU:HD13	2:F:400:ILE:HG23	1.70	0.72
2:B:131:ILE:HG22	2:B:133:PHE:HD2	1.53	0.72
2:F:171:GLY:H	2:F:314:THR:HB	1.54	0.72
2:C:131:ILE:HG23	2:C:133:PHE:HD2	1.55	0.71
2:C:135:ASN:HB3	2:C:307:VAL:HG13	1.69	0.71
2:E:226:GLU:OE2	2:E:249:LYS:HE2	1.90	0.71
2:C:3:LEU:O	2:C:7:LYS:HG2	1.90	0.71
2:F:270:LEU:HD11	2:F:274:TYR:CE2	2.25	0.71
2:A:169:GLY:H	2:A:172:GLN:HG2	1.55	0.71
2:A:217:THR:O	2:A:221:ARG:HG3	1.91	0.71
2:F:65:LEU:HB2	2:F:79:ILE:HB	1.72	0.71
2:B:321:ILE:HD11	2:B:332:TYR:CD2	2.25	0.71
2:A:369:GLU:HA	2:A:377:LEU:HD11	1.71	0.71
2:C:47:GLU:O	2:C:48:ASP:HB2	1.89	0.71
2:F:167:PRO:HD2	2:F:365:THR:CG2	2.21	0.71
2:B:131:ILE:HG22	2:B:133:PHE:CD2	2.25	0.71
2:B:169:GLY:H	2:B:172:GLN:HG3	1.56	0.71
2:B:228:VAL:HG12	2:B:242:VAL:HG13	1.73	0.71
2:B:170:ARG:HD3	2:B:259:ASP:OD2	1.91	0.71
2:C:269:ARG:NH1	2:C:272:ARG:HH12	1.87	0.71
2:D:60:ASP:HB2	2:D:62:PHE:CE2	2.26	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:268:THR:HG23	2:F:319:ALA:HA	1.72	0.71
2:F:369:GLU:HA	2:F:377:LEU:HD13	1.71	0.71
2:C:173:ARG:HD3	2:C:301:PHE:O	1.91	0.71
2:D:141:ALA:O	2:D:370:LEU:HB3	1.89	0.71
2:F:411:ASP:O	2:F:415:MSE:HB2	1.90	0.71
2:B:253:LEU:O	2:B:258:LYS:HB2	1.90	0.70
2:C:10:PRO:HG2	2:C:13:GLU:OE2	1.90	0.70
2:A:173:ARG:NH1	2:A:173:ARG:HB2	2.06	0.70
2:C:375:GLU:CD	2:C:375:GLU:H	1.94	0.70
2:D:24:GLU:O	2:D:26:LEU:HD23	1.91	0.70
2:C:275:ASN:HD21	2:C:290:ASP:H	1.38	0.70
2:D:396:MSE:O	2:D:400:ILE:HG13	1.91	0.70
2:F:346:SER:HB3	2:F:349:ILE:HG13	1.71	0.70
2:A:86:ILE:HG23	2:A:91:LEU:HB2	1.73	0.70
2:C:167:PRO:HD2	2:C:365:THR:CG2	2.22	0.70
2:D:352:LYS:O	2:D:353:ARG:HB2	1.91	0.70
2:F:266:SER:HB2	2:F:269:ARG:H	1.55	0.70
2:D:390:MSE:CE	2:D:395:ALA:HA	2.16	0.70
2:D:66:ARG:HG2	2:D:66:ARG:HH11	1.54	0.70
2:E:211:GLU:HG3	2:E:212:ARG:H	1.56	0.70
2:C:356:PRO:HB2	2:C:396:MSE:HE2	1.73	0.69
2:E:18:GLY:O	2:E:23:LEU:HB2	1.92	0.69
2:B:158:THR:OG1	2:B:356:PRO:HG3	1.91	0.69
2:D:231:THR:OG1	2:D:233:ASP:HB2	1.91	0.69
2:E:139:LEU:HD22	2:E:367:LYS:CD	2.23	0.69
2:F:168:ILE:CG1	2:F:341:MSE:HE3	2.21	0.69
2:B:144:ARG:HG2	2:B:145:LEU:N	2.08	0.69
2:D:23:LEU:CG	2:D:41:GLN:HG3	2.22	0.69
2:A:184:LYS:HG2	2:A:185:THR:N	2.05	0.69
2:C:356:PRO:O	2:C:358:ILE:N	2.26	0.69
2:C:141:ALA:CA	2:C:371:LEU:HD23	2.22	0.69
2:A:405:MSE:SE	2:A:415:MSE:HE1	2.42	0.69
2:C:171:GLY:N	2:C:314:THR:HG22	2.08	0.69
2:D:372:THR:OG1	2:D:377:LEU:HD12	1.92	0.69
2:E:343:LEU:HD11	2:E:358:ILE:HG23	1.74	0.69
2:F:275:ASN:ND2	2:F:289:VAL:HA	2.08	0.69
2:C:91:LEU:HD13	2:C:97:ILE:CD1	2.21	0.69
2:A:140:HIS:HA	2:A:306:ASN:ND2	2.08	0.69
2:A:405:MSE:SE	2:A:415:MSE:HE2	2.41	0.69
2:D:272:ARG:CG	2:D:272:ARG:HH11	2.06	0.69
2:F:15:ILE:HD13	2:F:27:ALA:HA	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:173:ARG:HD2	2:A:301:PHE:O	1.92	0.69
2:B:139:LEU:O	2:B:141:ALA:N	2.26	0.68
2:A:131:ILE:CG2	2:A:133:PHE:HD2	2.06	0.68
2:A:265:ASP:O	2:A:318:THR:CB	2.30	0.68
2:B:210:ASP:OD1	2:B:232:PHE:HA	1.93	0.68
2:C:214:GLU:HG2	2:C:215:GLU:N	2.09	0.68
2:E:321:ILE:HD11	2:E:332:TYR:CG	2.28	0.68
2:C:236:ALA:HA	2:C:239:HIS:HD2	1.57	0.68
2:A:252:ARG:NH1	2:A:255:GLU:CD	2.47	0.68
2:D:222:LEU:N	2:D:222:LEU:HD23	2.08	0.68
2:F:252:ARG:HA	2:F:255:GLU:OE1	1.93	0.68
2:F:382:ILE:O	2:F:386:ILE:CG2	2.41	0.68
2:C:252:ARG:NH1	2:C:255:GLU:OE2	2.26	0.68
2:D:131:ILE:HG21	2:D:133:PHE:CD2	2.23	0.68
2:E:272:ARG:HE	2:E:327:MSE:CG	2.06	0.68
2:F:402:LYS:NZ	2:F:415:MSE:HE1	2.07	0.68
2:B:105:LYS:O	2:B:108:GLU:HB2	1.94	0.68
2:C:141:ALA:CB	2:C:370:LEU:HB3	2.12	0.68
2:A:173:ARG:HH22	2:B:214:GLU:CD	1.97	0.68
2:A:272:ARG:NE	2:A:327:MSE:SE	2.77	0.68
2:C:79:ILE:HD13	2:C:101:ILE:CG2	2.19	0.68
2:D:170:ARG:NH1	2:D:202:CYS:SG	2.66	0.68
2:E:141:ALA:HB3	2:E:370:LEU:CB	2.23	0.68
2:E:169:GLY:N	2:E:172:GLN:HG2	2.07	0.68
2:F:138:PRO:HD2	2:F:306:ASN:O	1.94	0.68
2:A:187:LEU:HD21	2:A:343:LEU:HD23	1.76	0.68
2:B:244:GLU:CD	2:B:296:ARG:HH21	1.96	0.68
2:C:99:GLY:HA3	2:C:115:LYS:O	1.94	0.68
2:C:260:VAL:HG12	2:C:261:ILE:N	2.09	0.68
2:D:341:MSE:CE	2:D:342:GLU:N	2.56	0.68
2:B:137:THR:HG21	2:B:305:ARG:NH1	2.09	0.67
2:B:355:PHE:O	2:B:356:PRO:C	2.29	0.67
2:C:226:GLU:OE2	2:C:249:LYS:HE2	1.94	0.67
2:F:6:LEU:HD22	2:F:14:LEU:CD2	2.23	0.67
2:F:355:PHE:HA	3:F:420:HOH:O	1.94	0.67
2:D:136:LEU:N	2:D:136:LEU:HD23	2.07	0.67
2:D:184:LYS:NZ	2:D:265:ASP:OD2	2.28	0.67
2:B:329:GLU:OE1	2:B:329:GLU:HA	1.94	0.67
2:E:337:GLY:O	2:F:212:ARG:NH1	2.26	0.67
2:C:275:ASN:ND2	2:C:290:ASP:H	1.92	0.67
2:D:402:LYS:O	2:D:405:MSE:HG2	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:18:GLY:O	2:F:23:LEU:HB2	1.94	0.67
2:B:143:SER:OG	2:B:170:ARG:HD2	1.95	0.67
2:C:236:ALA:HA	2:C:239:HIS:CD2	2.29	0.67
2:A:66:ARG:NH1	2:A:66:ARG:HG2	2.07	0.67
2:B:348:LYS:HD2	2:B:392:GLU:OE1	1.94	0.67
2:D:268:THR:O	2:D:272:ARG:HG2	1.94	0.67
2:B:264:LEU:HD22	2:B:300:PHE:CE2	2.30	0.67
2:D:356:PRO:O	2:D:358:ILE:HG13	1.95	0.67
2:D:136:LEU:O	2:D:138:PRO:CD	2.42	0.67
2:C:137:THR:HG22	2:D:214:GLU:HB3	1.75	0.67
2:E:252:ARG:NH1	2:E:255:GLU:OE2	2.28	0.67
2:E:137:THR:HG22	2:E:305:ARG:HB2	1.77	0.67
2:F:367:LYS:HB3	2:F:370:LEU:HD12	1.76	0.67
2:D:341:MSE:C	2:D:341:MSE:CE	2.63	0.66
2:F:212:ARG:O	2:F:216:VAL:HG23	1.95	0.66
2:A:207:LEU:HD23	2:A:264:LEU:HD13	1.77	0.66
2:B:173:ARG:HD3	2:B:304:ALA:HB3	1.76	0.66
2:B:356:PRO:HB2	2:B:396:MSE:HE2	1.77	0.66
2:C:341:MSE:HE3	2:C:342:GLU:N	2.09	0.66
2:C:141:ALA:HB1	2:C:370:LEU:HB2	1.69	0.66
2:C:398:PHE:CE1	2:C:402:LYS:HE3	2.30	0.66
2:C:141:ALA:HB1	2:C:370:LEU:C	2.16	0.66
2:C:388:HIS:HB3	2:C:389:PRO:HD3	1.77	0.66
2:E:366:ARG:HG3	2:E:366:ARG:NH1	2.11	0.66
2:F:390:MSE:HE1	2:F:398:PHE:CD1	2.31	0.66
2:A:172:GLN:NE2	2:A:371:LEU:HD11	2.10	0.66
2:B:272:ARG:CD	2:B:327:MSE:SE	2.93	0.66
2:C:160:ARG:CG	2:C:408:THR:HG23	2.25	0.66
2:D:343:LEU:HA	2:D:363:SER:HB3	1.76	0.66
2:D:49:ILE:HG22	2:D:101:ILE:HD11	1.76	0.66
2:C:171:GLY:HA2	2:C:313:LEU:O	1.96	0.66
2:C:187:LEU:O	2:C:191:ILE:HG13	1.96	0.66
2:D:160:ARG:HD2	2:D:408:THR:HG23	1.78	0.66
2:B:141:ALA:HB3	2:B:370:LEU:HD12	1.76	0.66
2:A:296:ARG:HB2	2:A:297:PRO:HD3	1.77	0.66
2:E:289:VAL:HB	2:E:327:MSE:CE	2.27	0.66
2:A:50:PHE:CE1	2:A:100:LYS:HG2	2.31	0.65
2:D:341:MSE:HE2	2:D:342:GLU:CA	2.24	0.65
2:D:42:HIS:O	2:D:42:HIS:ND1	2.29	0.65
2:C:173:ARG:NH2	2:D:214:GLU:OE1	2.25	0.65
2:A:131:ILE:HG22	2:A:133:PHE:CD2	2.28	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:252:ARG:NH1	2:A:255:GLU:OE2	2.28	0.65
2:C:174:GLY:HA2	2:C:341:MSE:HE2	1.77	0.65
2:E:66:ARG:HH11	2:E:66:ARG:HG2	1.62	0.65
2:F:211:GLU:HG3	2:F:212:ARG:N	2.11	0.65
2:B:352:LYS:O	2:B:352:LYS:HG3	1.96	0.65
2:F:390:MSE:CE	2:F:398:PHE:CG	2.75	0.65
2:D:23:LEU:HG	2:D:41:GLN:HG3	1.79	0.65
2:E:49:ILE:CG2	2:E:101:ILE:HG13	2.26	0.65
2:A:171:GLY:H	2:A:314:THR:HB	1.60	0.65
2:C:89:PHE:HB2	2:C:91:LEU:HD21	1.79	0.65
2:D:377:LEU:HD23	2:D:381:TRP:CD1	2.32	0.65
2:D:6:LEU:O	2:D:9:THR:HG23	1.97	0.65
2:D:130:LYS:NZ	2:E:12:SER:HB3	2.12	0.65
2:F:381:TRP:O	2:F:385:LYS:HG3	1.96	0.65
2:F:390:MSE:CE	2:F:398:PHE:CB	2.75	0.65
2:F:160:ARG:HD2	2:F:408:THR:HB	1.79	0.65
2:A:41:GLN:C	2:A:43:ALA:H	1.99	0.64
2:B:289:VAL:CG1	2:B:330:VAL:HG11	2.28	0.64
2:C:251:LYS:O	2:C:255:GLU:HG3	1.97	0.64
2:E:7:LYS:HE2	2:E:77:ASP:OD1	1.97	0.64
2:A:379:LYS:HD3	2:A:412:PHE:HB2	1.79	0.64
2:F:296:ARG:HB2	2:F:297:PRO:HD3	1.79	0.64
2:C:30:ARG:HH11	2:C:30:ARG:HG3	1.62	0.64
2:C:356:PRO:O	2:C:358:ILE:CG1	2.43	0.64
2:E:132:LEU:HA	2:E:135:ASN:HD22	1.61	0.64
2:A:144:ARG:HH21	2:A:167:PRO:HB3	1.63	0.64
2:C:169:GLY:H	2:C:172:GLN:CG	2.09	0.64
2:C:173:ARG:NH1	2:C:304:ALA:O	2.31	0.64
2:E:58:LEU:HD12	2:E:59:GLN:H	1.63	0.64
2:A:382:ILE:O	2:A:386:ILE:HG22	1.97	0.64
2:C:289:VAL:CG1	2:C:330:VAL:HG11	2.25	0.64
2:F:360:TYR:HE2	2:F:384:ARG:HE	1.44	0.64
2:D:130:LYS:HA	2:E:27:ALA:O	1.98	0.64
2:B:321:ILE:O	2:B:322:ASP:HB2	1.98	0.63
2:B:173:ARG:NH2	2:C:212:ARG:HB3	2.12	0.63
2:E:39:LEU:HB3	2:E:111:PHE:CZ	2.32	0.63
2:A:6:LEU:O	2:A:9:THR:HG23	1.98	0.63
2:B:167:PRO:HD2	2:B:365:THR:CG2	2.28	0.63
2:C:228:VAL:CG1	2:C:242:VAL:HG13	2.28	0.63
2:A:144:ARG:NH2	2:A:167:PRO:HB3	2.13	0.63
2:B:131:ILE:HG21	2:B:133:PHE:CD2	2.32	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:320:LEU:HD12	3:B:421:HOH:O	1.98	0.63
2:D:272:ARG:CB	2:D:272:ARG:HH11	2.11	0.63
2:A:6:LEU:HD22	2:A:14:LEU:HD21	1.81	0.63
2:B:238:ARG:NH1	2:B:241:GLN:OE1	2.31	0.63
2:C:355:PHE:CB	2:C:356:PRO:HD3	2.27	0.63
2:E:268:THR:CG2	2:E:320:LEU:H	2.10	0.63
2:F:268:THR:CG2	2:F:320:LEU:H	2.10	0.63
2:A:236:ALA:HA	2:A:239:HIS:CD2	2.31	0.63
2:B:228:VAL:HG12	2:B:242:VAL:CG1	2.29	0.63
2:C:167:PRO:O	2:C:365:THR:HG21	1.99	0.63
2:C:47:GLU:HG2	2:C:48:ASP:H	1.62	0.63
2:E:137:THR:HG21	2:E:305:ARG:NH1	2.13	0.63
2:F:185:THR:HB	3:F:423:HOH:O	1.99	0.63
2:A:264:LEU:HD22	2:A:300:PHE:CE2	2.32	0.63
2:B:294:LEU:CD1	2:B:334:GLU:HG3	2.28	0.63
2:B:102:ARG:HB3	2:B:114:LEU:HD12	1.81	0.63
2:B:169:GLY:H	2:B:172:GLN:CG	2.12	0.62
2:D:135:ASN:HB3	2:D:307:VAL:CG1	2.29	0.62
2:E:138:PRO:HD2	2:E:306:ASN:O	1.98	0.62
2:B:104:PRO:HA	2:B:108:GLU:OE1	1.99	0.62
2:D:156:ASP:O	2:D:160:ARG:HG2	1.97	0.62
2:E:1:MSE:HG3	2:E:2:ASN:H	1.64	0.62
2:E:341:MSE:HE2	2:E:341:MSE:O	1.96	0.62
2:A:302:GLY:O	2:A:305:ARG:NH2	2.29	0.62
2:C:3:LEU:HD12	2:C:39:LEU:HD11	1.80	0.62
2:D:39:LEU:HB3	2:D:111:PHE:CZ	2.35	0.62
2:D:289:VAL:HG11	2:D:330:VAL:CG1	2.24	0.62
2:E:140:HIS:CA	2:E:306:ASN:HB2	2.28	0.62
2:E:381:TRP:CH2	2:F:353:ARG:HD3	2.35	0.62
2:C:356:PRO:HB2	2:C:396:MSE:CE	2.27	0.62
2:D:268:THR:HG22	2:D:319:ALA:HA	1.81	0.62
2:D:172:GLN:NE2	2:D:371:LEU:HD11	2.14	0.62
2:E:173:ARG:NH2	2:F:214:GLU:OE2	2.32	0.62
2:B:343:LEU:HD11	2:B:358:ILE:HG12	1.81	0.62
2:B:379:LYS:HD3	2:B:412:PHE:HB2	1.80	0.62
2:C:1:MSE:CG	2:C:2:ASN:H	2.13	0.62
2:C:269:ARG:HH11	2:C:272:ARG:NH1	1.94	0.62
2:C:140:HIS:CB	2:C:306:ASN:CB	2.77	0.62
2:F:274:TYR:CD2	2:F:297:PRO:HG3	2.35	0.62
2:D:139:LEU:HD13	2:E:214:GLU:CG	2.26	0.62
2:F:412:PHE:O	2:F:416:MSE:HG2	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:267:ILE:HG22	2:C:318:THR:O	2.00	0.62
2:A:145:LEU:HD21	2:A:170:ARG:HG3	1.81	0.62
2:A:341:MSE:O	2:A:341:MSE:CE	2.45	0.62
2:E:55:LEU:HB2	2:E:65:LEU:CD2	2.30	0.62
2:A:266:SER:OG	2:A:269:ARG:HB2	1.99	0.61
2:A:140:HIS:CB	2:A:306:ASN:HB2	2.29	0.61
2:E:207:LEU:HD11	2:E:242:VAL:HG12	1.82	0.61
2:F:353:ARG:HH11	2:F:353:ARG:HG3	1.65	0.61
2:A:49:ILE:CG2	2:A:101:ILE:CG1	2.77	0.61
2:F:173:ARG:N	2:F:340:ASN:OD1	2.30	0.61
2:A:166:SER:OG	2:A:343:LEU:HD13	2.01	0.61
2:C:136:LEU:O	2:C:138:PRO:HD3	2.00	0.61
2:D:330:VAL:HG12	2:D:331:ILE:N	2.15	0.61
2:A:174:GLY:CA	2:A:341:MSE:HE2	2.30	0.61
2:A:261:ILE:CG1	2:A:314:THR:HG23	2.29	0.61
2:D:341:MSE:HE3	2:D:342:GLU:N	2.14	0.61
2:E:396:MSE:HE3	2:E:400:ILE:HD11	1.83	0.61
2:A:209:ILE:HD13	2:A:270:LEU:HD13	1.82	0.61
2:A:238:ARG:NH1	2:A:241:GLN:OE1	2.33	0.61
2:A:272:ARG:HD2	2:A:327:MSE:SE	2.51	0.61
2:C:4:THR:HG22	2:C:5:GLU:H	1.63	0.61
2:C:139:LEU:HD11	2:D:218:GLU:OE1	2.01	0.61
2:D:260:VAL:HG12	2:D:261:ILE:N	2.16	0.61
2:E:140:HIS:HA	2:E:306:ASN:CB	2.31	0.61
2:E:236:ALA:CB	2:E:277:VAL:HG23	2.31	0.61
2:C:352:LYS:HD2	2:C:393:ILE:HD12	1.83	0.61
2:F:268:THR:HG21	2:F:320:LEU:N	2.15	0.61
2:A:173:ARG:N	2:A:340:ASN:OD1	2.28	0.61
2:C:383:LEU:O	2:C:387:ILE:HG13	2.00	0.60
2:C:47:GLU:HG2	2:C:48:ASP:N	2.16	0.60
2:C:4:THR:HG23	2:C:5:GLU:N	2.16	0.60
2:D:54:VAL:CG2	2:D:249:LYS:HD2	2.30	0.60
2:F:191:ILE:O	2:F:195:ILE:HG13	2.01	0.60
2:D:247:ILE:O	2:D:250:ALA:HB3	2.02	0.60
2:E:157:LEU:O	2:E:161:VAL:HG23	2.01	0.60
2:C:290:ASP:OD1	2:C:290:ASP:C	2.39	0.60
2:E:141:ALA:O	2:E:371:LEU:HG	2.02	0.60
2:E:136:LEU:CD1	2:F:221:ARG:HH21	2.14	0.60
2:A:209:ILE:HD11	2:A:243:ALA:HB2	1.83	0.60
2:A:275:ASN:HD21	2:A:289:VAL:HA	1.67	0.60
2:D:354:VAL:HG11	2:D:396:MSE:HB3	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:30:ARG:HG3	2:C:30:ARG:NH1	2.16	0.60
2:C:412:PHE:CE2	2:C:416:MSE:SE	3.04	0.60
2:E:266:SER:H	2:E:318:THR:HG1	1.46	0.60
2:F:6:LEU:O	2:F:9:THR:HG23	2.02	0.60
2:A:144:ARG:HH11	2:A:146:ARG:NE	1.97	0.60
2:C:272:ARG:CG	2:C:272:ARG:HH11	2.01	0.60
2:F:247:ILE:O	2:F:250:ALA:HB3	2.02	0.60
2:C:174:GLY:CA	2:C:341:MSE:HE2	2.31	0.60
2:D:132:LEU:HD13	2:D:251:LYS:HG2	1.83	0.60
2:B:245:MSE:HA	2:B:245:MSE:HE2	1.84	0.60
2:F:135:ASN:HB3	2:F:307:VAL:CG2	2.31	0.60
2:A:49:ILE:CG2	2:A:101:ILE:HG13	2.32	0.59
2:C:4:THR:CG2	2:C:5:GLU:H	2.15	0.59
2:D:245:MSE:HA	2:D:245:MSE:CE	2.32	0.59
2:D:386:ILE:HG13	2:D:386:ILE:O	2.01	0.59
2:E:268:THR:HG22	2:E:319:ALA:HA	1.84	0.59
2:A:1:MSE:CG	2:A:2:ASN:H	2.10	0.59
2:C:85:GLN:NE2	2:C:113:LEU:O	2.29	0.59
2:E:49:ILE:HG22	2:E:101:ILE:CG1	2.31	0.59
2:F:167:PRO:HD2	2:F:365:THR:HG22	1.84	0.59
2:E:131:ILE:CG2	2:E:133:PHE:H	2.14	0.59
2:D:136:LEU:HD12	2:E:221:ARG:NH2	2.17	0.59
2:E:4:THR:HB	2:E:52:ASP:OD1	2.01	0.59
2:F:58:LEU:HD12	2:F:59:GLN:H	1.67	0.59
2:D:23:LEU:HD21	2:D:41:GLN:HG3	1.83	0.59
2:D:136:LEU:HD12	2:E:221:ARG:HH21	1.67	0.59
2:F:189:GLN:O	2:F:193:GLN:HG3	2.02	0.59
2:F:238:ARG:NH1	2:F:241:GLN:OE1	2.35	0.59
2:F:23:LEU:HG	2:F:41:GLN:HG3	1.84	0.59
2:B:139:LEU:CD1	2:C:214:GLU:HG3	2.32	0.59
2:D:144:ARG:NH2	2:D:163:ASP:OD1	2.33	0.59
2:E:36:PHE:CE2	2:E:40:LYS:HD2	2.37	0.59
2:F:272:ARG:CG	2:F:272:ARG:HH11	2.14	0.59
2:A:411:ASP:O	2:A:415:MSE:HG3	2.02	0.59
2:B:407:LYS:HG2	2:B:408:THR:HG23	1.83	0.59
2:C:56:GLU:HG3	2:C:245:MSE:SE	2.53	0.59
2:C:377:LEU:HA	2:C:380:MSE:HE2	1.85	0.59
2:C:3:LEU:O	2:C:7:LYS:CG	2.50	0.59
2:B:407:LYS:CG	2:B:408:THR:HG23	2.32	0.59
2:C:379:LYS:CG	2:C:412:PHE:CG	2.82	0.59
2:D:377:LEU:HD23	2:D:381:TRP:HD1	1.64	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:268:THR:HG21	2:E:320:LEU:H	1.68	0.59
2:E:411:ASP:O	2:E:415:MSE:CG	2.50	0.59
2:A:167:PRO:O	2:A:365:THR:HG21	2.03	0.59
2:A:383:LEU:O	2:A:387:ILE:HG13	2.02	0.59
2:C:214:GLU:HG2	2:C:215:GLU:H	1.68	0.59
2:E:142:ASN:HD21	2:E:306:ASN:HD21	1.51	0.59
2:E:152:GLY:CA	2:E:407:LYS:CE	2.74	0.59
2:A:187:LEU:HD21	2:A:343:LEU:CD2	2.33	0.59
2:C:379:LYS:C	2:C:379:LYS:HD2	2.23	0.59
2:D:23:LEU:CD2	2:D:41:GLN:HG3	2.33	0.59
2:E:142:ASN:OD1	2:E:306:ASN:ND2	2.35	0.59
2:E:30:ARG:O	2:E:33:ASP:N	2.36	0.59
2:A:257:LYS:HD3	2:A:309:GLU:O	2.01	0.58
2:A:390:MSE:HE1	2:A:398:PHE:CB	2.32	0.58
2:B:161:VAL:HG21	2:B:396:MSE:HE1	1.84	0.58
2:C:160:ARG:NE	2:C:408:THR:H	2.01	0.58
2:C:141:ALA:HB3	2:C:370:LEU:HB2	1.45	0.58
2:D:341:MSE:HE2	2:D:342:GLU:N	2.18	0.58
2:A:272:ARG:HE	2:A:327:MSE:SE	2.36	0.58
2:D:171:GLY:H	2:D:314:THR:HG22	1.68	0.58
2:F:294:LEU:O	2:F:297:PRO:HD2	2.03	0.58
2:A:1:MSE:HG3	2:A:2:ASN:N	2.11	0.58
2:B:266:SER:HA	2:B:318:THR:O	2.02	0.58
2:C:15:ILE:CD1	2:C:27:ALA:HA	2.33	0.58
2:C:160:ARG:HE	2:C:408:THR:H	1.52	0.58
2:F:402:LYS:HZ3	2:F:415:MSE:HE1	1.66	0.58
2:D:137:THR:CG2	2:D:305:ARG:HB2	2.32	0.58
2:E:272:ARG:NE	2:E:327:MSE:SE	2.86	0.58
2:F:307:VAL:HG13	2:F:309:GLU:HG2	1.85	0.58
2:C:205:MSE:CE	2:C:246:VAL:HG13	2.33	0.58
2:C:167:PRO:HG2	2:C:368:GLU:HG2	1.86	0.58
2:C:42:HIS:ND1	2:C:42:HIS:O	2.37	0.58
2:D:30:ARG:O	2:D:31:LYS:C	2.42	0.58
2:A:390:MSE:CE	2:A:398:PHE:HB3	2.33	0.58
2:C:56:GLU:CD	2:C:66:ARG:HH11	2.06	0.58
2:E:141:ALA:CB	2:E:370:LEU:CD1	2.73	0.58
2:F:2:ASN:OD1	2:F:4:THR:HG22	2.02	0.58
1:H:4:DC:N3	2:C:66:ARG:NH2	2.52	0.58
2:A:337:GLY:O	2:B:212:ARG:HD3	2.03	0.58
2:C:338:THR:O	2:D:212:ARG:HG2	2.04	0.58
2:F:376:GLU:O	2:F:380:MSE:HG3	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:169:GLY:H	2:C:172:GLN:HG3	1.68	0.58
2:E:137:THR:HG22	2:E:305:ARG:CB	2.33	0.58
2:B:298:LYS:NZ	2:B:334:GLU:O	2.36	0.58
2:C:375:GLU:OE1	2:C:375:GLU:N	2.29	0.58
2:F:211:GLU:HG3	2:F:212:ARG:H	1.67	0.58
2:A:144:ARG:CG	2:A:145:LEU:N	2.64	0.57
2:A:385:LYS:CE	2:B:353:ARG:HH12	2.15	0.57
2:D:139:LEU:O	2:D:141:ALA:N	2.37	0.57
2:A:294:LEU:CD1	2:A:334:GLU:HG3	2.33	0.57
2:C:231:THR:C	2:C:233:ASP:H	2.06	0.57
2:E:49:ILE:HG22	2:E:101:ILE:HG13	1.85	0.57
2:E:323:THR:OG1	2:E:325:SER:HB3	2.04	0.57
2:E:36:PHE:HE2	2:E:40:LYS:HD2	1.69	0.57
2:F:168:ILE:HD13	2:F:316:ILE:HD11	1.86	0.57
2:A:373:THR:HB	2:A:375:GLU:OE1	2.03	0.57
2:B:231:THR:OG1	2:B:233:ASP:HB2	2.04	0.57
2:D:144:ARG:HD2	2:D:371:LEU:O	2.03	0.57
2:E:268:THR:HB	2:E:331:ILE:HG21	1.86	0.57
2:F:356:PRO:C	2:F:358:ILE:H	2.07	0.57
2:B:307:VAL:HG12	2:B:309:GLU:H	1.69	0.57
2:B:407:LYS:O	2:B:408:THR:OG1	2.21	0.57
2:F:359:ASP:C	2:F:359:ASP:OD1	2.42	0.57
2:B:198:ASN:N	2:B:198:ASN:HD22	2.02	0.57
2:C:131:ILE:HG23	2:C:133:PHE:CD2	2.38	0.57
2:B:206:VAL:HB	2:B:227:VAL:HG22	1.85	0.57
2:C:131:ILE:HA	2:C:255:GLU:OE2	2.04	0.57
2:C:15:ILE:HD13	2:C:27:ALA:HA	1.85	0.57
2:D:133:PHE:CB	3:E:430:HOH:O	2.42	0.57
2:E:254:VAL:CG1	2:E:307:VAL:HG21	2.34	0.57
2:E:173:ARG:NH2	2:F:212:ARG:HD2	2.19	0.57
2:F:30:ARG:O	2:F:33:ASP:N	2.38	0.57
2:D:230:SER:HB3	2:D:242:VAL:HG21	1.87	0.57
2:D:388:HIS:HB3	2:D:389:PRO:HD3	1.85	0.57
2:E:167:PRO:O	2:E:365:THR:HG21	2.04	0.57
2:F:294:LEU:HD11	2:F:334:GLU:HG3	1.86	0.57
2:C:139:LEU:CD1	2:D:218:GLU:OE1	2.53	0.57
2:D:275:ASN:HD22	2:D:289:VAL:HG23	1.69	0.57
2:F:100:LYS:O	2:F:114:LEU:HB3	2.05	0.57
2:A:140:HIS:CA	2:A:306:ASN:HB3	2.35	0.57
2:E:131:ILE:HG23	2:E:133:PHE:HD2	1.68	0.57
2:F:56:GLU:OE2	2:F:241:GLN:NE2	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:266:SER:HG	2:A:269:ARG:H	1.50	0.56
2:D:169:GLY:N	2:D:172:GLN:HG2	2.15	0.56
2:F:185:THR:O	2:F:189:GLN:HG3	2.04	0.56
2:F:268:THR:CG2	2:F:319:ALA:HA	2.35	0.56
2:E:146:ARG:NH2	2:E:376:GLU:OE1	2.38	0.56
2:E:95:ASP:OD2	2:F:28:ARG:NH1	2.31	0.56
2:F:274:TYR:HD2	2:F:297:PRO:HG3	1.69	0.56
2:E:195:ILE:HD13	2:E:261:ILE:HD12	1.87	0.56
2:A:1:MSE:N	3:A:420:HOH:O	2.37	0.56
2:A:161:VAL:HG22	2:A:399:LEU:HD13	1.88	0.56
2:A:172:GLN:HE22	2:A:371:LEU:HD11	1.68	0.56
2:B:261:ILE:HG12	2:B:314:THR:HG21	1.85	0.56
2:D:2:ASN:OD1	2:D:4:THR:HG22	2.05	0.56
2:B:261:ILE:HA	2:B:314:THR:HG23	1.88	0.56
2:D:268:THR:CG2	2:D:319:ALA:HA	2.35	0.56
2:A:138:PRO:HD2	2:A:306:ASN:O	2.06	0.56
2:C:133:PHE:CB	3:D:422:HOH:O	2.52	0.56
2:C:160:ARG:NE	2:C:408:THR:HG23	2.20	0.56
2:C:141:ALA:CA	2:C:371:LEU:CD2	2.68	0.56
2:E:174:GLY:HA3	2:E:341:MSE:HE2	1.87	0.56
2:E:167:PRO:HD2	2:E:365:THR:CG2	2.35	0.56
2:F:264:LEU:HB3	2:F:317:ALA:HA	1.87	0.56
2:A:173:ARG:NH2	2:B:214:GLU:OE2	2.25	0.56
2:B:372:THR:HB	2:B:376:GLU:HB3	1.88	0.56
2:B:416:MSE:O	2:B:417:LYS:CB	2.51	0.56
2:D:272:ARG:HG3	2:D:272:ARG:NH1	2.20	0.56
1:L:4:DC:H5	2:F:110:TYR:CZ	2.24	0.56
2:F:138:PRO:C	2:F:140:HIS:H	2.08	0.56
2:F:68:ALA:C	2:F:70:SER:H	2.07	0.56
2:A:169:GLY:H	2:A:172:GLN:HG3	1.68	0.56
2:D:130:LYS:HZ2	2:E:12:SER:HB3	1.68	0.56
2:E:327:MSE:O	2:E:328:ASP:C	2.44	0.56
2:F:245:MSE:HA	2:F:245:MSE:HE2	1.87	0.56
2:D:275:ASN:ND2	2:D:289:VAL:HA	2.21	0.56
2:E:139:LEU:HD22	2:E:367:LYS:CG	2.36	0.56
2:E:290:ASP:OD1	2:E:292:ASN:N	2.39	0.56
2:E:92:ARG:NH2	2:E:131:ILE:HD11	2.21	0.56
2:F:169:GLY:H	2:F:172:GLN:CD	2.08	0.56
2:F:168:ILE:HD13	2:F:316:ILE:CD1	2.36	0.56
2:A:44:LYS:O	2:A:45:SER:HB2	2.06	0.56
2:B:316:ILE:HD12	2:B:341:MSE:HE2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:31:LYS:O	2:E:35:ILE:HD12	2.06	0.56
2:B:355:PHE:O	2:B:357:ALA:N	2.39	0.55
2:C:416:MSE:O	2:C:417:LYS:CB	2.51	0.55
2:D:136:LEU:C	2:D:138:PRO:HD3	2.26	0.55
2:F:162:LEU:HD12	2:F:187:LEU:HD11	1.88	0.55
2:A:357:ALA:O	2:A:358:ILE:HG13	2.05	0.55
2:C:355:PHE:HB2	2:C:356:PRO:CD	2.34	0.55
2:E:289:VAL:HB	2:E:327:MSE:HE3	1.87	0.55
2:E:376:GLU:O	2:E:380:MSE:HG3	2.05	0.55
2:C:205:MSE:HE2	2:C:246:VAL:HG13	1.88	0.55
2:E:405:MSE:O	2:E:406:THR:HG23	2.05	0.55
2:D:296:ARG:O	2:D:299:ARG:HB2	2.06	0.55
2:D:303:ALA:O	2:D:304:ALA:C	2.43	0.55
2:E:377:LEU:HD23	2:E:381:TRP:HE1	1.72	0.55
2:F:141:ALA:O	2:F:370:LEU:HB3	2.06	0.55
2:F:169:GLY:O	2:F:172:GLN:HG3	2.06	0.55
2:F:353:ARG:HG3	2:F:353:ARG:NH1	2.19	0.55
2:F:49:ILE:HG22	2:F:101:ILE:CD1	2.31	0.55
2:B:240:VAL:HG13	2:B:274:TYR:CZ	2.42	0.55
2:B:272:ARG:NE	2:B:327:MSE:SE	2.89	0.55
1:L:3:DC:O2	2:F:109:ARG:HB2	2.06	0.55
2:F:85:GLN:NE2	2:F:113:LEU:O	2.32	0.55
2:F:252:ARG:O	2:F:255:GLU:HB2	2.06	0.55
2:C:257:LYS:HE2	2:C:309:GLU:O	2.07	0.55
2:A:88:ARG:HG3	2:A:88:ARG:O	2.07	0.55
2:B:244:GLU:OE2	2:B:296:ARG:NH2	2.37	0.55
2:F:184:LYS:HD2	2:F:318:THR:HG21	1.88	0.55
2:B:154:THR:O	2:B:157:LEU:HB2	2.07	0.55
2:C:113:LEU:HD21	2:C:116:VAL:HG22	1.89	0.55
2:D:252:ARG:NH1	2:D:255:GLU:OE2	2.39	0.55
2:E:144:ARG:HG3	2:E:145:LEU:N	2.21	0.55
2:E:187:LEU:HG	2:E:191:ILE:HD11	1.89	0.55
2:E:91:LEU:HD13	2:E:97:ILE:CD1	2.37	0.55
2:B:206:VAL:HG22	2:B:263:LEU:HB2	1.89	0.55
2:B:245:MSE:CA	2:B:245:MSE:HE2	2.37	0.55
2:E:140:HIS:HA	2:E:306:ASN:HB2	1.88	0.55
2:F:382:ILE:HD13	2:F:416:MSE:HE1	1.87	0.55
2:F:60:ASP:CB	2:F:62:PHE:HE2	2.20	0.55
2:C:26:LEU:HB3	2:C:29:MSE:HG2	1.89	0.55
2:C:308:GLU:HB3	2:C:309:GLU:OE2	2.07	0.55
2:C:382:ILE:O	2:C:383:LEU:C	2.45	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:252:ARG:HH11	2:D:255:GLU:CD	2.10	0.55
2:D:294:LEU:CD1	2:D:334:GLU:HG3	2.38	0.55
2:E:139:LEU:HD22	2:E:367:LYS:HG3	1.87	0.55
2:E:381:TRP:CD2	2:F:353:ARG:NH1	2.75	0.55
2:F:376:GLU:HA	2:F:379:LYS:HD2	1.88	0.55
2:C:1:MSE:HG3	2:C:2:ASN:N	2.22	0.54
2:F:160:ARG:O	2:F:164:LEU:HG	2.07	0.54
2:A:263:LEU:HD22	2:A:316:ILE:HB	1.88	0.54
2:A:390:MSE:CE	2:A:395:ALA:HA	2.24	0.54
2:D:173:ARG:HD3	2:D:301:PHE:O	2.06	0.54
2:E:141:ALA:HB3	2:E:370:LEU:HD13	1.84	0.54
2:D:139:LEU:CD1	2:E:214:GLU:HG3	2.32	0.54
2:F:275:ASN:HD21	2:F:289:VAL:HA	1.73	0.54
2:B:289:VAL:HG11	2:B:330:VAL:CG1	2.36	0.54
2:E:343:LEU:HD11	2:E:358:ILE:CG2	2.36	0.54
2:E:359:ASP:C	2:E:359:ASP:OD1	2.46	0.54
2:E:368:GLU:HA	2:E:371:LEU:HD12	1.89	0.54
2:F:264:LEU:HD23	2:F:317:ALA:HB1	1.88	0.54
2:B:146:ARG:NH2	2:B:376:GLU:OE1	2.40	0.54
2:B:139:LEU:HA	2:C:214:GLU:HB2	1.89	0.54
2:C:7:LYS:HA	2:C:35:ILE:HD11	1.90	0.54
2:E:140:HIS:CB	2:E:306:ASN:CB	2.78	0.54
2:F:60:ASP:CB	2:F:62:PHE:CE2	2.88	0.54
2:B:171:GLY:H	2:B:314:THR:HB	1.73	0.54
2:B:321:ILE:CD1	2:B:332:TYR:CG	2.88	0.54
2:C:296:ARG:HB2	2:C:297:PRO:HD3	1.90	0.54
2:D:147:MSE:HE1	2:D:191:ILE:HA	1.89	0.54
2:A:7:LYS:HA	2:A:35:ILE:HD11	1.90	0.54
2:C:56:GLU:CD	2:C:66:ARG:NH1	2.61	0.54
2:D:321:ILE:HD11	2:D:332:TYR:CE2	2.42	0.54
2:F:11:VAL:O	2:F:15:ILE:HG13	2.08	0.54
2:F:206:VAL:HG22	2:F:263:LEU:HD12	1.89	0.54
2:F:258:LYS:O	2:F:312:SER:N	2.40	0.54
2:C:309:GLU:N	2:C:309:GLU:OE2	2.41	0.54
2:D:272:ARG:HD2	2:D:327:MSE:SE	2.57	0.54
2:E:236:ALA:HB1	2:E:277:VAL:HG23	1.89	0.54
2:E:59:GLN:NE2	2:E:59:GLN:O	2.40	0.54
2:F:380:MSE:HG2	2:F:412:PHE:CZ	2.42	0.54
2:A:39:LEU:HD13	2:A:111:PHE:CZ	2.43	0.54
2:A:194:SER:O	2:A:198:ASN:HB2	2.08	0.54
2:B:365:THR:HG23	2:B:368:GLU:HG2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:294:LEU:HD12	2:C:334:GLU:HG3	1.90	0.54
2:A:187:LEU:O	2:A:191:ILE:HG13	2.08	0.53
2:C:381:TRP:HB3	2:D:353:ARG:HH21	1.71	0.53
2:C:402:LYS:HD3	2:C:415:MSE:HE1	1.89	0.53
2:D:119:VAL:O	2:D:120:ASN:HB2	2.07	0.53
2:E:65:LEU:HD21	2:E:97:ILE:HD12	1.89	0.53
2:F:253:LEU:O	2:F:258:LYS:HB2	2.08	0.53
1:L:3:DC:H4'	1:L:4:DC:O5'	2.08	0.53
2:A:161:VAL:HG11	2:A:396:MSE:CE	2.34	0.53
2:B:272:ARG:HE	2:B:327:MSE:CG	2.21	0.53
2:D:228:VAL:HG12	2:D:242:VAL:CG1	2.38	0.53
2:E:173:ARG:HH21	2:F:212:ARG:CD	2.19	0.53
2:F:280:ALA:HA	2:F:290:ASP:OD2	2.09	0.53
2:B:137:THR:CG2	2:B:305:ARG:HH11	2.21	0.53
2:C:169:GLY:H	2:C:172:GLN:HG2	1.74	0.53
2:C:132:LEU:HD22	2:C:251:LYS:HD3	1.90	0.53
2:F:219:MSE:HG3	2:F:223:VAL:HG23	1.91	0.53
2:F:241:GLN:O	2:F:242:VAL:C	2.45	0.53
2:B:67:SER:HB2	2:B:69:ASP:OD1	2.08	0.53
2:D:164:LEU:O	2:D:380:MSE:HE3	2.09	0.53
2:F:355:PHE:O	2:F:357:ALA:N	2.41	0.53
2:F:403:LEU:C	2:F:405:MSE:H	2.12	0.53
2:B:140:HIS:HA	2:B:306:ASN:HD22	1.74	0.53
2:B:290:ASP:C	2:B:290:ASP:OD1	2.46	0.53
2:C:348:LYS:HD2	2:C:392:GLU:OE1	2.09	0.53
2:D:290:ASP:OD1	2:D:292:ASN:HB3	2.07	0.53
2:E:3:LEU:HD12	2:E:39:LEU:HD11	1.90	0.53
2:A:170:ARG:NH1	2:A:201:ASP:OD2	2.42	0.53
2:E:298:LYS:O	2:E:302:GLY:N	2.27	0.53
2:B:173:ARG:HH22	2:C:212:ARG:HB3	1.73	0.53
2:E:228:VAL:HG12	2:E:242:VAL:HG13	1.91	0.53
2:F:86:ILE:HA	2:F:91:LEU:HD12	1.90	0.53
2:B:173:ARG:HD2	2:B:301:PHE:O	2.08	0.53
2:E:272:ARG:NH1	2:E:272:ARG:CG	2.62	0.53
2:F:56:GLU:HG3	2:F:245:MSE:CE	2.36	0.53
1:J:3:DC:H4'	1:J:4:DC:C5'	2.38	0.53
2:B:144:ARG:NH2	2:B:163:ASP:CG	2.62	0.53
2:B:91:LEU:HD22	2:B:97:ILE:HD11	1.89	0.53
2:C:173:ARG:NH2	2:D:213:PRO:HD2	2.24	0.53
2:D:171:GLY:H	2:D:314:THR:CG2	2.21	0.53
2:D:211:GLU:HG3	2:D:215:GLU:HB3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:15:ILE:CD1	2:F:27:ALA:HA	2.39	0.53
2:C:415:MSE:N	3:C:421:HOH:O	2.42	0.53
2:D:26:LEU:HB3	2:D:29:MSE:SE	2.59	0.53
2:E:140:HIS:CA	2:E:306:ASN:CB	2.87	0.53
2:D:60:ASP:HB2	2:D:62:PHE:HE2	1.70	0.52
2:E:147:MSE:HE1	2:E:195:ILE:HG12	1.90	0.52
2:F:144:ARG:HD3	2:F:146:ARG:NE	2.24	0.52
2:F:162:LEU:CD1	2:F:187:LEU:HD11	2.39	0.52
2:A:387:ILE:HA	2:A:390:MSE:SE	2.59	0.52
2:A:136:LEU:HD13	2:B:221:ARG:HH21	1.74	0.52
2:B:341:MSE:SE	2:B:341:MSE:C	2.98	0.52
2:E:23:LEU:HD21	2:E:41:GLN:CG	2.33	0.52
2:F:382:ILE:CD1	2:F:416:MSE:HE1	2.38	0.52
2:A:62:PHE:HE1	2:A:64:PHE:HE2	1.57	0.52
2:B:240:VAL:HG13	2:B:274:TYR:CE1	2.44	0.52
2:B:245:MSE:HA	2:B:245:MSE:CE	2.39	0.52
2:B:307:VAL:HG12	2:B:309:GLU:N	2.22	0.52
2:E:187:LEU:HD21	2:E:343:LEU:HD23	1.91	0.52
2:A:166:SER:HA	2:A:365:THR:HG22	1.91	0.52
2:B:144:ARG:CG	2:B:145:LEU:N	2.71	0.52
2:B:173:ARG:CD	2:B:301:PHE:O	2.58	0.52
2:D:275:ASN:ND2	2:D:289:VAL:HG23	2.24	0.52
2:E:266:SER:HB2	2:E:269:ARG:H	1.74	0.52
2:C:294:LEU:HD13	2:C:334:GLU:HG3	1.88	0.52
2:E:105:LYS:N	2:E:108:GLU:OE1	2.41	0.52
2:A:406:THR:HB	2:A:410:ASP:HB2	1.91	0.52
2:C:141:ALA:O	2:C:370:LEU:O	2.27	0.52
2:D:382:ILE:O	2:D:386:ILE:HG22	2.09	0.52
2:D:5:GLU:O	2:D:9:THR:HG22	2.10	0.52
2:E:274:TYR:O	2:E:278:VAL:HB	2.09	0.52
2:F:52:ASP:HA	2:F:97:ILE:O	2.09	0.52
2:C:173:ARG:CD	2:C:301:PHE:O	2.57	0.52
2:E:55:LEU:HB2	2:E:65:LEU:HD23	1.91	0.52
2:C:268:THR:HA	2:C:331:ILE:HG21	1.92	0.52
2:C:343:LEU:HD11	2:C:358:ILE:HD13	1.92	0.52
2:E:214:GLU:HG2	2:E:215:GLU:N	2.24	0.52
2:E:170:ARG:HD3	2:E:259:ASP:OD2	2.09	0.52
2:E:378:GLN:O	2:E:382:ILE:HG13	2.10	0.52
2:A:173:ARG:CD	2:A:301:PHE:O	2.58	0.52
2:B:269:ARG:NH1	2:B:272:ARG:NH1	2.41	0.52
2:D:244:GLU:OE2	2:D:274:TYR:OH	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:156:ASP:O	2:B:160:ARG:HB2	2.10	0.52
2:B:141:ALA:CB	2:B:370:LEU:HB2	2.36	0.52
2:C:131:ILE:HG22	2:C:134:GLU:HG2	1.92	0.52
2:C:26:LEU:HD22	2:C:29:MSE:HE3	1.92	0.52
2:D:272:ARG:HG3	2:D:272:ARG:HH11	1.72	0.52
2:D:71:SER:HA	2:D:228:VAL:HG13	1.92	0.52
2:E:137:THR:HG21	2:E:305:ARG:CZ	2.40	0.52
2:E:264:LEU:HB3	2:E:317:ALA:HB2	1.92	0.52
2:F:132:LEU:HD13	2:F:251:LYS:HA	1.91	0.52
2:A:272:ARG:CD	2:A:327:MSE:SE	3.09	0.51
2:B:139:LEU:HD13	2:C:214:GLU:HG3	1.91	0.51
2:C:71:SER:OG	2:C:228:VAL:HA	2.10	0.51
2:B:355:PHE:HB2	2:B:356:PRO:HD2	1.92	0.51
2:C:6:LEU:O	2:C:9:THR:HG23	2.09	0.51
1:J:4:DC:H5	2:D:110:TYR:CZ	2.28	0.51
2:E:56:GLU:CD	2:E:66:ARG:HE	2.14	0.51
2:B:316:ILE:HD12	2:B:341:MSE:HE3	1.92	0.51
2:C:265:ASP:O	2:C:266:SER:CB	2.58	0.51
2:E:321:ILE:HD11	2:E:332:TYR:CB	2.40	0.51
2:B:236:ALA:O	2:B:240:VAL:HG23	2.10	0.51
2:B:274:TYR:HE1	2:B:296:ARG:CZ	2.23	0.51
2:D:46:GLY:O	2:D:47:GLU:HB2	2.10	0.51
2:F:208:LEU:HB2	2:F:229:ALA:CB	2.40	0.51
2:F:39:LEU:HD23	3:F:425:HOH:O	2.10	0.51
2:F:160:ARG:CD	2:F:408:THR:HB	2.39	0.51
2:F:72:TYR:CD2	2:F:245:MSE:HG2	2.46	0.51
2:E:168:ILE:HA	2:E:172:GLN:HG3	1.92	0.51
2:E:209:ILE:HG22	2:E:210:ASP:HB2	1.93	0.51
2:E:254:VAL:HG11	2:E:307:VAL:HG21	1.92	0.51
2:E:349:ILE:HD12	2:E:357:ALA:O	2.11	0.51
1:L:3:DC:O2	2:F:109:ARG:N	2.40	0.51
2:F:266:SER:HA	2:F:318:THR:O	2.11	0.51
2:F:5:GLU:O	2:F:9:THR:HG22	2.10	0.51
2:D:140:HIS:O	2:D:141:ALA:HB2	2.10	0.51
2:D:207:LEU:HD23	2:D:264:LEU:HD13	1.92	0.51
2:E:30:ARG:O	2:E:32:GLN:N	2.44	0.51
2:F:326:LYS:O	2:F:330:VAL:HG23	2.11	0.51
2:F:294:LEU:CD1	2:F:334:GLU:HG3	2.41	0.51
2:D:226:GLU:OE2	2:D:249:LYS:HE3	2.10	0.51
2:F:14:LEU:O	2:F:38:ILE:HD11	2.11	0.51
2:A:175:LEU:H	2:A:341:MSE:CE	2.23	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:154:THR:HA	2:B:157:LEU:HG	1.91	0.51
2:B:137:THR:CG2	2:B:305:ARG:NH1	2.73	0.51
2:C:265:ASP:O	2:C:266:SER:HB2	2.09	0.51
1:L:4:DC:H5	2:F:110:TYR:HH	1.59	0.51
2:F:381:TRP:HB3	2:F:385:LYS:HE3	1.92	0.51
2:F:390:MSE:HE1	2:F:398:PHE:CB	2.34	0.51
2:C:170:ARG:HD3	2:C:259:ASP:OD2	2.10	0.51
2:C:260:VAL:CG1	2:C:261:ILE:N	2.73	0.51
2:E:92:ARG:O	2:E:95:ASP:HB2	2.11	0.51
2:A:405:MSE:O	2:A:406:THR:CG2	2.56	0.51
2:B:352:LYS:C	2:B:354:VAL:H	2.15	0.51
2:C:1:MSE:CG	2:C:2:ASN:N	2.74	0.51
2:E:30:ARG:O	2:E:31:LYS:C	2.50	0.51
2:E:326:LYS:O	2:E:329:GLU:HB2	2.10	0.51
2:E:382:ILE:O	2:E:386:ILE:CG2	2.59	0.51
2:A:369:GLU:HG2	2:A:370:LEU:HD12	1.94	0.50
2:D:73:LEU:HB2	2:D:238:ARG:NH2	2.26	0.50
2:D:248:GLU:O	2:D:249:LYS:C	2.49	0.50
2:E:136:LEU:CD1	2:F:221:ARG:NH2	2.67	0.50
2:D:264:LEU:HD12	2:D:265:ASP:N	2.25	0.50
2:F:293:ALA:O	2:F:295:HIS:N	2.45	0.50
2:A:172:GLN:HA	2:A:340:ASN:HD21	1.76	0.50
2:A:236:ALA:CA	2:A:239:HIS:HD2	2.21	0.50
2:A:390:MSE:CE	2:A:398:PHE:CB	2.90	0.50
2:B:402:LYS:HD3	2:B:405:MSE:CE	2.41	0.50
2:B:71:SER:OG	2:B:229:ALA:N	2.41	0.50
2:C:23:LEU:CG	2:C:41:GLN:HG3	2.41	0.50
2:E:382:ILE:O	2:E:386:ILE:HG23	2.12	0.50
2:E:130:LYS:HE2	2:F:11:VAL:HB	1.92	0.50
2:F:355:PHE:O	2:F:356:PRO:C	2.47	0.50
2:C:406:THR:OG1	2:C:411:ASP:N	2.45	0.50
2:C:415:MSE:CG	2:C:415:MSE:O	2.53	0.50
2:A:42:HIS:CE1	3:A:420:HOH:O	2.63	0.50
2:B:376:GLU:O	2:B:380:MSE:HG3	2.11	0.50
2:B:390:MSE:HE2	2:B:394:ASP:HB3	1.93	0.50
2:F:380:MSE:HG2	2:F:412:PHE:HZ	1.76	0.50
2:F:64:PHE:HA	2:F:79:ILE:O	2.11	0.50
2:D:132:LEU:HB3	2:D:251:LYS:HD3	1.93	0.50
2:F:356:PRO:HB2	2:F:396:MSE:HE2	1.93	0.50
2:F:68:ALA:C	2:F:70:SER:N	2.63	0.50
2:C:70:SER:O	2:C:71:SER:C	2.49	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:139:LEU:C	2:B:141:ALA:N	2.64	0.50
2:C:177:VAL:CG1	2:C:321:ILE:HD13	2.38	0.50
2:C:377:LEU:HD12	2:C:380:MSE:HE2	1.94	0.50
2:C:91:LEU:N	2:C:91:LEU:HD23	2.27	0.50
2:D:205:MSE:HE3	2:D:226:GLU:OE2	2.10	0.50
2:D:369:GLU:HA	2:D:377:LEU:CD1	2.41	0.50
2:D:65:LEU:HD11	2:D:97:ILE:HB	1.93	0.50
2:E:92:ARG:CZ	2:E:131:ILE:HD11	2.42	0.50
2:E:132:LEU:HD22	2:E:251:LYS:CD	2.32	0.50
2:F:141:ALA:HB3	2:F:370:LEU:HD13	1.93	0.50
2:A:50:PHE:HE1	2:A:100:LYS:HG2	1.74	0.50
2:C:137:THR:HG23	2:C:305:ARG:HB2	1.94	0.50
2:C:138:PRO:HD2	2:C:306:ASN:O	2.12	0.50
2:D:120:ASN:O	2:D:121:PHE:HB2	2.12	0.50
2:D:252:ARG:NH1	2:D:255:GLU:CD	2.65	0.50
2:E:103:PRO:HA	2:E:111:PHE:CD1	2.47	0.50
2:E:123:LYS:O	2:E:126:ASN:N	2.44	0.50
2:A:137:THR:HG22	2:A:305:ARG:HD3	1.93	0.49
2:B:268:THR:HG21	2:B:320:LEU:N	2.20	0.49
2:B:352:LYS:HB3	2:B:354:VAL:HG23	1.93	0.49
2:A:307:VAL:HB	2:A:311:GLY:O	2.11	0.49
2:E:152:GLY:N	2:E:407:LYS:CE	2.75	0.49
2:A:268:THR:O	2:A:272:ARG:HG2	2.12	0.49
2:B:227:VAL:O	2:B:227:VAL:HG12	2.13	0.49
2:D:123:LYS:O	2:D:125:GLU:N	2.46	0.49
2:D:169:GLY:O	2:D:172:GLN:HG2	2.13	0.49
2:D:260:VAL:CG1	2:D:261:ILE:N	2.75	0.49
2:D:399:LEU:O	2:D:403:LEU:HD12	2.11	0.49
2:E:91:LEU:HD13	2:E:97:ILE:HD11	1.93	0.49
2:F:144:ARG:HD3	2:F:146:ARG:HE	1.77	0.49
2:F:267:ILE:HG22	2:F:318:THR:O	2.13	0.49
2:A:403:LEU:C	2:A:405:MSE:H	2.16	0.49
2:C:139:LEU:HD13	2:C:367:LYS:HD2	1.93	0.49
2:C:275:ASN:ND2	2:C:289:VAL:HA	2.27	0.49
2:D:405:MSE:HE2	2:D:405:MSE:HA	1.95	0.49
2:E:343:LEU:CD1	2:E:358:ILE:HG23	2.43	0.49
2:F:141:ALA:HB1	2:F:370:LEU:HB3	1.88	0.49
2:F:399:LEU:HD22	2:F:403:LEU:HD11	1.95	0.49
2:B:52:ASP:HA	2:B:97:ILE:O	2.12	0.49
2:E:211:GLU:HG3	2:E:212:ARG:N	2.27	0.49
2:B:160:ARG:CZ	2:B:407:LYS:HA	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:348:LYS:HD2	2:D:392:GLU:OE1	2.12	0.49
2:E:409:ASN:C	2:E:411:ASP:H	2.16	0.49
2:F:182:ALA:HB1	2:F:345:LEU:HB3	1.94	0.49
2:A:44:LYS:O	2:A:45:SER:CB	2.60	0.49
2:B:268:THR:CG2	2:B:319:ALA:HA	2.43	0.49
2:C:250:ALA:O	2:C:254:VAL:HG23	2.13	0.49
2:C:254:VAL:HG21	2:C:313:LEU:HB2	1.94	0.49
2:C:378:GLN:O	2:C:382:ILE:HD12	2.13	0.49
2:E:49:ILE:CG2	2:E:101:ILE:CG1	2.91	0.49
2:E:66:ARG:HG2	2:E:66:ARG:NH1	2.28	0.49
2:A:198:ASN:HB3	2:A:199:HIS:CD2	2.48	0.49
2:A:228:VAL:HG12	2:A:242:VAL:CG1	2.43	0.49
2:B:382:ILE:O	2:B:386:ILE:HG22	2.12	0.49
2:C:158:THR:O	2:C:162:LEU:HB2	2.12	0.49
2:C:346:SER:HB3	2:C:349:ILE:HG13	1.95	0.49
2:E:207:LEU:HD13	2:E:246:VAL:HG21	1.93	0.49
2:E:338:THR:O	2:F:212:ARG:HD3	2.13	0.49
2:A:189:GLN:O	2:A:193:GLN:HG3	2.12	0.48
2:A:146:ARG:NH2	2:A:376:GLU:OE1	2.46	0.48
2:A:57:ILE:HG13	2:A:93:THR:HG22	1.94	0.48
2:A:86:ILE:HA	2:A:91:LEU:HD12	1.94	0.48
2:B:238:ARG:NH1	2:B:242:VAL:HG23	2.28	0.48
2:B:321:ILE:HD11	2:B:332:TYR:CB	2.43	0.48
2:C:55:LEU:HD12	2:C:64:PHE:O	2.13	0.48
2:C:71:SER:OG	2:C:229:ALA:N	2.39	0.48
2:E:355:PHE:CD2	3:E:424:HOH:O	2.55	0.48
2:F:207:LEU:HD11	2:F:242:VAL:HG12	1.89	0.48
2:A:252:ARG:HH11	2:A:255:GLU:CD	2.14	0.48
2:A:303:ALA:O	2:A:305:ARG:NE	2.39	0.48
2:A:341:MSE:C	2:A:341:MSE:CE	2.76	0.48
2:B:58:LEU:HD12	2:B:59:GLN:H	1.77	0.48
2:C:167:PRO:CD	2:C:365:THR:CG2	2.90	0.48
2:D:206:VAL:HG22	2:D:263:LEU:HB2	1.95	0.48
2:D:261:ILE:HG12	2:D:314:THR:CG2	2.39	0.48
2:E:290:ASP:OD1	2:E:290:ASP:C	2.52	0.48
2:A:321:ILE:HD11	2:A:332:TYR:CD2	2.47	0.48
2:B:173:ARG:HH22	2:C:214:GLU:CD	2.17	0.48
2:D:156:ASP:OD1	2:D:160:ARG:HG2	2.13	0.48
2:E:131:ILE:HG22	2:E:134:GLU:HG2	1.95	0.48
2:E:144:ARG:HH21	2:E:163:ASP:CG	2.16	0.48
2:F:1:MSE:HG3	2:F:2:ASN:H	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:74:ALA:HA	2:D:78:ASP:OD2	2.12	0.48
2:E:236:ALA:HB3	2:E:277:VAL:HG23	1.95	0.48
2:F:6:LEU:O	2:F:9:THR:CG2	2.61	0.48
2:A:275:ASN:ND2	2:A:289:VAL:HA	2.27	0.48
2:C:167:PRO:N	2:C:365:THR:HG21	2.29	0.48
2:F:264:LEU:HD23	2:F:317:ALA:CB	2.44	0.48
2:F:359:ASP:OD1	2:F:362:ARG:HB2	2.14	0.48
2:A:289:VAL:CG1	2:A:330:VAL:HG11	2.43	0.48
2:A:372:THR:HG21	2:A:380:MSE:HE2	1.96	0.48
2:A:41:GLN:C	2:A:43:ALA:N	2.67	0.48
2:C:120:ASN:HB3	2:C:256:HIS:CD2	2.48	0.48
2:D:184:LYS:HG3	2:D:318:THR:HG21	1.95	0.48
2:D:390:MSE:HE1	2:D:398:PHE:CD2	2.49	0.48
2:E:356:PRO:CB	2:E:396:MSE:CE	2.82	0.48
2:D:147:MSE:CE	2:D:191:ILE:HG23	2.41	0.48
2:D:57:ILE:H	2:D:93:THR:HB	1.78	0.48
2:E:252:ARG:NH1	2:E:252:ARG:N	2.62	0.48
2:E:411:ASP:CG	2:E:412:PHE:N	2.67	0.48
2:F:46:GLY:O	2:F:47:GLU:HB2	2.13	0.48
2:A:245:MSE:HE3	2:A:245:MSE:CA	2.40	0.48
2:A:39:LEU:O	2:A:49:ILE:HD11	2.14	0.48
2:D:206:VAL:HB	2:D:227:VAL:HG22	1.96	0.48
2:F:138:PRO:O	2:F:140:HIS:N	2.47	0.48
2:A:91:LEU:HD22	2:A:97:ILE:HD11	1.94	0.48
2:B:144:ARG:HH21	2:B:163:ASP:CG	2.18	0.48
2:B:234:GLU:CD	2:B:238:ARG:HG2	2.33	0.48
2:C:187:LEU:HD12	2:C:187:LEU:O	2.14	0.48
2:E:1:MSE:CG	2:E:2:ASN:H	2.26	0.48
1:K:3:DC:H4'	1:K:4:DC:O5'	2.13	0.48
2:A:170:ARG:NH1	2:A:202:CYS:SG	2.87	0.47
2:B:272:ARG:HE	2:B:327:MSE:SE	2.47	0.47
2:C:355:PHE:CB	2:C:356:PRO:CD	2.92	0.47
2:D:271:ALA:HB3	2:D:331:ILE:HD13	1.96	0.47
2:E:137:THR:CG2	2:E:305:ARG:CD	2.90	0.47
2:A:178:ALA:HB2	2:A:345:LEU:HD12	1.96	0.47
2:C:207:LEU:HD11	2:C:242:VAL:HG12	1.96	0.47
2:E:123:LYS:O	2:E:125:GLU:N	2.47	0.47
2:E:245:MSE:HE2	2:E:245:MSE:HA	1.96	0.47
2:E:393:ILE:HG12	2:E:393:ILE:H	1.37	0.47
2:F:257:LYS:HD3	2:F:309:GLU:O	2.14	0.47
2:F:254:VAL:O	2:F:257:LYS:N	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:146:ARG:NH2	2:C:376:GLU:OE1	2.42	0.47
2:D:131:ILE:HG22	2:D:133:PHE:N	2.18	0.47
2:D:131:ILE:HG22	2:D:132:LEU:N	2.28	0.47
2:E:366:ARG:CG	2:E:366:ARG:NH1	2.74	0.47
2:F:2:ASN:HD22	2:F:50:PHE:HB2	1.79	0.47
1:L:4:DC:H42	2:F:66:ARG:HH12	1.62	0.47
2:A:137:THR:HG21	2:A:305:ARG:NH1	2.29	0.47
2:A:144:ARG:NH1	2:A:163:ASP:OD1	2.47	0.47
2:A:266:SER:OG	2:A:269:ARG:CB	2.63	0.47
2:A:296:ARG:HB2	2:A:297:PRO:CD	2.44	0.47
2:B:356:PRO:C	2:B:358:ILE:H	2.17	0.47
2:B:70:SER:HB3	2:B:73:LEU:HB3	1.95	0.47
2:E:144:ARG:NH2	2:E:163:ASP:CG	2.67	0.47
2:A:173:ARG:NH2	2:B:212:ARG:HB3	2.30	0.47
2:A:175:LEU:N	2:A:341:MSE:CE	2.78	0.47
2:C:406:THR:OG1	2:C:407:LYS:N	2.47	0.47
2:D:144:ARG:NH1	2:D:376:GLU:OE2	2.48	0.47
2:D:141:ALA:HB1	2:D:371:LEU:HG	1.95	0.47
2:D:23:LEU:HD21	2:D:41:GLN:CG	2.44	0.47
2:E:175:LEU:H	2:E:341:MSE:CE	2.28	0.47
2:E:49:ILE:HG22	2:E:101:ILE:HG12	1.96	0.47
2:A:49:ILE:HG22	2:A:101:ILE:O	2.15	0.47
2:A:145:LEU:HD21	2:A:170:ARG:CG	2.44	0.47
2:C:30:ARG:O	2:C:31:LYS:C	2.52	0.47
2:E:131:ILE:HG23	2:E:133:PHE:CD2	2.49	0.47
2:C:137:THR:HG22	2:D:214:GLU:CB	2.44	0.47
2:C:228:VAL:HG12	2:C:242:VAL:HG13	1.94	0.47
2:C:177:VAL:HG11	2:C:321:ILE:CD1	2.36	0.47
2:D:293:ALA:O	2:D:295:HIS:N	2.47	0.47
2:D:294:LEU:HD13	2:D:334:GLU:HG3	1.95	0.47
2:D:66:ARG:HG2	2:D:66:ARG:NH1	2.27	0.47
2:E:157:LEU:HD13	2:E:400:ILE:HG23	1.97	0.47
2:E:294:LEU:C	2:E:297:PRO:HD2	2.35	0.47
2:D:60:ASP:CB	2:D:62:PHE:HE2	2.27	0.47
2:D:134:GLU:OE2	2:E:29:MSE:O	2.32	0.47
1:K:4:DC:N4	2:E:78:ASP:OD2	2.48	0.47
2:B:173:ARG:CD	2:B:304:ALA:HB3	2.43	0.47
2:C:140:HIS:HA	2:C:306:ASN:HD22	1.79	0.47
2:C:377:LEU:HD12	2:C:380:MSE:CE	2.45	0.47
2:D:372:THR:HG22	2:D:376:GLU:CD	2.34	0.47
2:E:169:GLY:O	2:E:171:GLY:N	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:205:MSE:O	2:E:262:ILE:HA	2.15	0.47
2:E:390:MSE:HE2	2:E:395:ALA:N	2.30	0.47
2:A:284:VAL:HG12	2:A:284:VAL:O	2.15	0.47
2:B:54:VAL:HG21	2:B:249:LYS:HD2	1.97	0.47
2:B:387:ILE:HG22	2:B:387:ILE:O	2.13	0.47
2:C:264:LEU:HD22	2:C:300:PHE:CE2	2.50	0.47
2:D:267:ILE:HG23	2:D:268:THR:N	2.30	0.47
2:E:23:LEU:CD2	2:E:41:GLN:HG3	2.33	0.47
2:B:102:ARG:HB3	2:B:114:LEU:CD1	2.45	0.47
2:B:140:HIS:CB	2:B:306:ASN:HB3	2.44	0.47
2:B:402:LYS:HD3	2:B:405:MSE:HE2	1.97	0.47
2:C:296:ARG:O	2:C:299:ARG:HB2	2.15	0.47
2:C:56:GLU:CG	2:C:245:MSE:HE1	2.45	0.47
2:D:169:GLY:H	2:D:172:GLN:HG3	1.74	0.47
2:E:416:MSE:O	2:E:417:LYS:CB	2.55	0.47
2:A:105:LYS:HG3	2:A:108:GLU:OE1	2.16	0.46
2:A:228:VAL:CG1	2:A:242:VAL:HG13	2.45	0.46
2:B:250:ALA:HB1	2:B:313:LEU:CD1	2.45	0.46
2:C:1:MSE:HG3	2:C:2:ASN:H	1.79	0.46
2:C:4:THR:O	2:C:7:LYS:HG3	2.15	0.46
2:E:409:ASN:O	2:E:411:ASP:N	2.49	0.46
2:F:356:PRO:C	2:F:358:ILE:N	2.69	0.46
2:B:247:ILE:O	2:B:251:LYS:HG3	2.15	0.46
2:B:270:LEU:O	2:B:273:ALA:HB3	2.15	0.46
2:C:206:VAL:HB	2:C:227:VAL:HG22	1.98	0.46
2:D:131:ILE:HA	2:D:255:GLU:OE2	2.15	0.46
2:D:264:LEU:HD12	2:D:264:LEU:C	2.35	0.46
2:F:191:ILE:O	2:F:195:ILE:CG1	2.62	0.46
2:A:144:ARG:HH11	2:A:146:ARG:HG3	1.81	0.46
2:A:205:MSE:HE2	2:A:246:VAL:HG13	1.97	0.46
2:A:175:LEU:HD13	2:A:301:PHE:CZ	2.48	0.46
2:A:139:LEU:HA	2:B:214:GLU:HB2	1.97	0.46
2:B:299:ARG:O	2:B:300:PHE:C	2.54	0.46
2:C:159:ALA:O	2:C:163:ASP:HB2	2.15	0.46
2:C:175:LEU:H	2:C:341:MSE:CE	2.28	0.46
2:C:266:SER:OG	2:C:269:ARG:HG2	2.16	0.46
2:C:387:ILE:CG2	2:C:395:ALA:HB1	2.45	0.46
2:A:160:ARG:HD3	2:A:403:LEU:HD22	1.97	0.46
2:A:184:LYS:HD2	2:A:318:THR:HG21	1.97	0.46
2:A:411:ASP:O	2:A:415:MSE:CG	2.64	0.46
2:E:347:ARG:O	2:E:351:GLU:HG2	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:88:ARG:O	2:E:88:ARG:HG3	2.15	0.46
2:A:264:LEU:HB3	2:A:317:ALA:CB	2.45	0.46
2:C:349:ILE:HG22	2:C:354:VAL:HB	1.97	0.46
2:D:205:MSE:HE3	2:D:226:GLU:CD	2.35	0.46
2:E:267:ILE:HG22	2:E:318:THR:O	2.15	0.46
2:E:66:ARG:NH1	2:E:74:ALA:HA	2.30	0.46
2:F:105:LYS:O	2:F:106:GLU:C	2.54	0.46
2:A:173:ARG:HH11	2:A:173:ARG:HB2	1.79	0.46
2:E:162:LEU:CD1	2:E:187:LEU:HD11	2.46	0.46
2:E:294:LEU:HA	2:E:297:PRO:HG2	1.96	0.46
2:F:264:LEU:HB3	2:F:317:ALA:CB	2.45	0.46
2:F:379:LYS:HB3	2:F:412:PHE:CD1	2.51	0.46
2:A:100:LYS:O	2:A:114:LEU:N	2.42	0.46
2:A:24:GLU:O	2:A:26:LEU:CD2	2.55	0.46
2:D:308:GLU:CD	2:E:221:ARG:HH22	2.19	0.46
2:E:136:LEU:N	2:E:136:LEU:HD23	2.30	0.46
2:F:7:LYS:HA	2:F:35:ILE:HD11	1.98	0.46
1:K:3:DC:O2	2:E:109:ARG:HB2	2.15	0.46
2:B:134:GLU:OE1	2:C:31:LYS:N	2.41	0.46
2:E:6:LEU:HD23	2:E:6:LEU:HA	1.80	0.46
2:A:172:GLN:OE1	2:A:340:ASN:ND2	2.49	0.46
2:D:161:VAL:HG21	2:D:396:MSE:CE	2.28	0.46
2:D:341:MSE:HE3	2:D:343:LEU:N	2.31	0.46
2:E:139:LEU:O	2:E:140:HIS:CB	2.63	0.46
2:F:184:LYS:NZ	2:F:265:ASP:OD2	2.49	0.46
2:F:347:ARG:O	2:F:351:GLU:HG2	2.16	0.46
2:B:356:PRO:HB2	2:B:396:MSE:CE	2.44	0.46
2:C:189:GLN:O	2:C:193:GLN:HG3	2.16	0.46
2:C:60:ASP:HB3	2:C:62:PHE:CE2	2.51	0.46
2:D:245:MSE:HA	2:D:245:MSE:HE3	1.97	0.46
2:D:140:HIS:HA	2:D:306:ASN:CB	2.45	0.46
2:B:135:ASN:HB3	2:B:307:VAL:HG13	1.98	0.45
2:C:261:ILE:HG12	2:C:314:THR:HG23	1.97	0.45
2:E:173:ARG:HH22	2:F:214:GLU:CD	2.18	0.45
2:F:159:ALA:O	2:F:163:ASP:HB2	2.15	0.45
2:F:207:LEU:HD12	2:F:228:VAL:O	2.16	0.45
2:F:210:ASP:OD1	2:F:232:PHE:HA	2.16	0.45
2:A:141:ALA:O	2:A:370:LEU:C	2.55	0.45
2:B:168:ILE:HD11	2:B:341:MSE:HE2	1.97	0.45
2:B:308:GLU:HB3	2:B:309:GLU:OE2	2.16	0.45
2:B:71:SER:OG	2:B:228:VAL:HA	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:160:ARG:CD	2:D:408:THR:CG2	2.82	0.45
2:D:66:ARG:CG	2:D:66:ARG:HH11	2.26	0.45
2:F:135:ASN:CB	2:F:307:VAL:HG22	2.37	0.45
2:F:390:MSE:HE1	2:F:398:PHE:CD2	2.49	0.45
2:C:390:MSE:HB3	2:C:394:ASP:HB3	1.99	0.45
2:D:160:ARG:CD	2:D:408:THR:HG23	2.45	0.45
2:F:207:LEU:HD11	2:F:242:VAL:HG13	1.94	0.45
2:F:355:PHE:HB2	2:F:356:PRO:HD2	1.92	0.45
2:A:195:ILE:HG21	2:A:204:LEU:HD13	1.98	0.45
2:B:346:SER:HB3	2:B:349:ILE:HD12	1.98	0.45
2:C:186:MSE:O	2:C:187:LEU:C	2.54	0.45
2:C:356:PRO:O	2:C:357:ALA:C	2.53	0.45
2:D:272:ARG:HH11	2:D:272:ARG:HB3	1.81	0.45
2:B:409:ASN:C	2:B:411:ASP:H	2.20	0.45
2:B:65:LEU:HB2	2:B:79:ILE:HB	1.97	0.45
2:C:114:LEU:HD21	2:C:115:LYS:NZ	2.30	0.45
2:D:304:ALA:O	2:D:305:ARG:HB3	2.16	0.45
2:E:252:ARG:HA	2:E:252:ARG:HH11	1.81	0.45
2:D:381:TRP:CE3	2:E:353:ARG:HD3	2.52	0.45
2:A:141:ALA:O	2:A:370:LEU:O	2.35	0.45
2:D:123:LYS:HB2	2:D:126:ASN:CG	2.37	0.45
2:E:161:VAL:HG21	2:E:396:MSE:HE1	1.99	0.45
2:E:295:HIS:CD2	2:F:233:ASP:O	2.70	0.45
2:E:390:MSE:HE2	2:E:395:ALA:HA	1.98	0.45
2:E:95:ASP:OD1	2:E:120:ASN:ND2	2.38	0.45
2:F:158:THR:HA	2:F:356:PRO:HG2	1.98	0.45
2:F:57:ILE:HB	2:F:93:THR:HG22	1.97	0.45
2:A:178:ALA:HA	2:A:179:PRO:HD3	1.74	0.45
2:A:304:ALA:O	2:A:305:ARG:HB3	2.16	0.45
2:B:173:ARG:CG	2:B:304:ALA:HB3	2.47	0.45
2:C:231:THR:C	2:C:233:ASP:N	2.69	0.45
2:C:277:VAL:O	2:C:279:PRO:HD3	2.17	0.45
2:C:347:ARG:O	2:C:348:LYS:C	2.54	0.45
2:E:6:LEU:O	2:E:9:THR:HG23	2.15	0.45
2:F:32:GLN:HB3	2:F:76:PRO:HD2	1.98	0.45
2:A:116:VAL:HG12	2:A:124:PRO:HG3	1.98	0.45
2:A:266:SER:HB2	2:A:320:LEU:HG	1.98	0.45
2:A:385:LYS:HE2	2:B:353:ARG:NH1	2.22	0.45
2:C:289:VAL:HG11	2:C:330:VAL:CG1	2.30	0.45
2:C:349:ILE:HA	2:C:393:ILE:HD13	1.98	0.45
2:C:379:LYS:HD3	2:C:412:PHE:CD1	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:144:ARG:CG	2:D:145:LEU:N	2.79	0.45
2:E:26:LEU:HD22	2:E:29:MSE:SE	2.67	0.45
2:F:247:ILE:HB	2:F:300:PHE:CE1	2.52	0.45
2:B:274:TYR:HE1	2:B:296:ARG:NH2	2.15	0.45
2:D:49:ILE:HG22	2:D:101:ILE:CD1	2.44	0.45
2:D:238:ARG:NH1	2:D:242:VAL:HG22	2.32	0.45
2:D:267:ILE:HG22	2:D:318:THR:O	2.17	0.45
2:E:73:LEU:O	2:E:74:ALA:C	2.54	0.45
2:F:46:GLY:C	2:F:48:ASP:H	2.20	0.45
2:A:388:HIS:HB3	2:A:389:PRO:HD3	1.99	0.45
2:C:131:ILE:O	2:C:132:LEU:C	2.55	0.45
2:D:219:MSE:HB2	2:D:219:MSE:HE2	1.91	0.45
2:D:254:VAL:C	2:D:256:HIS:H	2.20	0.45
2:F:208:LEU:HB2	2:F:229:ALA:HB2	1.98	0.45
2:D:52:ASP:HA	2:D:97:ILE:O	2.18	0.44
2:E:211:GLU:HG2	2:E:215:GLU:HB3	1.99	0.44
2:E:252:ARG:NH1	2:E:255:GLU:CD	2.70	0.44
2:C:133:PHE:HB2	3:D:422:HOH:O	2.16	0.44
2:C:137:THR:O	2:C:137:THR:HG22	2.17	0.44
2:D:104:PRO:HB3	2:D:108:GLU:HB2	1.98	0.44
2:D:29:MSE:HG3	2:D:34:ILE:HG12	1.99	0.44
2:F:156:ASP:OD1	2:F:159:ALA:HB3	2.16	0.44
2:F:331:ILE:O	2:F:332:TYR:C	2.53	0.44
2:B:173:ARG:HG3	2:B:304:ALA:HB3	2.00	0.44
2:B:294:LEU:HD11	2:B:334:GLU:HG3	1.99	0.44
2:B:399:LEU:HD13	2:B:403:LEU:CD1	2.47	0.44
2:E:252:ARG:O	2:E:255:GLU:HB2	2.18	0.44
2:F:71:SER:HB3	2:F:228:VAL:HG13	1.99	0.44
2:F:369:GLU:OE2	2:F:370:LEU:HG	2.17	0.44
2:B:130:LYS:HZ3	2:C:12:SER:H	1.66	0.44
2:C:231:THR:O	2:C:233:ASP:N	2.50	0.44
2:E:9:THR:HA	2:E:10:PRO:HD3	1.86	0.44
2:E:56:GLU:HB3	2:E:66:ARG:HE	1.82	0.44
2:F:79:ILE:HD13	2:F:101:ILE:HG21	1.99	0.44
2:F:402:LYS:HZ2	2:F:415:MSE:HE1	1.78	0.44
2:A:140:HIS:HA	2:A:306:ASN:CB	2.48	0.44
2:A:304:ALA:HB2	2:A:315:ILE:HG13	2.00	0.44
2:A:39:LEU:CD1	2:A:111:PHE:CZ	3.01	0.44
2:A:4:THR:HA	2:A:7:LYS:HG3	1.99	0.44
2:C:117:ASN:O	2:C:124:PRO:CG	2.65	0.44
2:F:416:MSE:O	2:F:417:LYS:HB2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:49:ILE:CG2	2:A:101:ILE:O	2.65	0.44
2:C:385:LYS:NZ	2:D:353:ARG:NH2	2.65	0.44
2:D:49:ILE:HG22	2:D:101:ILE:CG1	2.48	0.44
2:D:178:ALA:HA	2:D:179:PRO:HD3	1.71	0.44
2:D:26:LEU:O	2:D:29:MSE:HG2	2.17	0.44
2:D:383:LEU:O	2:D:386:ILE:HG23	2.18	0.44
2:F:73:LEU:O	2:F:74:ALA:C	2.51	0.44
2:D:99:GLY:HA3	2:D:115:LYS:O	2.18	0.44
2:D:209:ILE:HD13	2:D:209:ILE:HA	1.70	0.44
2:E:252:ARG:CA	2:E:252:ARG:HH11	2.31	0.44
2:E:359:ASP:OD1	2:E:362:ARG:HB2	2.16	0.44
2:F:254:VAL:C	2:F:256:HIS:N	2.71	0.44
2:F:184:LYS:HZ3	2:F:265:ASP:CG	2.21	0.44
2:A:26:LEU:O	2:A:27:ALA:C	2.56	0.44
2:C:385:LYS:HE3	2:C:385:LYS:HB2	1.68	0.44
2:E:207:LEU:HD21	2:E:243:ALA:HA	2.00	0.44
2:B:122:ASP:OD1	2:B:123:LYS:N	2.47	0.44
2:B:268:THR:HG21	3:B:420:HOH:O	2.17	0.44
2:C:228:VAL:HG12	2:C:242:VAL:CG1	2.48	0.44
2:E:175:LEU:N	2:E:341:MSE:CE	2.81	0.44
2:F:268:THR:O	2:F:272:ARG:HG2	2.18	0.44
1:J:3:DC:O2	2:D:109:ARG:N	2.49	0.44
2:A:247:ILE:O	2:A:251:LYS:HG3	2.18	0.43
2:A:294:LEU:HD21	2:A:331:ILE:HG12	1.99	0.43
2:B:306:ASN:OD1	2:B:306:ASN:C	2.56	0.43
2:A:1:MSE:CG	2:A:2:ASN:N	2.77	0.43
2:A:205:MSE:CE	2:A:249:LYS:HD3	2.48	0.43
2:B:143:SER:O	2:B:143:SER:OG	2.36	0.43
2:B:259:ASP:OD1	2:B:311:GLY:HA2	2.17	0.43
2:B:57:ILE:HG13	2:B:93:THR:HG22	2.00	0.43
2:C:175:LEU:N	2:C:341:MSE:CE	2.81	0.43
2:C:47:GLU:O	2:C:48:ASP:CB	2.64	0.43
2:C:81:VAL:HG12	2:C:86:ILE:HG13	1.99	0.43
2:E:268:THR:HG21	2:E:320:LEU:N	2.31	0.43
2:F:335:PHE:O	2:F:336:LYS:C	2.55	0.43
2:F:356:PRO:O	2:F:358:ILE:N	2.52	0.43
2:A:169:GLY:O	2:A:172:GLN:HG2	2.18	0.43
2:A:206:VAL:HG21	2:A:223:VAL:HG11	1.99	0.43
2:A:252:ARG:O	2:A:255:GLU:HB2	2.18	0.43
2:A:271:ALA:CB	2:A:331:ILE:HD13	2.45	0.43
2:D:147:MSE:HE1	2:D:191:ILE:CG2	2.41	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:49:ILE:O	2:A:100:LYS:HA	2.18	0.43
2:A:252:ARG:HA	2:A:252:ARG:HD3	1.70	0.43
2:A:137:THR:CG2	2:A:305:ARG:HD3	2.48	0.43
2:D:83:PRO:O	2:D:87:ARG:HG3	2.18	0.43
2:E:330:VAL:O	2:E:330:VAL:CG1	2.66	0.43
2:F:123:LYS:HB2	2:F:126:ASN:HB2	1.99	0.43
2:F:141:ALA:CB	2:F:370:LEU:HD13	2.49	0.43
2:F:388:HIS:HB3	2:F:389:PRO:HD3	2.00	0.43
1:H:4:DC:H5	2:C:110:TYR:CZ	2.35	0.43
2:A:205:MSE:HE3	2:A:249:LYS:HD3	2.00	0.43
2:B:272:ARG:NH1	2:B:272:ARG:CG	2.49	0.43
2:B:399:LEU:HD13	2:B:403:LEU:HD11	1.99	0.43
2:C:141:ALA:HB1	2:C:370:LEU:CA	2.49	0.43
2:E:355:PHE:HA	3:E:424:HOH:O	2.17	0.43
2:E:361:ASN:ND2	2:E:388:HIS:O	2.51	0.43
1:L:4:DC:H5	2:F:110:TYR:OH	2.00	0.43
2:C:294:LEU:C	2:C:297:PRO:HD2	2.39	0.43
2:F:272:ARG:NH1	2:F:272:ARG:CG	2.77	0.43
2:A:374:GLN:HA	2:A:377:LEU:HD12	2.00	0.43
2:A:6:LEU:HA	2:A:6:LEU:HD23	1.90	0.43
2:B:228:VAL:HG11	2:B:242:VAL:HG13	1.94	0.43
2:B:273:ALA:O	2:B:277:VAL:HG23	2.17	0.43
2:D:355:PHE:C	2:D:357:ALA:N	2.71	0.43
2:D:387:ILE:O	2:D:387:ILE:HG22	2.18	0.43
2:E:278:VAL:O	2:E:279:PRO:C	2.57	0.43
2:F:234:GLU:HB3	2:F:238:ARG:HG2	2.01	0.43
2:A:161:VAL:O	2:A:161:VAL:HG12	2.18	0.43
2:B:356:PRO:O	2:B:396:MSE:HE2	2.18	0.43
2:C:95:ASP:OD1	2:C:120:ASN:ND2	2.49	0.43
2:D:173:ARG:CD	2:D:301:PHE:O	2.67	0.43
2:E:169:GLY:H	2:E:172:GLN:HG3	1.75	0.43
2:B:139:LEU:O	2:B:140:HIS:C	2.57	0.43
2:B:383:LEU:O	2:B:386:ILE:HG23	2.18	0.43
2:C:56:GLU:HG3	2:C:245:MSE:HE1	2.01	0.43
2:D:379:LYS:HG3	2:D:412:PHE:CG	2.54	0.43
2:A:53:GLY:HA3	2:A:65:LEU:HB3	2.01	0.43
2:B:139:LEU:C	2:B:141:ALA:H	2.22	0.43
2:C:139:LEU:HD22	2:C:367:LYS:HG3	2.00	0.43
2:C:356:PRO:HD2	2:C:400:ILE:CD1	2.37	0.43
1:J:4:DC:H5	2:D:110:TYR:HH	1.60	0.43
2:C:333:GLU:OE1	2:D:325:SER:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:405:MSE:O	2:D:406:THR:CG2	2.59	0.43
2:E:132:LEU:HA	2:E:135:ASN:HD21	1.78	0.43
2:E:272:ARG:HH11	2:E:272:ARG:CG	1.97	0.43
2:F:144:ARG:HB2	2:F:371:LEU:HB3	2.00	0.43
2:A:26:LEU:HD12	2:A:34:ILE:HG23	2.01	0.42
2:B:166:SER:HA	2:B:365:THR:HG22	2.00	0.42
2:C:252:ARG:HD3	2:C:252:ARG:HA	1.65	0.42
2:D:381:TRP:CD2	2:E:353:ARG:HD3	2.54	0.42
2:F:161:VAL:HG12	2:F:358:ILE:HD12	2.00	0.42
2:B:407:LYS:HG3	2:B:408:THR:HG23	2.01	0.42
2:C:211:GLU:HG3	2:C:212:ARG:N	2.34	0.42
2:C:120:ASN:HB2	2:C:256:HIS:NE2	2.34	0.42
2:C:338:THR:O	2:D:212:ARG:CD	2.67	0.42
2:E:355:PHE:CG	3:E:424:HOH:O	2.72	0.42
2:F:144:ARG:NH2	2:F:163:ASP:O	2.51	0.42
2:F:205:MSE:HE2	2:F:246:VAL:HG13	2.01	0.42
2:A:372:THR:HG23	2:A:376:GLU:CG	2.49	0.42
2:E:23:LEU:HD23	2:E:23:LEU:HA	1.87	0.42
2:A:256:HIS:O	2:A:257:LYS:HB2	2.18	0.42
2:A:272:ARG:NH1	2:A:272:ARG:CG	2.53	0.42
2:A:28:ARG:HA	2:A:28:ARG:HD3	1.62	0.42
2:A:321:ILE:O	2:A:322:ASP:HB2	2.18	0.42
2:D:226:GLU:OE2	2:D:249:LYS:CE	2.67	0.42
2:D:2:ASN:OD1	2:D:2:ASN:C	2.57	0.42
2:E:186:MSE:HE2	2:E:355:PHE:HD2	1.80	0.42
2:F:247:ILE:HG23	2:F:248:GLU:N	2.34	0.42
2:A:264:LEU:HB3	2:A:317:ALA:HB2	2.02	0.42
2:A:341:MSE:HE2	2:A:341:MSE:HB3	1.86	0.42
2:B:137:THR:HG22	2:B:305:ARG:HD3	2.01	0.42
2:C:5:GLU:O	2:C:9:THR:HG22	2.20	0.42
2:D:21:MSE:HE2	2:D:41:GLN:HB3	2.00	0.42
2:E:102:ARG:HD3	2:E:114:LEU:HD13	2.02	0.42
2:E:131:ILE:HG21	2:E:131:ILE:HD13	1.76	0.42
2:E:20:ASN:C	2:E:22:GLY:H	2.21	0.42
2:E:70:SER:O	2:E:71:SER:HB2	2.20	0.42
2:F:383:LEU:O	2:F:383:LEU:HD23	2.19	0.42
2:A:228:VAL:CG1	2:A:242:VAL:CG1	2.97	0.42
2:A:207:LEU:HD13	2:A:246:VAL:HG21	2.02	0.42
2:A:2:ASN:OD1	2:A:4:THR:HG23	2.20	0.42
1:G:4:DC:O2	2:A:66:ARG:NH2	2.52	0.42
2:B:117:ASN:O	2:B:124:PRO:HD3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:176:ILE:HG21	2:D:176:ILE:HD13	1.77	0.42
2:F:393:ILE:O	2:F:394:ASP:C	2.58	0.42
2:A:21:MSE:HE2	2:A:41:GLN:HB3	2.01	0.42
2:B:252:ARG:HA	2:B:252:ARG:HD3	1.65	0.42
2:B:264:LEU:O	2:B:317:ALA:HA	2.20	0.42
2:B:184:LYS:HE2	2:B:320:LEU:HD21	2.00	0.42
2:B:70:SER:O	2:B:71:SER:C	2.58	0.42
2:E:388:HIS:HB3	2:E:389:PRO:HD3	2.02	0.42
2:E:54:VAL:O	2:E:65:LEU:HA	2.20	0.42
2:A:268:THR:HA	2:A:331:ILE:HG21	2.01	0.42
2:B:188:LEU:HD23	2:B:188:LEU:HA	1.90	0.42
2:D:138:PRO:HD3	2:D:308:GLU:HB2	2.02	0.42
2:D:254:VAL:C	2:D:256:HIS:N	2.73	0.42
2:E:4:THR:CB	2:E:52:ASP:OD1	2.68	0.42
1:L:4:DC:C5	2:F:110:TYR:OH	2.70	0.42
2:A:278:VAL:HA	2:A:279:PRO:HD3	1.84	0.42
2:A:41:GLN:O	2:A:43:ALA:N	2.52	0.42
2:B:369:GLU:HA	2:B:377:LEU:HD13	2.02	0.42
2:E:186:MSE:HE2	2:E:355:PHE:CE2	2.54	0.42
2:E:33:ASP:OD1	2:E:76:PRO:HG2	2.20	0.42
2:E:344:HIS:O	2:E:358:ILE:HA	2.20	0.42
2:E:58:LEU:HD12	2:E:59:GLN:N	2.32	0.42
2:A:85:GLN:NE2	2:A:113:LEU:O	2.38	0.42
2:A:211:GLU:HG3	2:A:212:ARG:N	2.35	0.42
2:A:140:HIS:CA	2:A:306:ASN:CB	2.96	0.42
2:B:139:LEU:HD21	2:B:367:LYS:HG3	2.02	0.42
2:C:356:PRO:C	2:C:358:ILE:N	2.73	0.42
2:D:212:ARG:HB3	2:D:214:GLU:OE2	2.20	0.42
2:E:296:ARG:HA	2:E:299:ARG:HB2	2.02	0.42
2:E:390:MSE:CE	2:E:395:ALA:HA	2.50	0.42
2:A:50:PHE:CD1	2:A:100:LYS:HG2	2.54	0.41
2:A:266:SER:OG	2:A:269:ARG:N	2.40	0.41
2:A:40:LYS:HE3	2:A:40:LYS:HB3	1.70	0.41
2:C:113:LEU:HD21	2:C:116:VAL:CG2	2.49	0.41
2:C:230:SER:HG	2:C:239:HIS:HD1	1.66	0.41
2:C:379:LYS:HZ1	2:C:412:PHE:HB2	1.79	0.41
2:D:137:THR:CG2	2:D:305:ARG:NH1	2.83	0.41
2:D:247:ILE:HA	2:D:247:ILE:HD12	1.89	0.41
2:F:141:ALA:CB	2:F:370:LEU:HB3	2.50	0.41
2:F:248:GLU:O	2:F:249:LYS:C	2.57	0.41
2:F:270:LEU:CD1	2:F:274:TYR:CE2	3.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:169:GLY:O	2:A:171:GLY:N	2.53	0.41
2:A:359:ASP:OD2	2:A:362:ARG:HD2	2.19	0.41
2:A:83:PRO:O	2:A:87:ARG:HG3	2.20	0.41
2:B:179:PRO:HA	2:B:321:ILE:O	2.20	0.41
2:C:24:GLU:O	2:C:25:ASN:C	2.58	0.41
2:C:303:ALA:O	2:C:304:ALA:C	2.58	0.41
2:E:210:ASP:HB2	2:E:269:ARG:HB3	2.01	0.41
2:E:294:LEU:O	2:E:297:PRO:HD2	2.20	0.41
2:E:29:MSE:HG3	2:E:34:ILE:HG13	2.02	0.41
2:E:71:SER:HA	2:E:228:VAL:HG13	2.02	0.41
2:F:30:ARG:O	2:F:31:LYS:C	2.59	0.41
2:A:62:PHE:HE1	2:A:64:PHE:CE2	2.35	0.41
2:C:209:ILE:HD13	2:C:209:ILE:HA	1.64	0.41
2:D:139:LEU:O	2:D:140:HIS:C	2.58	0.41
2:D:154:THR:O	2:D:157:LEU:CB	2.59	0.41
2:D:42:HIS:CG	2:D:42:HIS:O	2.72	0.41
2:E:264:LEU:HD22	2:E:300:PHE:CE2	2.56	0.41
2:E:137:THR:CG2	2:E:305:ARG:NH1	2.81	0.41
2:F:122:ASP:OD1	2:F:123:LYS:N	2.48	0.41
2:F:293:ALA:C	2:F:295:HIS:N	2.74	0.41
2:F:403:LEU:C	2:F:405:MSE:N	2.74	0.41
2:A:261:ILE:HA	2:A:314:THR:O	2.20	0.41
2:A:349:ILE:HG23	2:A:354:VAL:HB	2.02	0.41
2:A:57:ILE:CG1	2:A:93:THR:HG22	2.51	0.41
2:B:247:ILE:HA	2:B:247:ILE:HD12	1.86	0.41
2:C:199:HIS:HB3	2:C:202:CYS:SG	2.60	0.41
2:C:294:LEU:HA	2:C:297:PRO:HG2	2.01	0.41
2:D:252:ARG:HD3	2:D:252:ARG:HA	1.82	0.41
1:K:4:DC:H5	2:E:110:TYR:CZ	2.38	0.41
2:E:131:ILE:CG2	2:E:133:PHE:HD2	2.33	0.41
2:A:142:ASN:OD1	2:A:306:ASN:ND2	2.54	0.41
2:A:247:ILE:HD11	2:A:303:ALA:CB	2.51	0.41
2:A:73:LEU:O	2:A:74:ALA:C	2.57	0.41
2:B:296:ARG:O	2:B:297:PRO:C	2.57	0.41
2:B:138:PRO:HD2	2:B:306:ASN:O	2.20	0.41
2:D:396:MSE:HE3	2:D:400:ILE:HD11	2.01	0.41
2:F:169:GLY:O	2:F:172:GLN:CG	2.68	0.41
2:A:32:GLN:O	2:A:33:ASP:C	2.58	0.41
2:B:199:HIS:N	2:B:200:PRO:HD3	2.35	0.41
2:B:217:THR:O	2:B:218:GLU:C	2.59	0.41
2:C:248:GLU:O	2:C:249:LYS:C	2.58	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:60:ASP:CB	2:C:62:PHE:CE2	3.03	0.41
2:D:131:ILE:HG22	2:D:133:PHE:CD2	2.51	0.41
2:D:17:LEU:HD23	2:D:17:LEU:C	2.41	0.41
2:D:264:LEU:O	2:D:317:ALA:HA	2.21	0.41
2:E:206:VAL:HG22	2:E:263:LEU:HD12	2.01	0.41
2:F:387:ILE:HG12	2:F:390:MSE:SE	2.70	0.41
2:F:99:GLY:HA3	2:F:115:LYS:O	2.21	0.41
2:B:231:THR:C	2:B:233:ASP:N	2.72	0.41
2:D:66:ARG:NH1	2:D:78:ASP:OD2	2.54	0.41
2:F:131:ILE:O	2:F:132:LEU:C	2.58	0.41
2:F:6:LEU:HD22	2:F:14:LEU:HD21	2.02	0.41
2:A:299:ARG:O	2:A:300:PHE:C	2.58	0.41
2:A:161:VAL:CG1	2:A:358:ILE:HD12	2.47	0.41
2:B:144:ARG:NH1	2:B:372:THR:HG22	2.36	0.41
2:B:197:TYR:HD2	2:B:198:ASN:ND2	2.19	0.41
2:B:252:ARG:O	2:B:255:GLU:HB2	2.21	0.41
2:C:337:GLY:O	2:D:212:ARG:NH1	2.44	0.41
2:D:355:PHE:O	2:D:357:ALA:N	2.54	0.41
2:E:307:VAL:HB	2:E:311:GLY:O	2.21	0.41
2:F:264:LEU:HB3	2:F:317:ALA:CA	2.49	0.41
2:A:210:ASP:OD1	2:A:232:PHE:HA	2.20	0.41
2:B:139:LEU:HD23	2:B:367:LYS:HD2	2.01	0.41
2:B:184:LYS:NZ	2:B:265:ASP:OD2	2.54	0.41
2:D:176:ILE:O	2:D:318:THR:HA	2.20	0.41
2:D:56:GLU:HB2	2:D:245:MSE:SE	2.70	0.41
1:K:4:DC:H5	2:E:110:TYR:HH	1.67	0.41
2:D:130:LYS:HZ1	2:E:12:SER:HB3	1.85	0.41
2:E:400:ILE:O	2:E:404:ALA:HB2	2.21	0.41
2:F:320:LEU:HD23	2:F:320:LEU:N	2.36	0.41
2:F:383:LEU:C	2:F:383:LEU:HD23	2.41	0.41
2:F:62:PHE:HB3	2:F:83:PRO:HD3	2.02	0.41
2:A:273:ALA:O	2:A:277:VAL:HG23	2.21	0.41
2:A:393:ILE:H	2:A:393:ILE:HG13	1.75	0.41
2:A:386:ILE:HD11	2:A:398:PHE:CZ	2.56	0.41
2:B:144:ARG:HH11	2:B:372:THR:HG22	1.85	0.41
2:C:272:ARG:HD2	2:C:327:MSE:SE	2.67	0.41
2:D:26:LEU:HB3	2:D:29:MSE:HE3	2.03	0.41
2:E:269:ARG:O	2:E:270:LEU:C	2.59	0.41
2:E:406:THR:HB	2:E:407:LYS:H	1.68	0.41
2:F:146:ARG:C	2:F:147:MSE:HG3	2.40	0.41
2:F:144:ARG:HA	2:F:169:GLY:HA2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:341:MSE:HA	2:F:365:THR:HA	2.03	0.41
2:F:399:LEU:O	2:F:403:LEU:HD12	2.21	0.41
2:A:248:GLU:O	2:A:249:LYS:C	2.58	0.41
2:A:294:LEU:C	2:A:297:PRO:HD2	2.42	0.41
2:A:42:HIS:C	2:A:44:LYS:H	2.22	0.41
2:B:269:ARG:HH12	2:B:272:ARG:HH22	1.69	0.41
2:C:341:MSE:HA	2:C:365:THR:HA	2.02	0.41
2:C:348:LYS:O	2:C:349:ILE:C	2.59	0.41
2:C:166:SER:HA	2:C:365:THR:HG22	2.03	0.41
2:D:140:HIS:HA	2:D:306:ASN:HB2	2.03	0.41
2:D:157:LEU:HA	2:D:157:LEU:HD23	1.93	0.41
2:D:369:GLU:HA	2:D:377:LEU:HD13	2.02	0.41
2:F:294:LEU:C	2:F:297:PRO:HD2	2.41	0.41
2:A:3:LEU:O	2:A:3:LEU:HD23	2.21	0.40
2:B:234:GLU:HB3	2:B:238:ARG:HG2	2.03	0.40
2:D:113:LEU:HD12	2:D:113:LEU:HA	1.87	0.40
2:D:17:LEU:O	2:D:21:MSE:HG3	2.22	0.40
2:E:393:ILE:O	2:E:394:ASP:C	2.59	0.40
2:A:161:VAL:CG1	2:A:161:VAL:O	2.69	0.40
2:A:18:GLY:O	2:A:23:LEU:HB2	2.22	0.40
2:A:297:PRO:HB2	2:A:335:PHE:HZ	1.86	0.40
2:B:356:PRO:O	2:B:358:ILE:N	2.47	0.40
2:C:355:PHE:O	2:C:357:ALA:N	2.53	0.40
2:C:55:LEU:HD13	2:C:81:VAL:HG21	2.02	0.40
2:C:9:THR:OG1	2:C:14:LEU:HG	2.22	0.40
2:D:293:ALA:C	2:D:295:HIS:H	2.24	0.40
2:E:102:ARG:HG2	2:E:114:LEU:HD13	2.04	0.40
2:E:209:ILE:HA	2:E:209:ILE:HD13	1.61	0.40
2:F:369:GLU:HG2	2:F:370:LEU:N	2.36	0.40
2:A:251:LYS:O	2:A:252:ARG:C	2.59	0.40
2:A:173:ARG:HD3	2:A:304:ALA:HB3	2.03	0.40
2:A:309:GLU:N	2:A:309:GLU:OE2	2.46	0.40
2:B:352:LYS:HB3	2:B:354:VAL:CG2	2.52	0.40
2:C:399:LEU:HA	2:C:399:LEU:HD23	1.93	0.40
2:A:266:SER:HG	2:A:269:ARG:N	2.18	0.40
2:A:321:ILE:CG2	2:A:322:ASP:N	2.85	0.40
2:C:15:ILE:O	2:C:16:THR:C	2.60	0.40
2:C:178:ALA:HA	2:C:179:PRO:HD3	1.96	0.40
2:C:199:HIS:N	2:C:200:PRO:HD3	2.36	0.40
2:D:351:GLU:HA	2:D:351:GLU:OE1	2.21	0.40
2:E:256:HIS:O	2:E:257:LYS:HB2	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:274:TYR:CD2	2:E:297:PRO:HD3	2.57	0.40
2:F:205:MSE:HE3	2:F:226:GLU:OE1	2.21	0.40
2:F:262:ILE:HB	2:F:315:ILE:HG12	2.03	0.40
2:A:99:GLY:HA3	2:A:115:LYS:O	2.22	0.40
2:D:66:ARG:CG	2:D:66:ARG:NH1	2.84	0.40
2:E:173:ARG:N	2:E:340:ASN:OD1	2.40	0.40
2:E:4:THR:CG2	2:E:52:ASP:OD1	2.70	0.40
2:E:55:LEU:CB	2:E:65:LEU:HD23	2.51	0.40
2:E:137:THR:O	2:F:214:GLU:HA	2.21	0.40
2:F:29:MSE:HG3	2:F:34:ILE:HG12	2.03	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	
2	A	400/419 (96%)	363 (91%)	30 (8%)	7 (2%)	10	43
2	B	350/419 (84%)	306 (87%)	31 (9%)	13 (4%)	4	22
2	C	400/419 (96%)	354 (88%)	37 (9%)	9 (2%)	7	35
2	D	400/419 (96%)	352 (88%)	33 (8%)	15 (4%)	4	21
2	E	399/419 (95%)	346 (87%)	39 (10%)	14 (4%)	4	23
2	F	400/419 (96%)	352 (88%)	35 (9%)	13 (3%)	4	25
All	All	2349/2514 (93%)	2073 (88%)	205 (9%)	71 (3%)	5	27

All (71) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	357	ALA
2	B	140	HIS

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Mol	Chain	Res	Type
2	B	355	PHE
2	C	140	HIS
2	C	408	THR
2	D	45	SER
2	D	137	THR
2	D	140	HIS
2	D	266	SER
2	E	408	THR
2	F	355	PHE
2	A	25	ASN
2	A	170	ARG
2	C	25	ASN
2	C	266	SER
2	C	292	ASN
2	C	357	ALA
2	D	139	LEU
2	D	141	ALA
2	D	294	LEU
2	D	357	ALA
2	D	407	LYS
2	E	25	ASN
2	E	31	LYS
2	E	170	ARG
2	E	294	LEU
2	E	392	GLU
2	E	410	ASP
2	F	139	LEU
2	F	242	VAL
2	F	266	SER
2	F	357	ALA
2	F	404	ALA
2	A	42	HIS
2	A	45	SER
2	A	47	GLU
2	B	153	SER
2	B	266	SER
2	B	287	GLY
2	B	408	THR
2	C	355	PHE
2	E	27	ALA
2	E	154	THR
2	E	287	GLY

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Mol	Chain	Res	Type
2	E	358	ILE
2	F	45	SER
2	F	356	PRO
2	B	139	LEU
2	B	142	ASN
2	B	143	SER
2	B	292	ASN
2	D	20	ASN
2	D	405	MSE
2	E	413	PHE
2	F	23	LEU
2	F	341	MSE
2	B	356	PRO
2	B	357	ALA
2	C	48	ASP
2	D	106	GLU
2	E	266	SER
2	F	294	LEU
2	A	124	PRO
2	B	294	LEU
2	D	287	GLY
2	F	49	ILE
2	F	287	GLY
2	D	49	ILE
2	D	124	PRO
2	E	209	ILE
2	C	356	PRO

### 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	
2	A	350/343 (102%)	308 (88%)	42 (12%)	6	25
2	B	306/343 (89%)	273 (89%)	33 (11%)	7	29
2	C	350/343 (102%)	288 (82%)	62 (18%)	2	11

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	D	350/343 (102%)	291 (83%)	59 (17%)	2	12
2	E	349/343 (102%)	291 (83%)	58 (17%)	2	13
2	F	350/343 (102%)	309 (88%)	41 (12%)	6	25
All	All	2055/2058 (100%)	1760 (86%)	295 (14%)	4	18

All (295) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	4	THR
2	A	7	LYS
2	A	9	THR
2	A	11	VAL
2	A	12	SER
2	A	15	ILE
2	A	24	GLU
2	A	28	ARG
2	A	45	SER
2	A	52	ASP
2	A	70	SER
2	A	71	SER
2	A	73	LEU
2	A	82	SER
2	A	84	SER
2	A	88	ARG
2	A	132	LEU
2	A	137	THR
2	A	139	LEU
2	A	173	ARG
2	A	184	LYS
2	A	194	SER
2	A	203	VAL
2	A	210	ASP
2	A	222	LEU
2	A	224	LYS
2	A	245	MSE
2	A	252	ARG
2	A	268	THR
2	A	272	ARG
2	A	276	THR
2	A	289	VAL
2	A	299	ARG

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Mol	Chain	Res	Type
2	A	309	GLU
2	A	314	THR
2	A	321	ILE
2	A	341	MSE
2	A	342	GLU
2	A	365	THR
2	A	386	ILE
2	A	396	MSE
2	A	399	LEU
2	B	56	GLU
2	B	66	ARG
2	B	71	SER
2	B	93	THR
2	B	101	ILE
2	B	114	LEU
2	B	132	LEU
2	B	134	GLU
2	B	139	LEU
2	B	146	ARG
2	B	147	MSE
2	B	185	THR
2	B	198	ASN
2	B	252	ARG
2	B	268	THR
2	B	272	ARG
2	B	276	THR
2	B	289	VAL
2	B	290	ASP
2	B	299	ARG
2	B	301	PHE
2	B	314	THR
2	B	321	ILE
2	B	325	SER
2	B	354	VAL
2	B	356	PRO
2	B	363	SER
2	B	365	THR
2	B	377	LEU
2	B	383	LEU
2	B	386	ILE
2	B	399	LEU
2	B	406	THR

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Mol	Chain	Res	Type
2	C	1	MSE
2	C	2	ASN
2	C	3	LEU
2	C	4	THR
2	C	7	LYS
2	C	9	THR
2	C	17	LEU
2	C	24	GLU
2	C	40	LYS
2	C	48	ASP
2	C	49	ILE
2	C	52	ASP
2	C	56	GLU
2	C	66	ARG
2	C	69	ASP
2	C	82	SER
2	C	88	ARG
2	C	93	THR
2	C	129	ASN
2	C	131	ILE
2	C	132	LEU
2	C	139	LEU
2	C	146	ARG
2	C	163	ASP
2	C	181	LYS
2	C	190	ASN
2	C	194	SER
2	C	202	CYS
2	C	230	SER
2	C	231	THR
2	C	235	PRO
2	C	252	ARG
2	C	257	LYS
2	C	266	SER
2	C	272	ARG
2	C	276	THR
2	C	290	ASP
2	C	299	ARG
2	C	301	PHE
2	C	309	GLU
2	C	314	THR
2	C	318	THR

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Mol	Chain	Res	Type
2	C	321	ILE
2	C	325	SER
2	C	326	LYS
2	C	336	LYS
2	C	341	MSE
2	C	347	ARG
2	C	362	ARG
2	C	365	THR
2	C	367	LYS
2	C	379	LYS
2	C	383	LEU
2	C	384	ARG
2	C	386	ILE
2	C	393	ILE
2	C	399	LEU
2	C	406	THR
2	C	407	LYS
2	C	411	ASP
2	C	414	GLU
2	C	417	LYS
2	D	7	LYS
2	D	9	THR
2	D	11	VAL
2	D	12	SER
2	D	24	GLU
2	D	26	LEU
2	D	69	ASP
2	D	70	SER
2	D	84	SER
2	D	88	ARG
2	D	92	ARG
2	D	93	THR
2	D	114	LEU
2	D	115	LYS
2	D	130	LYS
2	D	131	ILE
2	D	132	LEU
2	D	134	GLU
2	D	137	THR
2	D	139	LEU
2	D	163	ASP
2	D	170	ARG

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Mol	Chain	Res	Type
2	D	184	LYS
2	D	186	MSE
2	D	194	SER
2	D	210	ASP
2	D	222	LEU
2	D	242	VAL
2	D	245	MSE
2	D	252	ARG
2	D	268	THR
2	D	272	ARG
2	D	276	THR
2	D	286	THR
2	D	296	ARG
2	D	299	ARG
2	D	305	ARG
2	D	309	GLU
2	D	312	SER
2	D	314	THR
2	D	318	THR
2	D	321	ILE
2	D	322	ASP
2	D	330	VAL
2	D	336	LYS
2	D	341	MSE
2	D	353	ARG
2	D	356	PRO
2	D	363	SER
2	D	365	THR
2	D	372	THR
2	D	374	GLN
2	D	377	LEU
2	D	386	ILE
2	D	393	ILE
2	D	396	MSE
2	D	399	LEU
2	D	405	MSE
2	D	416	MSE
2	E	1	MSE
2	E	3	LEU
2	E	4	THR
2	E	6	LEU
2	E	9	THR

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Mol	Chain	Res	Type
2	E	16	THR
2	E	24	GLU
2	E	28	ARG
2	E	31	LYS
2	E	40	LYS
2	E	44	LYS
2	E	69	ASP
2	E	84	SER
2	E	86	ILE
2	E	88	ARG
2	E	93	THR
2	E	131	ILE
2	E	132	LEU
2	E	137	THR
2	E	139	LEU
2	E	143	SER
2	E	146	ARG
2	E	162	LEU
2	E	163	ASP
2	E	184	LYS
2	E	186	MSE
2	E	194	SER
2	E	209	ILE
2	E	211	GLU
2	E	233	ASP
2	E	252	ARG
2	E	268	THR
2	E	272	ARG
2	E	276	THR
2	E	278	VAL
2	E	286	THR
2	E	289	VAL
2	E	296	ARG
2	E	299	ARG
2	E	309	GLU
2	E	314	THR
2	E	326	LYS
2	E	341	MSE
2	E	353	ARG
2	E	355	PHE
2	E	356	PRO
2	E	359	ASP

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Mol	Chain	Res	Type
2	E	365	THR
2	E	366	ARG
2	E	371	LEU
2	E	374	GLN
2	E	384	ARG
2	E	386	ILE
2	E	393	ILE
2	E	399	LEU
2	E	406	THR
2	E	407	LYS
2	E	413	PHE
2	F	3	LEU
2	F	7	LYS
2	F	9	THR
2	F	11	VAL
2	F	12	SER
2	F	24	GLU
2	F	40	LYS
2	F	45	SER
2	F	49	ILE
2	F	58	LEU
2	F	84	SER
2	F	93	THR
2	F	101	ILE
2	F	106	GLU
2	F	126	ASN
2	F	144	ARG
2	F	162	LEU
2	F	163	ASP
2	F	194	SER
2	F	195	ILE
2	F	202	CYS
2	F	245	MSE
2	F	261	ILE
2	F	266	SER
2	F	267	ILE
2	F	272	ARG
2	F	276	THR
2	F	299	ARG
2	F	305	ARG
2	F	307	VAL
2	F	308	GLU

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Mol	Chain	Res	Type
2	F	321	ILE
2	F	341	MSE
2	F	346	SER
2	F	356	PRO
2	F	359	ASP
2	F	365	THR
2	F	386	ILE
2	F	390	MSE
2	F	393	ILE
2	F	405	MSE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	275	ASN
2	A	306	ASN
2	B	198	ASN
2	B	199	HIS
2	B	275	ASN
2	C	41	GLN
2	C	275	ASN
2	C	306	ASN
2	D	41	GLN
2	D	126	ASN
2	D	129	ASN
2	D	172	GLN
2	D	275	ASN
2	E	59	GLN
2	E	129	ASN
2	E	135	ASN
2	E	275	ASN
2	E	295	HIS
2	E	306	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 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](#)

There are no ligands in this entry.

## 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	G	2/2 (100%)	0.88	0 100 100	150, 150, 150, 150	0
1	H	2/2 (100%)	2.21	1 (50%) 0 0	150, 150, 150, 150	0
1	J	2/2 (100%)	3.94	2 (100%) 0 0	150, 150, 150, 150	0
1	K	2/2 (100%)	2.99	1 (50%) 0 0	150, 150, 150, 150	0
1	L	2/2 (100%)	2.85	2 (100%) 0 0	150, 150, 150, 150	0
2	A	392/419 (93%)	0.44	37 (9%) 9 3	35, 69, 121, 127	0
2	B	345/419 (82%)	0.38	28 (8%) 13 5	30, 69, 114, 127	0
2	C	392/419 (93%)	0.10	8 (2%) 65 36	18, 44, 96, 113	0
2	D	392/419 (93%)	0.01	19 (4%) 31 12	14, 45, 77, 126	0
2	E	391/419 (93%)	0.04	11 (2%) 53 25	18, 47, 87, 126	0
2	F	392/419 (93%)	0.36	29 (7%) 15 6	36, 67, 114, 124	0
All	All	2314/2524 (91%)	0.23	138 (5%) 23 9	14, 57, 110, 150	0

All (138) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	51	GLY	7.6
2	F	47	GLU	6.9
2	F	286	THR	6.2
2	B	141	ALA	5.9
2	A	355	PHE	5.8
2	E	414	GLU	5.8
2	A	279	PRO	5.2
2	F	25	ASN	5.1
1	J	4	DC	4.7
2	A	414	GLU	4.6
2	A	406	THR	4.6
2	A	354	VAL	4.6

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Mol	Chain	Res	Type	RSRZ
2	A	141	ALA	4.3
2	F	126	ASN	4.2
2	A	46	GLY	4.2
2	F	368	GLU	4.2
2	F	406	THR	4.2
2	D	355	PHE	4.1
2	C	414	GLU	4.1
1	K	4	DC	4.1
2	D	414	GLU	4.0
2	C	48	ASP	4.0
2	C	352	LYS	3.9
2	A	392	GLU	3.9
2	B	355	PHE	3.8
2	A	166	SER	3.8
2	F	310	GLY	3.8
2	B	62	PHE	3.8
2	A	284	VAL	3.7
2	F	289	VAL	3.7
2	B	406	THR	3.7
2	E	406	THR	3.6
2	E	25	ASN	3.6
2	A	27	ALA	3.6
2	A	388	HIS	3.5
2	E	26	LEU	3.5
1	L	3	DC	3.5
2	F	50	PHE	3.5
2	A	233	ASP	3.4
2	F	308	GLU	3.4
2	D	23	LEU	3.4
2	C	25	ASN	3.3
2	F	130	LYS	3.3
2	A	417	LYS	3.2
1	J	3	DC	3.2
2	A	197	TYR	3.2
2	A	163	ASP	3.2
2	B	106	GLU	3.2
2	D	407	LYS	3.1
2	D	48	ASP	3.1
2	B	381	TRP	3.1
2	F	381	TRP	3.1
2	A	346	SER	3.0
2	A	363	SER	2.9

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Mol	Chain	Res	Type	RSRZ
2	A	412	PHE	2.9
2	F	139	LEU	2.9
2	F	48	ASP	2.9
2	B	111	PHE	2.8
2	B	143	SER	2.8
2	A	60	ASP	2.8
2	B	292	ASN	2.8
2	F	141	ALA	2.8
2	A	352	LYS	2.7
2	A	361	ASN	2.7
2	D	284	VAL	2.7
2	F	306	ASN	2.7
2	B	129	ASN	2.7
1	H	3	DC	2.6
2	B	317	ALA	2.6
2	F	404	ALA	2.6
2	D	412	PHE	2.6
2	B	140	HIS	2.6
2	D	126	ASN	2.6
2	F	136	LEU	2.6
2	A	378	GLN	2.6
2	C	417	LYS	2.6
2	D	109	ARG	2.6
2	A	317	ALA	2.6
2	F	193	GLN	2.6
2	B	63	GLY	2.5
2	A	165	ALA	2.5
2	F	137	THR	2.5
2	A	394	ASP	2.5
2	D	406	THR	2.5
2	F	285	LEU	2.5
2	A	28	ARG	2.5
2	F	290	ASP	2.5
2	F	280	ALA	2.5
2	F	170	ARG	2.4
2	B	125	GLU	2.4
2	B	60	ASP	2.4
2	B	412	PHE	2.4
2	A	285	LEU	2.4
2	B	113	LEU	2.4
2	B	259	ASP	2.4
2	A	193	GLN	2.4

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Mol	Chain	Res	Type	RSRZ
2	F	372	THR	2.4
2	D	60	ASP	2.4
2	E	285	LEU	2.3
2	A	198	ASN	2.3
2	B	59	GLN	2.3
2	B	417	LYS	2.3
2	D	417	LYS	2.3
2	E	393	ILE	2.3
2	A	47	GLU	2.3
2	A	343	LEU	2.2
2	D	47	GLU	2.2
2	C	292	ASN	2.2
2	E	50	PHE	2.2
1	L	4	DC	2.2
2	A	26	LEU	2.2
2	B	126	ASN	2.2
2	C	141	ALA	2.2
2	E	125	GLU	2.2
2	F	307	VAL	2.2
2	D	141	ALA	2.1
2	D	374	GLN	2.1
2	F	160	ARG	2.1
2	B	354	VAL	2.1
2	D	110	TYR	2.1
2	D	197	TYR	2.1
2	E	60	ASP	2.1
2	B	198	ASN	2.1
2	F	279	PRO	2.1
2	A	160	ARG	2.1
2	A	348	LYS	2.1
2	A	125	GLU	2.1
2	B	279	PRO	2.1
2	E	109	ARG	2.1
2	D	375	GLU	2.1
2	B	130	LYS	2.0
2	B	247	ILE	2.0
2	C	142	ASN	2.0
2	E	59	GLN	2.0
2	B	142	ASN	2.0
2	D	292	ASN	2.0
2	F	27	ALA	2.0
2	A	278	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](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.