



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:29 AM GMT

PDB ID : 2H1L
Title : The Structure of the Oncoprotein SV40 Large T Antigen and p53 Tumor
Suppressor Complex
Authors : Lilyestrom, W.
Deposited on : 2006-05-16
Resolution : 3.16 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

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

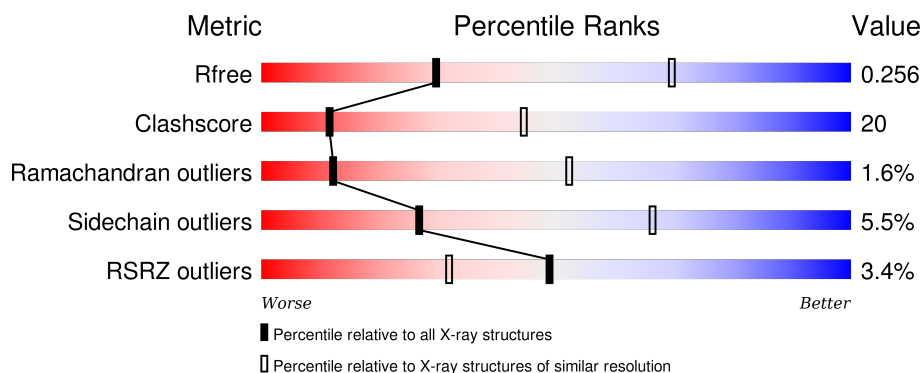
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.16 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1112 (3.20-3.12)
Clashscore	102246	1249 (3.20-3.12)
Ramachandran outliers	100387	1222 (3.20-3.12)
Sidechain outliers	100360	1221 (3.20-3.12)
RSRZ outliers	91569	1117 (3.20-3.12)

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

Mol	Chain	Length	Quality of chain
1	A	370	<div> <div>2%</div> <div>56% 38% . .</div> </div>
1	B	370	<div> <div>50% 43% 5% .</div> </div>
1	C	370	<div> <div>2%</div> <div>52% 41% 5% .</div> </div>
1	D	370	<div> <div>%</div> <div>55% 41% . .</div> </div>
1	E	370	<div> <div>%</div> <div>54% 39% . .</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	370	
1	G	370	
1	H	370	
1	I	370	
1	J	370	
1	K	370	
1	L	370	
2	M	203	
2	N	203	
2	O	203	
2	P	203	
2	Q	203	
2	R	203	
2	S	203	
2	T	203	
2	U	203	
2	V	203	
2	W	203	
2	X	203	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 53920 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Large T antigen.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	362	Total	C	N	O	S	0	0	0
			2933	1888	493	531	21			
1	B	362	Total	C	N	O	S	0	0	0
			2933	1888	493	531	21			
1	C	363	Total	C	N	O	S	0	0	0
			2940	1892	494	533	21			
1	D	362	Total	C	N	O	S	0	0	0
			2933	1888	493	531	21			
1	E	362	Total	C	N	O	S	0	0	0
			2933	1888	493	531	21			
1	F	363	Total	C	N	O	S	0	0	0
			2940	1892	494	533	21			
1	G	362	Total	C	N	O	S	0	0	0
			2933	1888	493	531	21			
1	H	362	Total	C	N	O	S	0	0	0
			2933	1888	493	531	21			
1	I	363	Total	C	N	O	S	0	0	0
			2940	1892	494	533	21			
1	J	362	Total	C	N	O	S	0	0	0
			2933	1888	493	531	21			
1	K	362	Total	C	N	O	S	0	0	0
			2933	1888	493	531	21			
1	L	363	Total	C	N	O	S	0	0	0
			2940	1892	494	533	21			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	258	GLY	-	CLONING ARTIFACT	UNP Q9NP68
A	259	SER	-	CLONING ARTIFACT	UNP Q9NP68
B	258	GLY	-	CLONING ARTIFACT	UNP Q9NP68
B	259	SER	-	CLONING ARTIFACT	UNP Q9NP68
C	258	GLY	-	CLONING ARTIFACT	UNP Q9NP68

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Chain	Residue	Modelled	Actual	Comment	Reference
C	259	SER	-	CLONING ARTIFACT	UNP Q9NP68
D	258	GLY	-	CLONING ARTIFACT	UNP Q9NP68
D	259	SER	-	CLONING ARTIFACT	UNP Q9NP68
E	258	GLY	-	CLONING ARTIFACT	UNP Q9NP68
E	259	SER	-	CLONING ARTIFACT	UNP Q9NP68
F	258	GLY	-	CLONING ARTIFACT	UNP Q9NP68
F	259	SER	-	CLONING ARTIFACT	UNP Q9NP68
G	258	GLY	-	CLONING ARTIFACT	UNP Q9NP68
G	259	SER	-	CLONING ARTIFACT	UNP Q9NP68
H	258	GLY	-	CLONING ARTIFACT	UNP Q9NP68
H	259	SER	-	CLONING ARTIFACT	UNP Q9NP68
I	258	GLY	-	CLONING ARTIFACT	UNP Q9NP68
I	259	SER	-	CLONING ARTIFACT	UNP Q9NP68
J	258	GLY	-	CLONING ARTIFACT	UNP Q9NP68
J	259	SER	-	CLONING ARTIFACT	UNP Q9NP68
K	258	GLY	-	CLONING ARTIFACT	UNP Q9NP68
K	259	SER	-	CLONING ARTIFACT	UNP Q9NP68
L	258	GLY	-	CLONING ARTIFACT	UNP Q9NP68
L	259	SER	-	CLONING ARTIFACT	UNP Q9NP68

- Molecule 2 is a protein called Cellular tumor antigen p53.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	M	199	Total	C	N	O	S	0	0	0
			1556	959	286	295	16			
2	N	199	Total	C	N	O	S	0	0	0
			1556	959	286	295	16			
2	O	199	Total	C	N	O	S	0	0	0
			1556	959	286	295	16			
2	P	199	Total	C	N	O	S	0	0	0
			1556	959	286	295	16			
2	Q	199	Total	C	N	O	S	0	0	0
			1556	959	286	295	16			
2	R	199	Total	C	N	O	S	0	0	0
			1556	959	286	295	16			
2	S	199	Total	C	N	O	S	0	0	0
			1556	959	286	295	16			
2	T	199	Total	C	N	O	S	0	0	0
			1556	959	286	295	16			
2	U	199	Total	C	N	O	S	0	0	0
			1556	959	286	295	16			
2	V	199	Total	C	N	O	S	0	0	0
			1556	959	286	295	16			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	W	199	Total	C	N	O	S	0	0	0
			1556	959	286	295	16			
2	X	199	Total	C	N	O	S	0	0	0
			1556	959	286	295	16			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	90	GLY	-	CLONING ARTIFACT	UNP Q9NP68
M	91	SER	-	CLONING ARTIFACT	UNP Q9NP68
N	90	GLY	-	CLONING ARTIFACT	UNP Q9NP68
N	91	SER	-	CLONING ARTIFACT	UNP Q9NP68
O	90	GLY	-	CLONING ARTIFACT	UNP Q9NP68
O	91	SER	-	CLONING ARTIFACT	UNP Q9NP68
P	90	GLY	-	CLONING ARTIFACT	UNP Q9NP68
P	91	SER	-	CLONING ARTIFACT	UNP Q9NP68
Q	90	GLY	-	CLONING ARTIFACT	UNP Q9NP68
Q	91	SER	-	CLONING ARTIFACT	UNP Q9NP68
R	90	GLY	-	CLONING ARTIFACT	UNP Q9NP68
R	91	SER	-	CLONING ARTIFACT	UNP Q9NP68
S	90	GLY	-	CLONING ARTIFACT	UNP Q9NP68
S	91	SER	-	CLONING ARTIFACT	UNP Q9NP68
T	90	GLY	-	CLONING ARTIFACT	UNP Q9NP68
T	91	SER	-	CLONING ARTIFACT	UNP Q9NP68
U	90	GLY	-	CLONING ARTIFACT	UNP Q9NP68
U	91	SER	-	CLONING ARTIFACT	UNP Q9NP68
V	90	GLY	-	CLONING ARTIFACT	UNP Q9NP68
V	91	SER	-	CLONING ARTIFACT	UNP Q9NP68
W	90	GLY	-	CLONING ARTIFACT	UNP Q9NP68
W	91	SER	-	CLONING ARTIFACT	UNP Q9NP68
X	90	GLY	-	CLONING ARTIFACT	UNP Q9NP68
X	91	SER	-	CLONING ARTIFACT	UNP Q9NP68

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

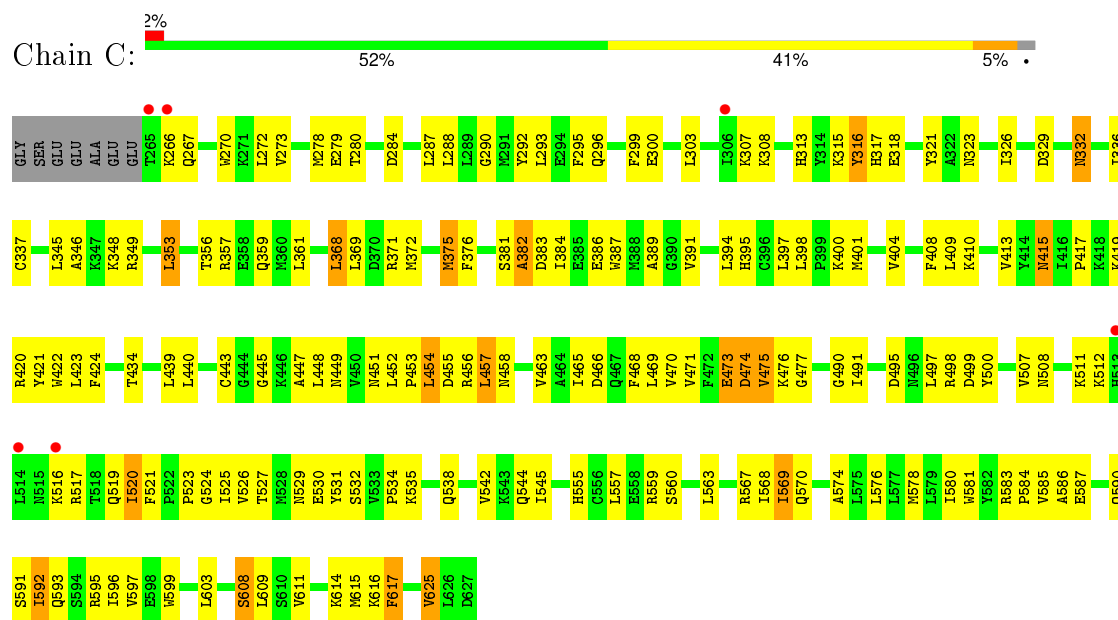
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	P	1	Total	Zn	0	0
			1	1		
3	K	1	Total	Zn	0	0
			1	1		
3	B	1	Total	Zn	0	0
			1	1		

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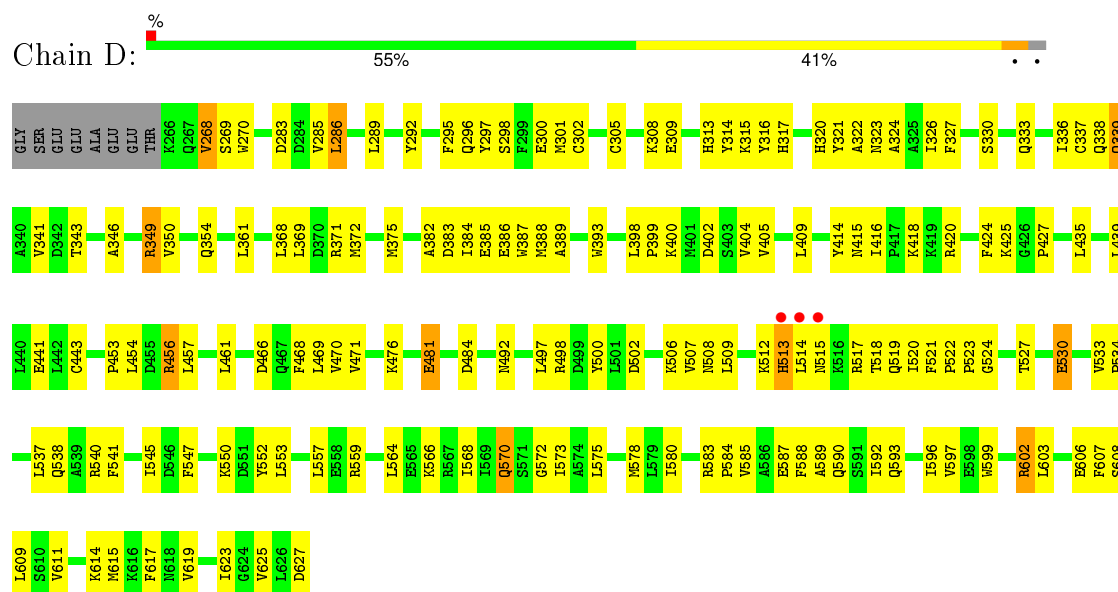
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	W	1	Total 1	Zn 1	0	0
3	N	1	Total 1	Zn 1	0	0
3	X	1	Total 1	Zn 1	0	0
3	S	1	Total 1	Zn 1	0	0
3	J	1	Total 1	Zn 1	0	0
3	E	1	Total 1	Zn 1	0	0
3	V	1	Total 1	Zn 1	0	0
3	A	1	Total 1	Zn 1	0	0
3	R	1	Total 1	Zn 1	0	0
3	M	1	Total 1	Zn 1	0	0
3	D	1	Total 1	Zn 1	0	0
3	I	1	Total 1	Zn 1	0	0
3	U	1	Total 1	Zn 1	0	0
3	L	1	Total 1	Zn 1	0	0
3	G	1	Total 1	Zn 1	0	0
3	Q	1	Total 1	Zn 1	0	0
3	H	1	Total 1	Zn 1	0	0
3	C	1	Total 1	Zn 1	0	0
3	T	1	Total 1	Zn 1	0	0
3	O	1	Total 1	Zn 1	0	0
3	F	1	Total 1	Zn 1	0	0

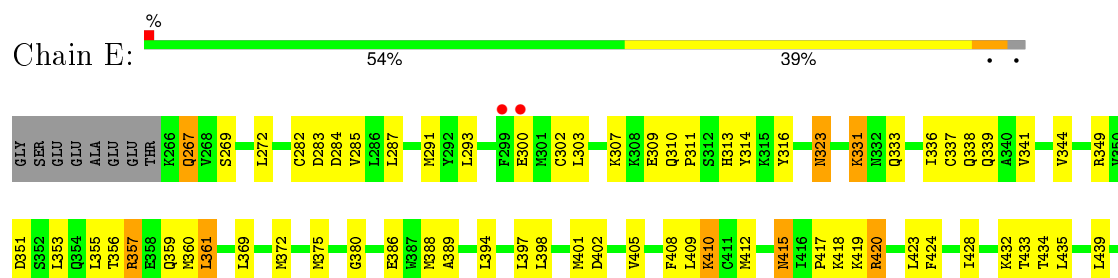
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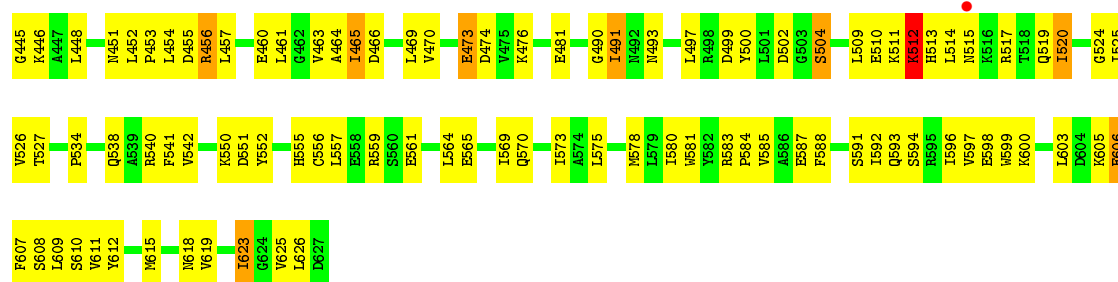


• Molecule 1: Large T antigen

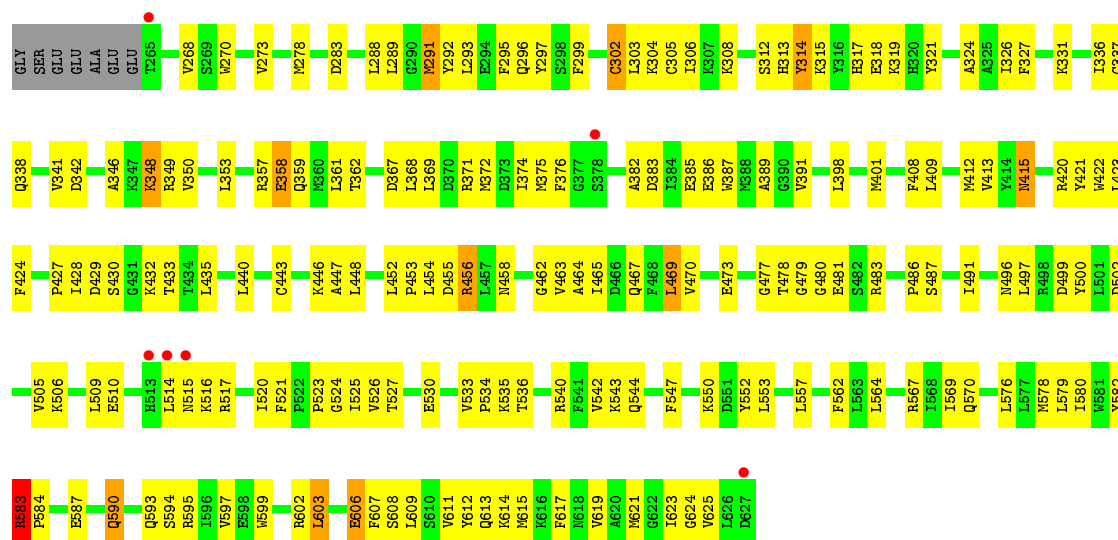


• Molecule 1: Large T antigen

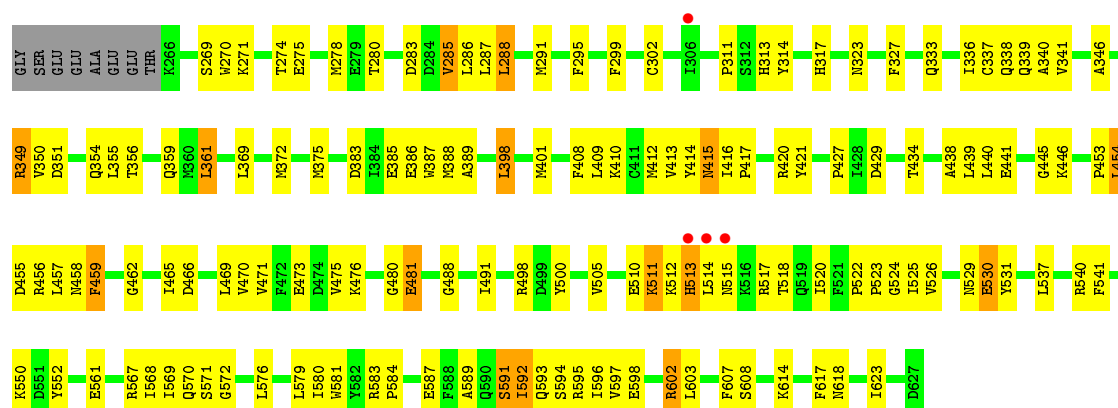




• Molecule 1: Large T antigen

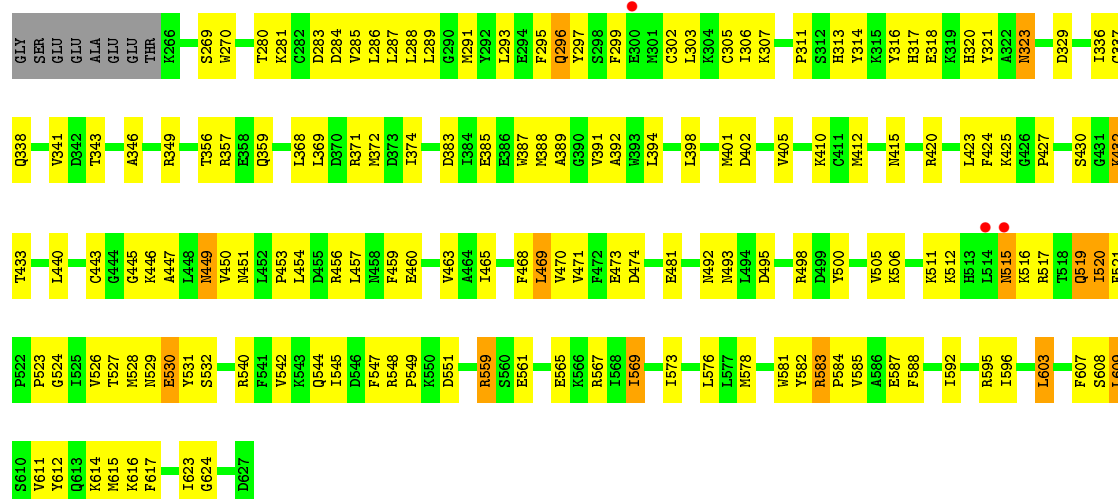


• Molecule 1: Large T antigen

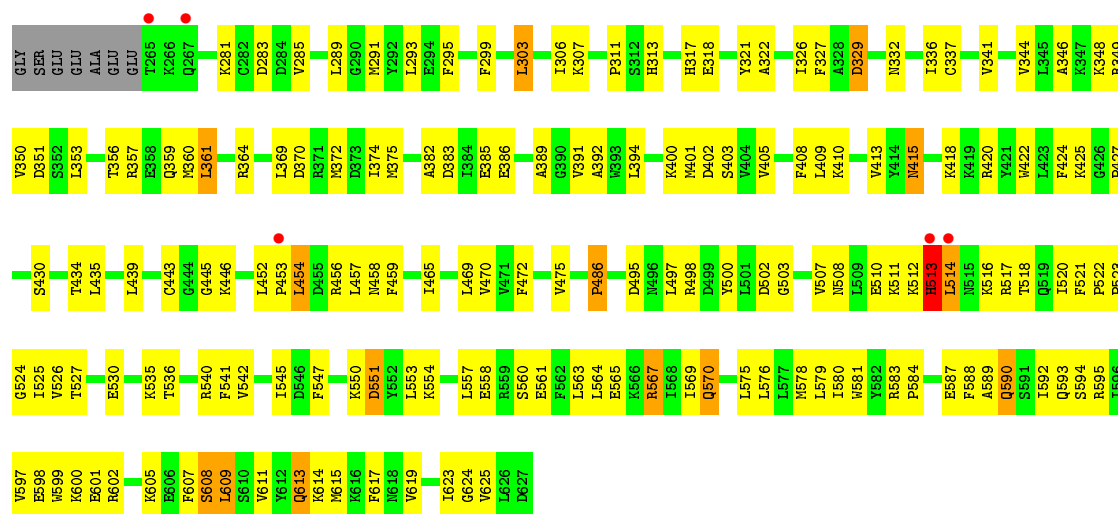


• Molecule 1: Large T antigen

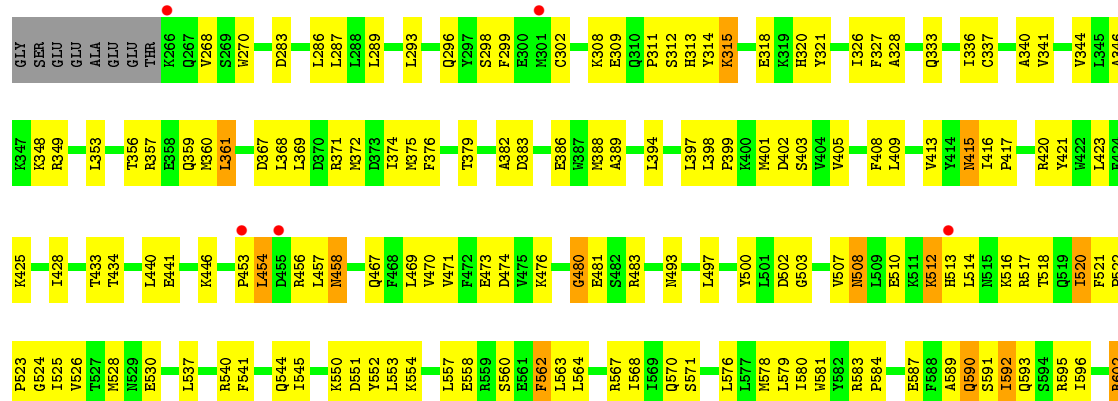


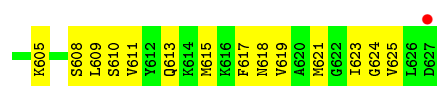


• Molecule 1: Large T antigen

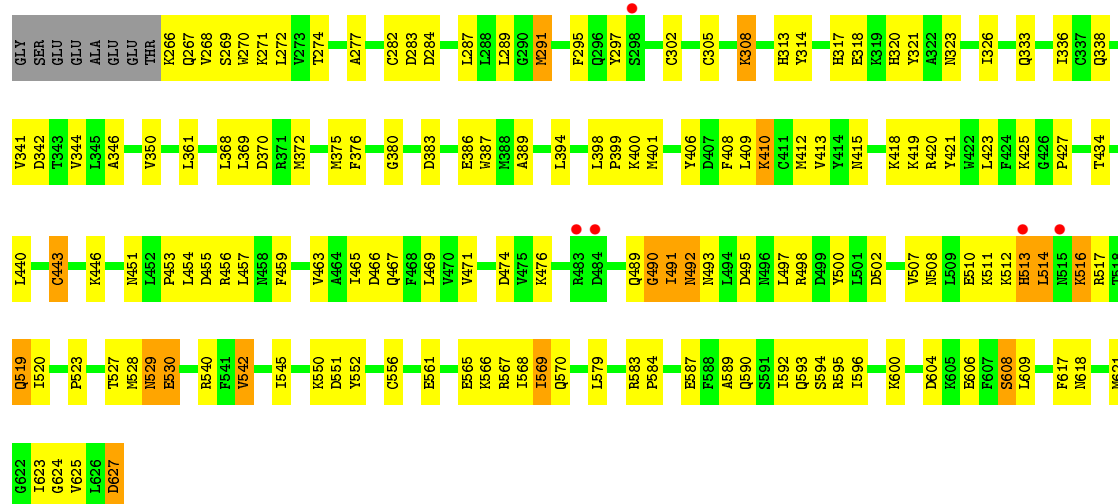


• Molecule 1: Large T antigen

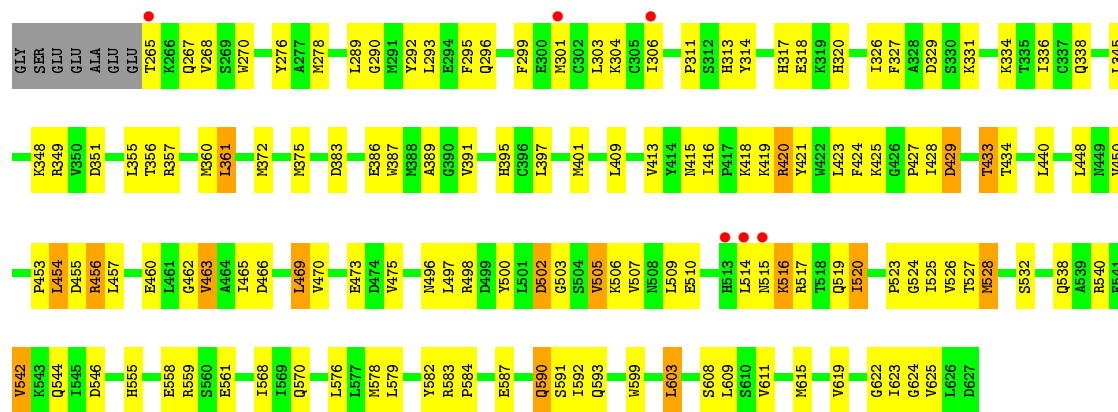




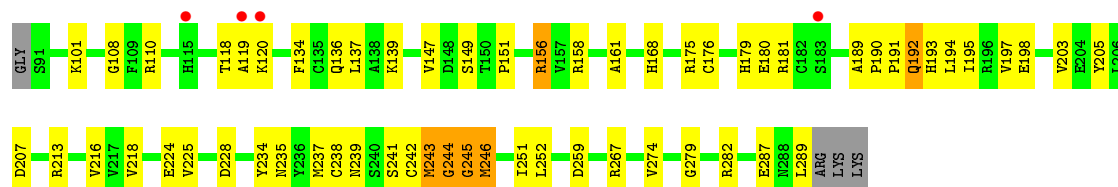
• Molecule 1: Large T antigen



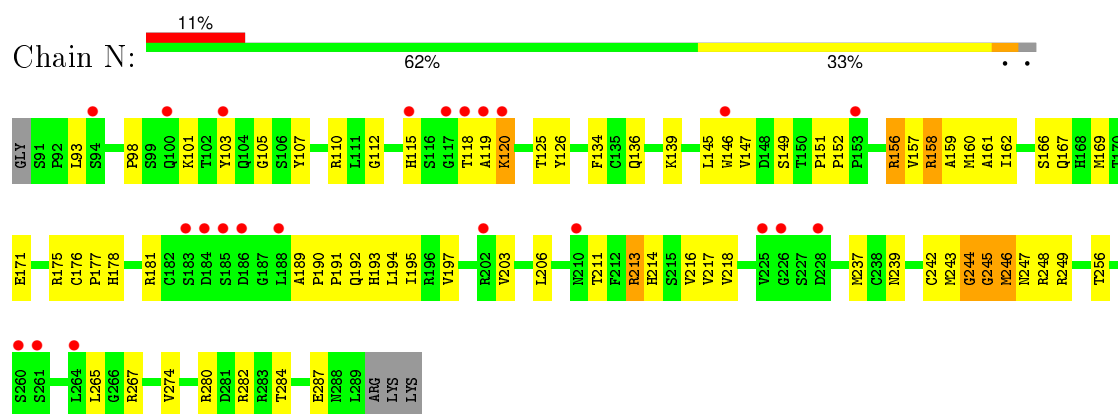
• Molecule 1: Large T antigen



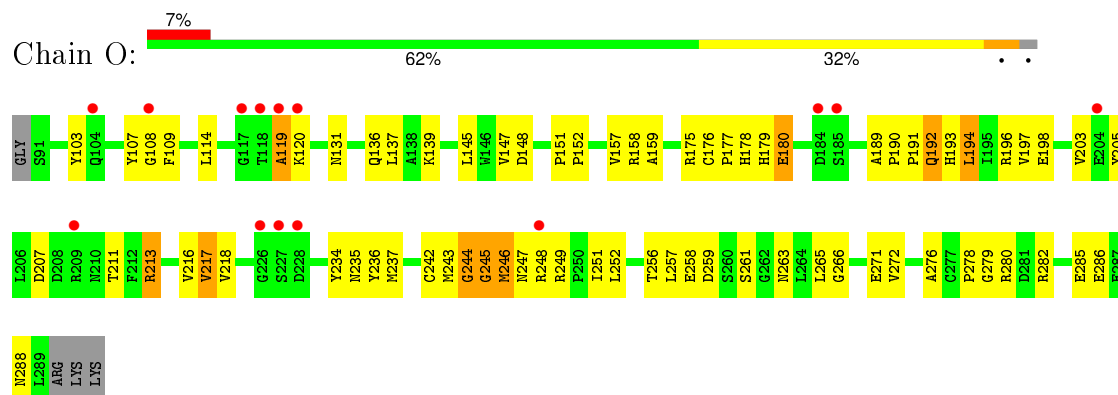
• Molecule 2: Cellular tumor antigen p53



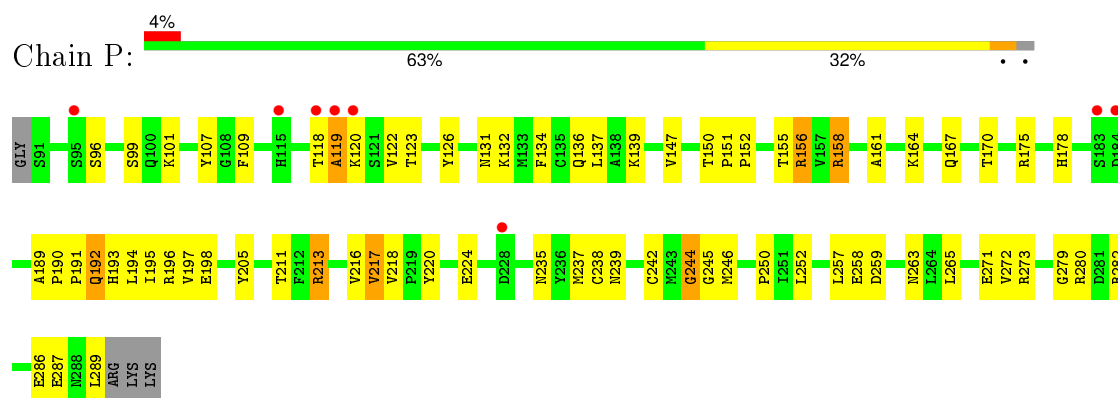
• Molecule 2: Cellular tumor antigen p53



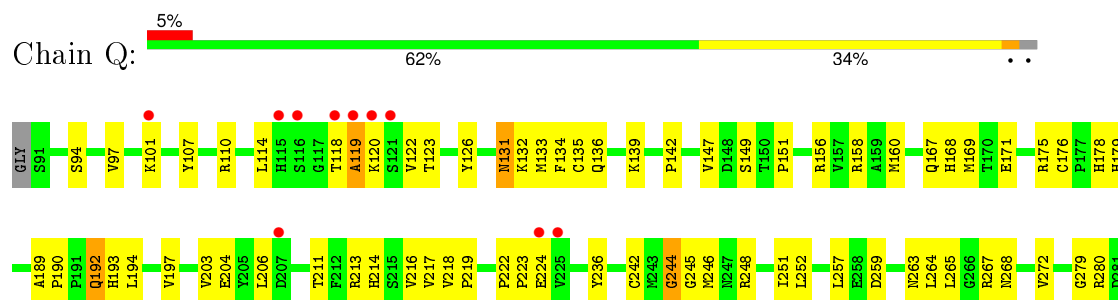
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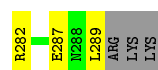


• Molecule 2: Cellular tumor antigen p53

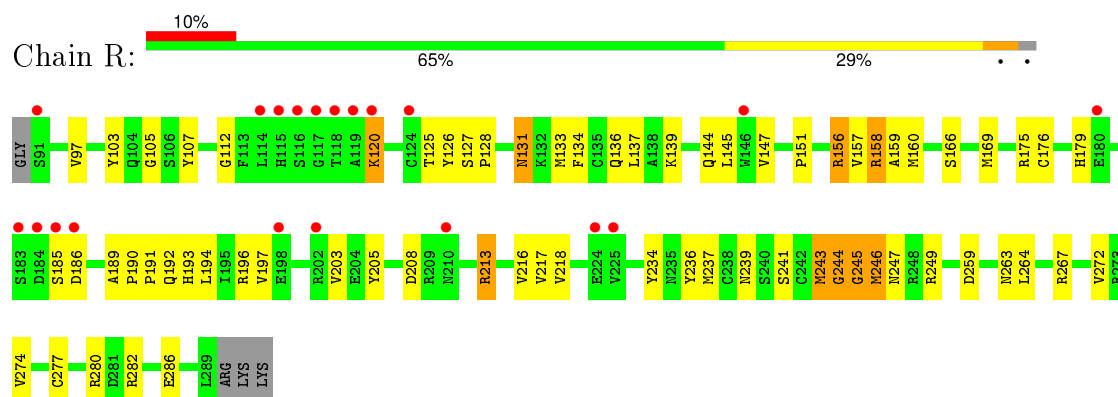


• Molecule 2: Cellular tumor antigen p53

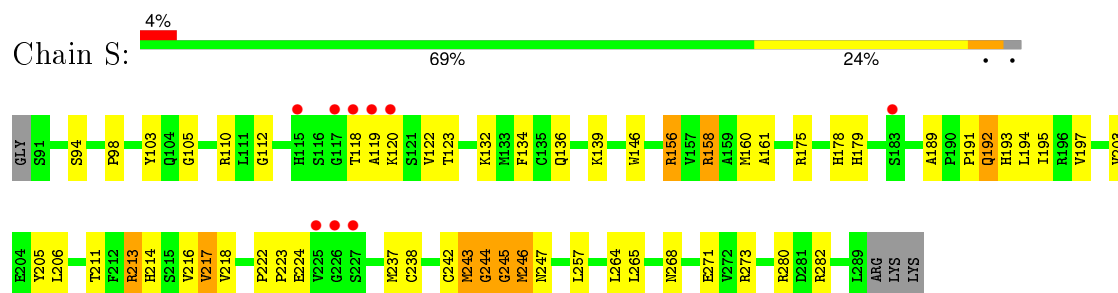




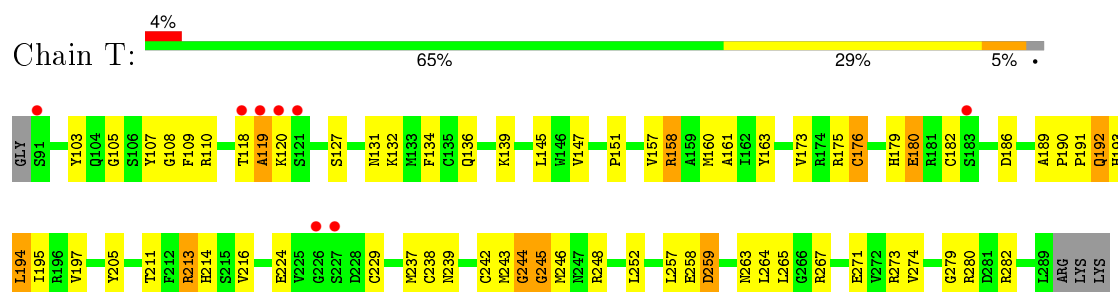
• Molecule 2: Cellular tumor antigen p53



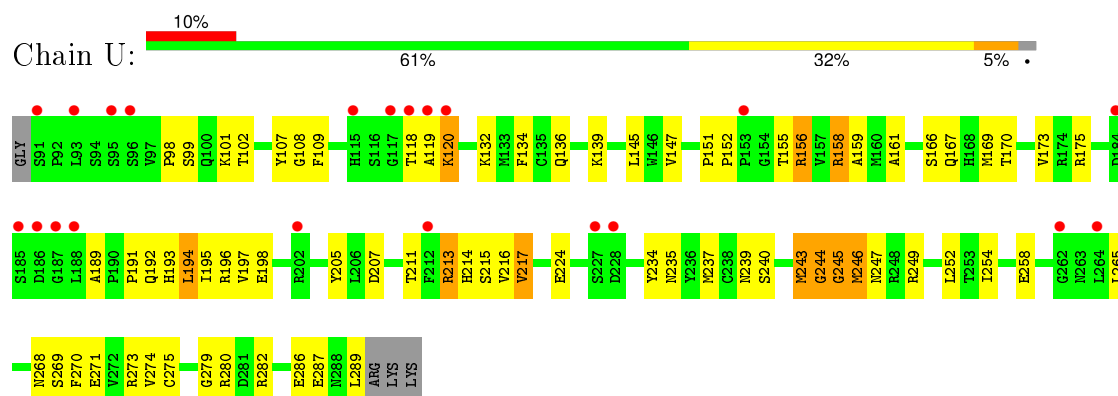
• Molecule 2: Cellular tumor antigen p53



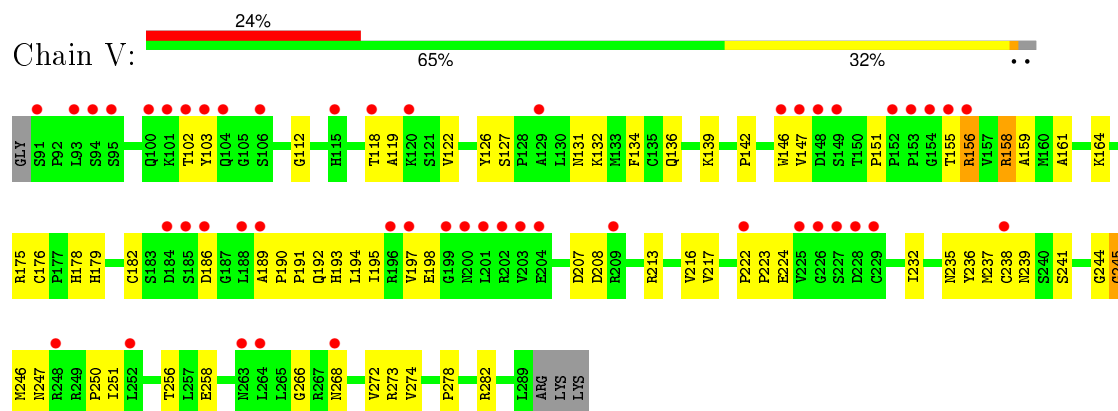
• Molecule 2: Cellular tumor antigen p53



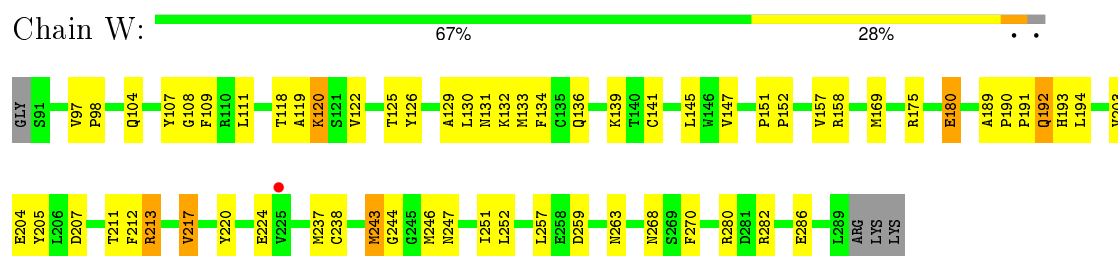
• Molecule 2: Cellular tumor antigen p53



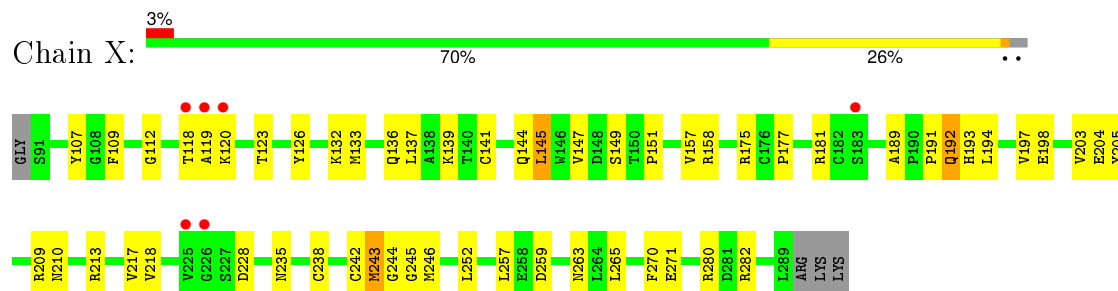
- Molecule 2: Cellular tumor antigen p53



- Molecule 2: Cellular tumor antigen p53



- Molecule 2: Cellular tumor antigen p53



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	127.02Å 182.72Å 262.06Å 90.00° 92.08° 90.00°	Depositor
Resolution (Å)	20.00 – 3.16 19.98 – 3.16	Depositor EDS
% Data completeness (in resolution range)	97.3 (20.00-3.16) 97.0 (19.98-3.16)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.13 (at 3.15Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.261 , 0.308 0.252 , 0.256	Depositor DCC
R_{free} test set	15189 reflections (7.69%)	DCC
Wilson B-factor (Å ²)	81.4	Xtriage
Anisotropy	0.595	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 42.6	EDS
Estimated twinning fraction	0.000 for h,-k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtriage
Outliers	0 of 197864 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	53920	wwPDB-VP
Average B, all atoms (Å ²)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.15% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.57	0/2992	0.67	0/4030
1	B	0.55	0/2992	0.63	0/4030
1	C	0.56	0/2999	0.63	0/4040
1	D	0.59	0/2992	0.68	0/4030
1	E	0.61	0/2992	0.67	0/4030
1	F	0.59	0/2999	0.67	0/4040
1	G	0.64	0/2992	0.70	1/4030 (0.0%)
1	H	0.60	0/2992	0.68	0/4030
1	I	0.55	0/2999	0.63	0/4040
1	J	0.52	0/2992	0.61	0/4030
1	K	0.62	0/2992	0.68	0/4030
1	L	0.67	0/2999	0.71	0/4040
2	M	0.55	1/1592 (0.1%)	0.64	0/2160
2	N	0.44	0/1592	0.57	0/2160
2	O	0.47	0/1592	0.61	0/2160
2	P	0.51	0/1592	0.62	0/2160
2	Q	0.47	0/1592	0.60	0/2160
2	R	0.46	1/1592 (0.1%)	0.59	0/2160
2	S	0.52	1/1592 (0.1%)	0.63	0/2160
2	T	0.49	1/1592 (0.1%)	0.61	0/2160
2	U	0.49	1/1592 (0.1%)	0.59	0/2160
2	V	0.46	1/1592 (0.1%)	0.54	0/2160
2	W	0.60	1/1592 (0.1%)	0.65	0/2160
2	X	0.62	1/1592 (0.1%)	0.68	0/2160
All	All	0.56	8/55036 (0.0%)	0.65	1/74320 (0.0%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	M	243	MET	SD-CE	7.60	2.20	1.77
2	U	243	MET	SD-CE	6.29	2.13	1.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	X	243	MET	SD-CE	6.17	2.12	1.77
2	T	176	CYS	CB-SG	-5.89	1.72	1.81
2	W	243	MET	SD-CE	5.65	2.09	1.77
2	S	243	MET	SD-CE	5.52	2.08	1.77
2	V	238	CYS	CB-SG	5.14	1.91	1.82
2	R	243	MET	SD-CE	5.07	2.06	1.77

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	349	ARG	NE-CZ-NH1	-5.27	117.66	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2933	0	2982	129	0
1	B	2933	0	2982	163	0
1	C	2940	0	2989	177	0
1	D	2933	0	2982	144	0
1	E	2933	0	2982	142	0
1	F	2940	0	2989	162	0
1	G	2933	0	2982	129	0
1	H	2933	0	2982	144	0
1	I	2940	0	2989	150	0
1	J	2933	0	2982	152	0
1	K	2933	0	2982	130	0
1	L	2940	0	2989	133	0
2	M	1556	0	1514	40	0
2	N	1556	0	1515	59	0
2	O	1556	0	1513	65	0
2	P	1556	0	1513	55	0
2	Q	1556	0	1513	48	0
2	R	1556	0	1513	52	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	S	1556	0	1513	54	0
2	T	1556	0	1513	56	0
2	U	1556	0	1514	64	0
2	V	1556	0	1515	40	0
2	W	1556	0	1513	41	0
2	X	1556	0	1513	43	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
3	I	1	0	0	0	0
3	J	1	0	0	0	0
3	K	1	0	0	0	0
3	L	1	0	0	0	0
3	M	1	0	0	0	0
3	N	1	0	0	0	0
3	O	1	0	0	0	0
3	P	1	0	0	0	0
3	Q	1	0	0	0	0
3	R	1	0	0	0	0
3	S	1	0	0	0	0
3	T	1	0	0	0	0
3	U	1	0	0	0	0
3	V	1	0	0	0	0
3	W	1	0	0	0	0
3	X	1	0	0	0	0
All	All	53920	0	53974	2203	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 20.

All (2203) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:291:MET:SD	1:G:291:MET:CE	2.04	1.46
2:T:243:MET:CE	2:T:243:MET:SD	2.04	1.46
2:N:243:MET:SD	2:N:243:MET:CE	2.03	1.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:243:MET:CE	2:R:243:MET:SD	2.06	1.43
2:W:243:MET:CE	2:W:243:MET:SD	2.09	1.41
2:S:243:MET:CE	2:S:243:MET:SD	2.08	1.41
2:X:243:MET:SD	2:X:243:MET:CE	2.12	1.38
2:U:243:MET:CE	2:U:243:MET:SD	2.13	1.37
2:M:243:MET:SD	2:M:243:MET:CE	2.20	1.28
1:G:415:ASN:ND2	1:G:420:ARG:HD2	1.69	1.06
2:O:198:GLU:HB2	2:O:235:ASN:HD21	1.22	1.00
1:A:446:LYS:HG2	1:A:467:GLN:HE21	1.27	0.98
1:A:415:ASN:HD21	1:A:420:ARG:HH11	1.12	0.96
1:C:520:ILE:H	1:C:520:ILE:HD13	1.30	0.96
2:Q:158:ARG:HG3	2:Q:217:VAL:HG22	1.46	0.95
1:J:520:ILE:H	1:J:520:ILE:HD12	1.30	0.94
2:M:136:GLN:HB2	2:M:139:LYS:HG3	1.50	0.93
1:G:361:LEU:HD11	1:G:409:LEU:HD22	1.51	0.90
1:K:267:GLN:HE21	1:K:268:VAL:HG12	1.34	0.90
1:B:269:SER:HB3	1:B:323:ASN:HD21	1.32	0.90
2:O:136:GLN:HB2	2:O:139:LYS:HG3	1.53	0.90
1:G:349:ARG:HH21	1:H:286:LEU:HD12	1.35	0.90
1:B:269:SER:HB3	1:B:323:ASN:ND2	1.86	0.90
1:H:559:ARG:HD2	1:H:624:GLY:H	1.36	0.89
1:L:415:ASN:ND2	1:L:420:ARG:HD2	1.88	0.89
1:G:415:ASN:HD21	1:G:420:ARG:HD2	1.28	0.89
1:K:583:ARG:HD3	1:K:587:GLU:OE1	1.73	0.88
1:H:349:ARG:HH22	1:H:515:ASN:HD21	1.20	0.88
2:P:175:ARG:HD3	2:P:191:PRO:O	1.74	0.87
1:H:415:ASN:HD21	1:H:420:ARG:HH11	1.22	0.87
1:B:415:ASN:HD21	1:B:420:ARG:HH11	1.17	0.87
1:B:415:ASN:ND2	1:B:420:ARG:HD2	1.89	0.87
1:I:465:ILE:HD12	1:I:511:LYS:HE3	1.56	0.87
1:E:351:ASP:HB3	1:E:355:LEU:HD12	1.54	0.87
1:G:581:TRP:HE1	2:S:246:MET:HE3	1.40	0.87
1:E:454:LEU:HB3	1:F:453:PRO:HG2	1.55	0.87
1:I:454:LEU:HA	1:I:457:LEU:HG	1.55	0.87
1:F:579:LEU:HD23	1:F:583:ARG:HG3	1.57	0.86
1:J:361:LEU:HD11	1:J:409:LEU:HD22	1.55	0.86
1:F:478:THR:HG22	1:F:487:SER:HB2	1.58	0.86
1:G:514:LEU:HA	1:H:512:LYS:HG3	1.57	0.85
1:B:449:ASN:HD21	1:B:451:ASN:HB2	1.41	0.85
1:E:466:ASP:H	1:E:519:GLN:HE22	1.22	0.85
1:C:284:ASP:HB3	1:C:287:LEU:HB3	1.56	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:415:ASN:ND2	1:E:420:ARG:HD2	1.92	0.85
1:G:349:ARG:HH11	1:G:517:ARG:HD2	1.39	0.84
1:A:520:ILE:HD12	1:A:520:ILE:H	1.40	0.84
1:C:398:LEU:HB2	1:C:401:MET:HE2	1.59	0.83
1:G:454:LEU:HA	1:G:457:LEU:HB2	1.60	0.83
1:F:385:GLU:HA	1:F:607:PHE:HZ	1.41	0.83
1:L:520:ILE:HD12	1:L:520:ILE:H	1.43	0.83
1:K:269:SER:H	1:K:323:ASN:HD21	1.21	0.83
1:J:408:PHE:CE1	1:J:525:ILE:HD11	2.14	0.83
1:H:608:SER:HB3	1:H:611:VAL:HG23	1.60	0.83
1:D:415:ASN:HD21	1:D:420:ARG:HH11	1.26	0.82
2:S:136:GLN:HB2	2:S:139:LYS:HG3	1.59	0.82
1:B:303:LEU:H	1:B:303:LEU:HD23	1.43	0.82
1:J:454:LEU:HB2	1:K:453:PRO:HG2	1.61	0.82
1:F:383:ASP:HB3	1:F:386:GLU:HG3	1.60	0.82
1:F:469:LEU:HD12	1:F:470:VAL:N	1.94	0.82
2:U:258:GLU:HA	2:U:265:LEU:HG	1.61	0.82
2:U:161:ALA:HB2	2:U:195:ILE:HD11	1.61	0.81
1:F:408:PHE:CE1	1:F:525:ILE:HD11	2.16	0.81
1:E:434:THR:HG23	1:E:570:GLN:HB3	1.63	0.81
1:I:517:ARG:HH12	1:J:286:LEU:HD12	1.45	0.80
1:K:415:ASN:HD21	1:K:420:ARG:HH11	1.29	0.80
1:G:349:ARG:NH1	1:G:517:ARG:HD2	1.96	0.80
1:A:428:ILE:H	1:A:428:ILE:HD12	1.46	0.80
1:B:302:CYS:O	1:B:306:ILE:HG13	1.80	0.80
2:T:136:GLN:HB2	2:T:139:LYS:HG3	1.63	0.80
1:G:465:ILE:HD12	1:G:511:LYS:HD2	1.64	0.80
2:R:175:ARG:HD3	2:R:191:PRO:O	1.83	0.79
1:A:415:ASN:ND2	1:A:420:ARG:HG2	1.98	0.79
1:E:451:ASN:HD21	1:E:476:LYS:H	1.31	0.79
1:A:415:ASN:HD21	1:A:420:ARG:NH1	1.80	0.78
1:H:454:LEU:HA	1:H:457:LEU:HB2	1.64	0.78
1:H:369:LEU:HD13	1:H:595:ARG:HD3	1.65	0.78
1:C:454:LEU:HB3	1:C:457:LEU:HD12	1.64	0.78
2:M:161:ALA:HB2	2:M:195:ILE:HD11	1.63	0.78
1:E:361:LEU:HD11	1:E:409:LEU:HD22	1.66	0.78
2:U:158:ARG:HH11	2:U:158:ARG:HB2	1.49	0.77
1:I:415:ASN:ND2	1:I:420:ARG:HD2	1.99	0.77
2:W:136:GLN:HB2	2:W:139:LYS:HG3	1.65	0.77
2:U:118:THR:HG22	2:U:282:ARG:HD3	1.66	0.77
2:X:175:ARG:HD3	2:X:191:PRO:O	1.83	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:466:ASP:H	1:E:519:GLN:NE2	1.83	0.77
1:H:559:ARG:HD2	1:H:624:GLY:N	2.00	0.77
1:H:415:ASN:ND2	1:H:420:ARG:HD2	1.99	0.76
1:K:434:THR:HG23	1:K:570:GLN:HB3	1.67	0.76
1:E:428:ILE:HD12	1:E:428:ILE:H	1.48	0.76
1:K:283:ASP:HA	1:K:341:VAL:HG13	1.66	0.76
1:I:623:ILE:HG22	1:I:624:GLY:H	1.49	0.76
1:A:415:ASN:HD22	1:A:420:ARG:HG2	1.50	0.76
1:K:466:ASP:H	1:K:519:GLN:NE2	1.84	0.76
1:E:520:ILE:HD12	1:F:567:ARG:HH12	1.51	0.76
2:O:198:GLU:HB2	2:O:235:ASN:ND2	1.99	0.76
1:D:285:VAL:HG21	1:D:338:GLN:NE2	2.01	0.76
1:A:434:THR:HG23	1:A:570:GLN:HG2	1.68	0.76
2:U:198:GLU:HB2	2:U:235:ASN:HD21	1.51	0.76
1:H:398:LEU:HD21	1:H:545:ILE:HG21	1.68	0.75
2:P:161:ALA:HB2	2:P:195:ILE:HD11	1.68	0.75
1:E:349:ARG:HH22	1:E:515:ASN:HD21	1.33	0.75
1:H:293:LEU:O	1:H:296:GLN:HG2	1.87	0.75
1:E:424:PHE:HB2	1:E:527:THR:HG22	1.69	0.75
2:Q:147:VAL:HG21	2:Q:151:PRO:HD3	1.67	0.75
1:G:453:PRO:HG2	1:L:454:LEU:HB2	1.68	0.75
1:I:418:LYS:HE3	1:I:540:ARG:HH12	1.51	0.75
1:J:584:PRO:HG2	1:J:587:GLU:HG3	1.68	0.74
1:C:409:LEU:O	1:C:413:VAL:HG23	1.87	0.74
1:F:349:ARG:CZ	1:F:517:ARG:HD3	2.16	0.74
2:Q:175:ARG:HH21	2:Q:179:HIS:HB3	1.51	0.74
1:C:451:ASN:HD21	1:C:475:VAL:HA	1.51	0.74
1:J:502:ASP:OD2	1:J:540:ARG:HD2	1.86	0.74
1:G:454:LEU:HB2	1:H:453:PRO:HG2	1.68	0.74
1:K:466:ASP:H	1:K:519:GLN:HE22	1.33	0.74
1:J:403:SER:HA	1:J:583:ARG:HH21	1.53	0.74
1:K:454:LEU:H	1:K:454:LEU:HD22	1.53	0.74
1:L:415:ASN:HD21	1:L:420:ARG:HD2	1.50	0.74
2:V:136:GLN:HB2	2:V:139:LYS:HG3	1.69	0.74
1:L:349:ARG:CZ	1:L:517:ARG:HD3	2.17	0.74
1:C:371:ARG:O	1:C:375:MET:HB2	1.88	0.73
1:A:355:LEU:HD22	1:A:359:GLN:HG2	1.70	0.73
1:J:420:ARG:HB3	1:J:523:PRO:HB3	1.70	0.73
1:L:389:ALA:HB1	1:L:625:VAL:HG21	1.69	0.73
1:D:599:TRP:O	1:D:603:LEU:HB2	1.88	0.73
1:C:608:SER:HB2	2:O:280:ARG:HD2	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:609:LEU:HG	2:W:246:MET:HE2	1.71	0.73
1:C:454:LEU:HA	1:C:457:LEU:HB2	1.70	0.73
1:H:470:VAL:O	1:H:524:GLY:HA3	1.89	0.73
1:E:331:LYS:N	1:E:331:LYS:HD2	2.04	0.73
1:K:446:LYS:HG2	1:K:467:GLN:OE1	1.89	0.73
2:R:191:PRO:HG2	2:R:192:GLN:HE21	1.54	0.73
2:T:118:THR:HG22	2:T:282:ARG:HD3	1.70	0.73
1:C:349:ARG:NH1	1:C:517:ARG:HD2	2.03	0.73
1:B:495:ASP:O	1:B:498:ARG:HG3	1.89	0.72
2:Q:158:ARG:HH21	2:Q:206:LEU:HD22	1.53	0.72
1:I:372:MET:HA	1:I:375:MET:HG2	1.69	0.72
1:I:349:ARG:HD2	1:I:517:ARG:CZ	2.20	0.72
1:J:402:ASP:HA	1:J:578:MET:HE3	1.70	0.72
1:E:415:ASN:HD21	1:E:420:ARG:HD2	1.54	0.72
1:J:401:MET:HG3	1:J:578:MET:HE1	1.72	0.72
1:C:420:ARG:HB3	1:C:523:PRO:HB3	1.70	0.72
2:N:158:ARG:HG3	2:N:217:VAL:HG22	1.72	0.72
2:X:136:GLN:HB2	2:X:139:LYS:HG3	1.70	0.72
1:L:415:ASN:HD21	1:L:420:ARG:HH11	1.35	0.71
1:J:454:LEU:HA	1:J:457:LEU:HB2	1.72	0.71
1:H:498:ARG:HB3	1:H:540:ARG:HH21	1.55	0.71
2:Q:136:GLN:HB2	2:Q:139:LYS:HG3	1.72	0.71
1:I:470:VAL:HG23	1:I:522:PRO:HG2	1.70	0.71
1:D:550:LYS:HB2	1:D:553:LEU:HD12	1.71	0.71
1:B:424:PHE:HB2	1:B:527:THR:HG22	1.72	0.71
1:B:417:PRO:HG3	1:C:567:ARG:HH21	1.54	0.71
1:A:453:PRO:HG3	1:F:454:LEU:HB3	1.72	0.71
1:I:357:ARG:HD3	1:I:413:VAL:O	1.91	0.70
1:C:498:ARG:NH2	1:D:476:LYS:HD3	2.06	0.70
1:B:351:ASP:OD2	1:B:355:LEU:HD11	1.92	0.70
1:L:619:VAL:HG22	1:L:625:VAL:HG12	1.73	0.70
1:L:268:VAL:HG11	1:L:327:PHE:HA	1.72	0.70
1:A:415:ASN:ND2	1:A:420:ARG:HH11	1.86	0.70
2:W:190:PRO:HB2	2:W:193:HIS:HD2	1.56	0.70
1:F:590:GLN:HA	1:F:593:GLN:HG3	1.70	0.70
1:G:469:LEU:C	1:G:469:LEU:HD12	2.12	0.70
1:C:495:ASP:O	1:C:498:ARG:HG3	1.92	0.70
2:N:190:PRO:HB2	2:N:193:HIS:HD2	1.57	0.70
1:J:520:ILE:CD1	1:J:520:ILE:H	2.03	0.70
1:E:491:ILE:O	1:E:491:ILE:HD13	1.92	0.70
1:B:415:ASN:HD21	1:B:420:ARG:HD2	1.53	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:414:TYR:HB3	1:G:416:ILE:HD11	1.74	0.70
1:L:623:ILE:HG22	1:L:624:GLY:H	1.55	0.69
1:H:432:LYS:CE	1:H:433:THR:H	2.05	0.69
2:V:147:VAL:HG21	2:V:151:PRO:HD3	1.74	0.69
1:F:608:SER:HB3	1:F:611:VAL:HG23	1.73	0.69
1:G:327:PHE:CZ	1:G:333:GLN:HB3	2.27	0.69
2:V:161:ALA:HB2	2:V:195:ILE:HD11	1.74	0.69
2:N:136:GLN:HB2	2:N:139:LYS:HG3	1.73	0.69
1:H:443:CYS:HB2	1:H:469:LEU:HD23	1.74	0.69
1:I:550:LYS:HB2	1:I:553:LEU:HD12	1.75	0.69
1:B:608:SER:HB2	2:N:280:ARG:NH1	2.07	0.69
1:L:590:GLN:NE2	1:L:590:GLN:H	1.90	0.69
1:K:491:ILE:HG22	1:K:492:ASN:HD22	1.58	0.69
1:J:415:ASN:HD21	1:J:420:ARG:HH11	1.41	0.68
1:G:476:LYS:HE2	1:L:496:ASN:ND2	2.08	0.68
1:C:273:VAL:HG22	1:C:292:TYR:CE2	2.28	0.68
1:G:409:LEU:O	1:G:413:VAL:HG23	1.93	0.68
1:D:470:VAL:HG23	1:D:522:PRO:HB2	1.74	0.68
1:G:415:ASN:HD21	1:G:420:ARG:HH11	1.42	0.68
1:C:465:ILE:HG23	1:C:517:ARG:HG2	1.74	0.68
1:J:434:THR:HG23	1:J:570:GLN:HB3	1.74	0.68
1:B:499:ASP:HB3	1:C:473:GLU:HG2	1.75	0.68
1:D:346:ALA:O	1:D:350:VAL:HG23	1.94	0.68
1:K:434:THR:HG21	1:K:569:ILE:HG12	1.75	0.68
1:C:375:MET:HE2	1:C:382:ALA:HB1	1.76	0.68
1:F:623:ILE:HG22	1:F:624:GLY:H	1.59	0.68
1:B:398:LEU:HD21	1:B:545:ILE:HG21	1.75	0.68
1:E:337:CYS:O	1:E:341:VAL:HG23	1.94	0.68
1:K:512:LYS:HG3	1:K:513:HIS:H	1.57	0.68
1:H:584:PRO:HD2	1:H:587:GLU:HG3	1.75	0.68
1:G:454:LEU:HD12	1:G:454:LEU:H	1.59	0.68
1:G:445:GLY:O	1:G:446:LYS:HG2	1.94	0.68
1:A:285:VAL:HG21	1:A:338:GLN:HE21	1.59	0.67
1:K:346:ALA:HB2	1:L:289:LEU:HD23	1.75	0.67
1:H:420:ARG:HB3	1:H:523:PRO:HB3	1.76	0.67
1:J:557:LEU:HD23	1:J:564:LEU:HD11	1.77	0.67
2:O:175:ARG:HD3	2:O:191:PRO:O	1.94	0.67
1:K:415:ASN:ND2	1:K:420:ARG:HD2	2.10	0.67
1:D:583:ARG:HD3	1:D:587:GLU:OE1	1.95	0.67
1:G:475:VAL:HG12	1:G:491:ILE:HD12	1.75	0.67
1:H:412:MET:CE	1:H:469:LEU:HB2	2.25	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:514:LEU:HD23	1:A:515:ASN:H	1.60	0.67
1:I:402:ASP:HA	1:I:578:MET:HE1	1.77	0.67
1:J:337:CYS:O	1:J:341:VAL:HG23	1.94	0.67
1:A:584:PRO:HG2	1:A:587:GLU:HG3	1.77	0.67
1:I:349:ARG:HD2	1:I:517:ARG:NH1	2.10	0.67
1:C:525:ILE:HG22	1:C:526:VAL:N	2.10	0.67
1:K:409:LEU:O	1:K:413:VAL:HG23	1.94	0.67
1:D:609:LEU:HD22	2:P:246:MET:HE1	1.75	0.67
1:G:420:ARG:HB3	1:G:523:PRO:HB3	1.76	0.67
2:V:190:PRO:HB2	2:V:193:HIS:HD2	1.60	0.67
2:P:119:ALA:O	2:P:279:GLY:HA3	1.95	0.67
2:O:147:VAL:HG21	2:O:151:PRO:HD3	1.77	0.67
1:L:349:ARG:HD3	1:L:517:ARG:NH1	2.10	0.66
1:F:520:ILE:HD12	1:F:520:ILE:H	1.59	0.66
1:B:283:ASP:HA	1:B:341:VAL:HG13	1.76	0.66
2:V:179:HIS:HA	2:V:182:CYS:SG	2.34	0.66
1:J:372:MET:HA	1:J:375:MET:HG2	1.77	0.66
1:H:440:LEU:HD13	1:H:471:VAL:HG23	1.77	0.66
1:I:470:VAL:O	1:I:524:GLY:HA3	1.96	0.66
1:I:357:ARG:HH11	1:I:357:ARG:HG2	1.61	0.66
1:L:454:LEU:HA	1:L:457:LEU:HB2	1.76	0.66
2:R:264:LEU:HD11	2:R:267:ARG:HB2	1.77	0.66
2:S:161:ALA:HB2	2:S:195:ILE:HD11	1.77	0.66
2:X:244:GLY:O	2:X:246:MET:N	2.29	0.66
1:K:383:ASP:HB3	1:K:386:GLU:HG3	1.76	0.66
1:B:369:LEU:HB2	1:B:595:ARG:HH11	1.60	0.66
1:C:516:LYS:O	1:C:517:ARG:HD3	1.96	0.66
1:H:349:ARG:HH22	1:H:515:ASN:ND2	1.94	0.66
1:B:520:ILE:CD1	1:C:567:ARG:HH12	2.07	0.66
1:L:270:TRP:CE2	1:L:336:ILE:HG12	2.30	0.66
1:H:281:LYS:HE2	1:H:281:LYS:HA	1.76	0.66
1:B:303:LEU:HA	1:B:306:ILE:HD11	1.77	0.66
2:T:161:ALA:HB2	2:T:195:ILE:HD11	1.77	0.66
1:L:383:ASP:HB3	1:L:386:GLU:HG3	1.78	0.66
1:F:599:TRP:O	1:F:603:LEU:HD12	1.96	0.66
1:A:285:VAL:HG21	1:A:338:GLN:NE2	2.11	0.65
1:I:402:ASP:HA	1:I:578:MET:CE	2.26	0.65
1:D:375:MET:O	1:D:382:ALA:HB3	1.96	0.65
2:R:176:CYS:SG	2:R:179:HIS:HB2	2.37	0.65
1:A:346:ALA:O	1:A:350:VAL:HG23	1.97	0.65
1:E:454:LEU:HB3	1:F:453:PRO:CG	2.25	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:576:LEU:O	1:J:580:ILE:HG12	1.96	0.65
2:U:136:GLN:HB2	2:U:139:LYS:HG3	1.79	0.65
1:L:498:ARG:HB3	1:L:540:ARG:HH12	1.61	0.65
1:D:316:TYR:HB3	1:D:320:HIS:HD2	1.62	0.65
1:H:402:ASP:HA	1:H:578:MET:HE3	1.78	0.65
2:R:147:VAL:HG21	2:R:151:PRO:HD3	1.77	0.65
1:E:593:GLN:O	1:E:597:VAL:HG23	1.97	0.65
2:T:158:ARG:HB2	2:T:158:ARG:HH11	1.60	0.65
2:O:108:GLY:HA3	2:O:148:ASP:OD2	1.97	0.65
2:T:239:ASN:HA	2:T:274:VAL:HB	1.78	0.65
1:B:349:ARG:HH11	1:B:349:ARG:HG2	1.61	0.65
2:V:158:ARG:HB2	2:V:158:ARG:HH11	1.62	0.65
2:U:175:ARG:HD3	2:U:191:PRO:O	1.97	0.65
1:C:454:LEU:HB2	1:D:453:PRO:HG2	1.79	0.65
1:E:428:ILE:HD12	1:E:428:ILE:N	2.12	0.64
1:L:454:LEU:HD12	1:L:454:LEU:H	1.61	0.64
1:B:454:LEU:HB2	1:C:453:PRO:HG2	1.79	0.64
1:B:412:MET:HE1	1:B:524:GLY:N	2.13	0.64
1:H:498:ARG:HB3	1:H:540:ARG:NH2	2.13	0.64
1:H:356:THR:HG22	1:H:359:GLN:OE1	1.97	0.64
1:J:408:PHE:HE1	1:J:525:ILE:HD11	1.62	0.64
2:T:259:ASP:OD2	2:T:263:ASN:HB2	1.98	0.64
1:L:583:ARG:NE	1:L:583:ARG:HA	2.12	0.64
1:E:451:ASN:ND2	1:E:476:LYS:H	1.95	0.64
2:P:137:LEU:O	2:P:139:LYS:HG2	1.98	0.64
1:I:458:ASN:HD22	1:J:456:ARG:NE	1.96	0.64
1:D:454:LEU:H	1:D:454:LEU:HD12	1.62	0.64
1:C:303:LEU:H	1:C:303:LEU:HD23	1.62	0.64
1:C:349:ARG:HH11	1:C:517:ARG:HD2	1.62	0.64
1:E:394:LEU:HD21	1:E:569:ILE:O	1.98	0.64
1:H:517:ARG:HG3	1:H:519:GLN:HG2	1.79	0.64
1:L:301:MET:O	1:L:303:LEU:HD22	1.97	0.64
1:H:283:ASP:HA	1:H:341:VAL:HG13	1.80	0.64
1:K:267:GLN:NE2	1:K:268:VAL:HG12	2.10	0.64
1:A:299:PHE:HB3	1:A:317:HIS:CD2	2.33	0.64
1:F:447:ALA:C	1:F:448:LEU:HD23	2.18	0.64
1:A:454:LEU:HA	1:A:457:LEU:HB2	1.79	0.64
1:J:423:LEU:HD23	1:J:544:GLN:HG3	1.79	0.64
2:Q:175:ARG:NH2	2:Q:179:HIS:HB3	2.13	0.64
1:C:293:LEU:O	1:C:296:GLN:HB3	1.98	0.64
1:J:389:ALA:HB1	1:J:625:VAL:HG21	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:590:GLN:HA	1:K:593:GLN:HG3	1.80	0.64
1:E:349:ARG:HH22	1:E:515:ASN:ND2	1.95	0.64
1:H:608:SER:HB3	1:H:611:VAL:CG2	2.26	0.63
1:I:498:ARG:NH2	1:J:476:LYS:HD3	2.13	0.63
1:B:434:THR:HG23	1:B:570:GLN:HB3	1.79	0.63
1:G:514:LEU:HD23	1:G:515:ASN:N	2.13	0.63
1:K:609:LEU:HD11	2:W:247:ASN:HB2	1.80	0.63
2:S:156:ARG:HB3	2:S:217:VAL:HG12	1.80	0.63
1:J:356:THR:O	1:J:360:MET:HG3	1.99	0.63
2:O:190:PRO:HB2	2:O:193:HIS:HD2	1.64	0.63
1:A:446:LYS:HG2	1:A:467:GLN:NE2	2.08	0.63
1:D:420:ARG:HG2	1:D:523:PRO:HB3	1.80	0.63
1:B:608:SER:HB2	2:N:280:ARG:HH11	1.63	0.63
1:I:535:LYS:HE2	1:J:428:ILE:HD12	1.80	0.63
2:P:259:ASP:OD2	2:P:263:ASN:HB2	1.98	0.63
1:B:576:LEU:O	1:B:580:ILE:HG12	1.99	0.63
1:B:569:ILE:H	1:B:569:ILE:HD13	1.64	0.63
1:F:303:LEU:H	1:F:303:LEU:HD22	1.64	0.63
1:B:421:TYR:CE1	1:B:523:PRO:HA	2.34	0.63
2:U:198:GLU:HB2	2:U:235:ASN:ND2	2.13	0.63
1:A:398:LEU:HB2	1:A:401:MET:CE	2.29	0.63
2:S:179:HIS:ND1	2:S:238:CYS:HA	2.14	0.63
2:X:197:VAL:HG11	2:X:218:VAL:HG11	1.81	0.62
1:B:272:LEU:HD23	1:B:323:ASN:HD22	1.64	0.62
1:D:405:VAL:HG21	1:D:575:LEU:HD22	1.81	0.62
2:N:161:ALA:HB2	2:N:195:ILE:HD11	1.81	0.62
1:C:376:PHE:CE1	1:C:384:ILE:HA	2.34	0.62
2:V:236:TYR:CE2	2:V:272:VAL:HG11	2.35	0.62
2:M:243:MET:HB2	2:M:243:MET:CE	2.29	0.62
1:A:372:MET:HA	1:A:375:MET:HG2	1.80	0.62
2:T:132:LYS:HE2	2:T:273:ARG:HB2	1.80	0.62
1:E:609:LEU:HG	2:Q:246:MET:HE2	1.81	0.62
1:E:284:ASP:HB3	1:E:287:LEU:HB3	1.82	0.62
1:B:350:VAL:HG21	1:C:290:GLY:HA3	1.81	0.62
1:F:576:LEU:O	1:F:580:ILE:HG12	1.99	0.62
2:S:175:ARG:NE	2:S:237:MET:HB2	2.15	0.62
2:T:244:GLY:O	2:T:246:MET:N	2.33	0.62
2:U:193:HIS:HE1	2:U:215:SER:H	1.48	0.62
1:E:465:ILE:HD11	1:E:509:LEU:HB2	1.80	0.62
1:I:516:LYS:O	1:I:517:ARG:HD3	2.00	0.62
2:X:243:MET:CE	2:X:243:MET:HB2	2.30	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:386:GLU:O	1:J:389:ALA:HB3	2.00	0.61
2:N:239:ASN:HA	2:N:274:VAL:HB	1.81	0.61
1:G:481:GLU:H	1:G:481:GLU:CD	2.02	0.61
1:J:415:ASN:ND2	1:J:420:ARG:HG2	2.14	0.61
1:C:500:TYR:CZ	1:C:507:VAL:HG11	2.35	0.61
1:K:289:LEU:HD11	1:K:333:GLN:HB3	1.82	0.61
1:B:389:ALA:HB1	1:B:625:VAL:HG21	1.82	0.61
1:C:434:THR:HG23	1:C:570:GLN:HB3	1.82	0.61
1:I:303:LEU:H	1:I:303:LEU:HD23	1.64	0.61
1:E:283:ASP:HA	1:E:341:VAL:HG13	1.81	0.61
2:S:103:TYR:CZ	2:S:105:GLY:HA2	2.36	0.61
1:B:332:ASN:O	1:B:336:ILE:HG13	2.00	0.61
1:B:454:LEU:HD12	1:B:454:LEU:N	2.16	0.61
1:I:303:LEU:O	1:I:306:ILE:HG22	2.00	0.61
1:J:579:LEU:C	1:J:581:TRP:H	2.02	0.61
2:P:198:GLU:HB2	2:P:235:ASN:HD21	1.65	0.61
1:L:361:LEU:HD11	1:L:409:LEU:HD22	1.82	0.61
1:J:369:LEU:HB2	1:J:595:ARG:NH1	2.16	0.61
1:H:402:ASP:HA	1:H:578:MET:CE	2.31	0.61
1:F:463:VAL:O	1:F:463:VAL:HG12	1.99	0.61
1:G:438:ALA:HA	1:G:570:GLN:O	2.00	0.61
1:E:481:GLU:H	1:E:481:GLU:CD	2.03	0.61
1:H:459:PHE:CE2	1:H:512:LYS:HD3	2.35	0.61
1:B:520:ILE:HD13	1:C:567:ARG:HH12	1.66	0.61
1:B:284:ASP:HB3	1:B:287:LEU:HB2	1.83	0.61
2:R:158:ARG:HB2	2:R:158:ARG:HH11	1.66	0.61
1:I:554:LYS:O	1:I:558:GLU:HG3	2.01	0.61
2:U:99:SER:HB2	2:U:101:LYS:HG2	1.83	0.61
1:L:520:ILE:N	1:L:520:ILE:HD12	2.14	0.61
1:I:418:LYS:HE3	1:I:540:ARG:NH1	2.15	0.61
1:L:389:ALA:HB1	1:L:625:VAL:CG2	2.31	0.61
2:O:191:PRO:HG2	2:O:192:GLN:HE21	1.65	0.61
1:D:589:ALA:O	1:D:592:ILE:HG22	2.01	0.61
2:R:137:LEU:O	2:R:139:LYS:HG2	2.01	0.61
1:B:372:MET:HE3	1:B:577:LEU:HG	1.83	0.61
2:R:244:GLY:O	2:R:246:MET:N	2.33	0.61
2:U:239:ASN:HA	2:U:274:VAL:HB	1.82	0.60
2:T:175:ARG:HD3	2:T:191:PRO:O	2.01	0.60
1:D:415:ASN:HD22	1:D:523:PRO:HG3	1.66	0.60
1:I:420:ARG:NH2	1:I:521:PHE:O	2.31	0.60
1:E:349:ARG:NH2	1:E:515:ASN:HD21	1.99	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:118:THR:HG22	2:Q:282:ARG:HD3	1.83	0.60
1:J:480:GLY:HA2	1:J:483:ARG:NH2	2.15	0.60
2:P:118:THR:HG22	2:P:282:ARG:HD3	1.82	0.60
1:A:470:VAL:O	1:A:524:GLY:HA3	2.01	0.60
2:X:107:TYR:O	2:X:147:VAL:HG23	2.01	0.60
1:B:272:LEU:HD23	1:B:323:ASN:ND2	2.16	0.60
2:Q:190:PRO:HB2	2:Q:193:HIS:HD2	1.66	0.60
1:F:415:ASN:HD21	1:F:420:ARG:HH11	1.48	0.60
1:K:440:LEU:HD22	1:K:471:VAL:HG21	1.83	0.60
1:C:398:LEU:CB	1:C:401:MET:HE2	2.32	0.60
1:K:420:ARG:HB3	1:K:523:PRO:HB3	1.83	0.60
2:N:175:ARG:HD3	2:N:191:PRO:O	2.01	0.60
1:F:303:LEU:HA	1:F:306:ILE:HG22	1.82	0.60
1:J:458:ASN:HB3	1:J:510:GLU:OE2	2.01	0.60
2:S:243:MET:CE	2:S:243:MET:HB2	2.31	0.60
2:P:136:GLN:HB2	2:P:139:LYS:HG3	1.83	0.60
1:C:593:GLN:O	1:C:597:VAL:HG23	2.01	0.60
1:I:614:LYS:O	1:I:617:PHE:HB3	2.02	0.60
1:I:346:ALA:HB2	1:J:289:LEU:HD23	1.84	0.60
2:Q:132:LYS:HD3	2:Q:134:PHE:CZ	2.36	0.60
1:I:563:LEU:HD11	1:I:625:VAL:HG21	1.84	0.60
1:F:358:GLU:HG2	1:F:413:VAL:HG11	1.84	0.60
2:Q:107:TYR:O	2:Q:147:VAL:HG23	2.02	0.60
1:B:564:LEU:HD23	1:B:569:ILE:HD11	1.82	0.60
1:J:583:ARG:HD2	1:J:587:GLU:OE1	2.02	0.60
2:S:158:ARG:HH11	2:S:158:ARG:HB2	1.67	0.60
1:C:584:PRO:HB3	2:O:243:MET:HA	1.83	0.60
1:K:529:ASN:O	1:K:530:GLU:HB3	2.02	0.60
1:A:418:LYS:NZ	1:A:540:ARG:HD3	2.16	0.60
1:G:299:PHE:HD2	1:G:299:PHE:H	1.50	0.60
2:Q:244:GLY:HA3	2:Q:248:ARG:HB2	1.83	0.60
1:B:456:ARG:HH21	1:B:512:LYS:HZ3	1.50	0.60
1:J:446:LYS:HG2	1:J:467:GLN:NE2	2.17	0.60
1:J:550:LYS:HB2	1:J:553:LEU:HD12	1.83	0.59
2:R:145:LEU:HD21	2:R:157:VAL:HG11	1.84	0.59
1:F:289:LEU:O	1:F:293:LEU:HG	2.02	0.59
1:I:285:VAL:HG22	1:I:341:VAL:HG21	1.83	0.59
1:E:401:MET:O	1:E:405:VAL:HG23	2.02	0.59
1:C:470:VAL:O	1:C:524:GLY:HA3	2.02	0.59
1:I:391:VAL:HG13	1:I:578:MET:HG3	1.84	0.59
1:J:369:LEU:HB2	1:J:595:ARG:HH11	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:160:MET:SD	2:R:213:ARG:HG2	2.41	0.59
1:H:285:VAL:HG21	1:H:338:GLN:NE2	2.18	0.59
1:A:420:ARG:HB3	1:A:523:PRO:HB3	1.85	0.59
1:C:520:ILE:H	1:C:520:ILE:CD1	2.05	0.59
2:M:137:LEU:O	2:M:139:LYS:HG2	2.03	0.59
1:D:354:GLN:CG	1:E:310:GLN:HE21	2.16	0.59
1:G:356:THR:OG1	1:G:359:GLN:HG3	2.03	0.59
1:G:520:ILE:HD12	1:G:520:ILE:H	1.64	0.59
1:K:410:LYS:HA	1:K:410:LYS:HE3	1.83	0.59
2:M:198:GLU:HB2	2:M:235:ASN:ND2	2.18	0.59
1:K:268:VAL:N	1:K:326:ILE:HG21	2.17	0.59
1:C:477:GLY:HA3	1:C:491:ILE:HD12	1.83	0.59
1:E:465:ILE:HD12	1:E:517:ARG:HB3	1.84	0.59
1:F:303:LEU:N	1:F:303:LEU:HD22	2.17	0.59
1:B:287:LEU:HD22	1:B:291:MET:HG3	1.84	0.59
1:A:609:LEU:O	1:A:613:GLN:HB2	2.03	0.59
1:C:400:LYS:O	1:C:404:VAL:HG23	2.02	0.59
2:U:147:VAL:HG21	2:U:151:PRO:HD3	1.85	0.59
1:H:372:MET:SD	1:H:576:LEU:HD23	2.42	0.59
2:M:147:VAL:HG21	2:M:151:PRO:HD3	1.84	0.59
1:J:344:VAL:O	1:J:348:LYS:HG2	2.02	0.59
1:I:337:CYS:O	1:I:341:VAL:HG23	2.02	0.59
1:H:469:LEU:HD12	1:H:470:VAL:N	2.17	0.58
1:B:356:THR:O	1:B:360:MET:HG3	2.03	0.58
2:X:132:LYS:HE3	2:X:271:GLU:OE2	2.01	0.58
1:D:592:ILE:O	1:D:596:ILE:HG12	2.03	0.58
1:C:590:GLN:HA	1:C:593:GLN:HG3	1.85	0.58
1:D:443:CYS:HB3	1:D:468:PHE:CD2	2.38	0.58
1:A:476:LYS:HB3	1:A:488:GLY:HA3	1.85	0.58
1:G:414:TYR:HB3	1:G:416:ILE:CD1	2.33	0.58
1:K:623:ILE:HD11	1:K:627:ASP:OD2	2.02	0.58
2:U:159:ALA:HB2	2:U:234:TYR:OH	2.03	0.58
1:K:608:SER:HB2	2:W:280:ARG:HH11	1.69	0.58
1:I:608:SER:HB2	2:U:280:ARG:NH1	2.17	0.58
2:S:122:VAL:HG12	2:S:123:THR:N	2.18	0.58
1:F:525:ILE:HG22	1:F:526:VAL:N	2.18	0.58
1:K:454:LEU:H	1:K:454:LEU:CD2	2.16	0.58
1:L:615:MET:O	1:L:619:VAL:HG23	2.02	0.58
1:C:473:GLU:HG3	1:C:474:ASP:H	1.68	0.58
1:B:584:PRO:HD2	1:B:587:GLU:HG3	1.85	0.58
1:F:614:LYS:O	1:F:617:PHE:HB3	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:274:THR:HG23	1:A:340:ALA:HA	1.84	0.58
1:A:273:VAL:HG22	1:A:292:TYR:CZ	2.38	0.58
1:B:415:ASN:HD21	1:B:420:ARG:NH1	1.95	0.58
1:B:417:PRO:HG3	1:C:567:ARG:NH2	2.17	0.58
1:F:617:PHE:O	1:F:621:MET:HG2	2.02	0.58
1:C:345:LEU:O	1:C:348:LYS:HB2	2.04	0.58
1:I:356:THR:OG1	1:I:359:GLN:HB2	2.03	0.58
2:V:158:ARG:HB3	2:V:256:THR:HB	1.85	0.58
1:A:451:ASN:HB3	1:F:496:ASN:ND2	2.19	0.58
2:V:175:ARG:HD3	2:V:191:PRO:O	2.03	0.58
1:A:385:GLU:HG2	1:A:626:LEU:HD21	1.86	0.58
1:J:552:TYR:HB2	1:J:619:VAL:O	2.04	0.58
1:B:495:ASP:HB3	1:C:476:LYS:HZ2	1.69	0.58
1:H:432:LYS:CD	1:H:433:THR:H	2.17	0.58
1:L:579:LEU:HD22	1:L:583:ARG:HG3	1.86	0.58
1:H:559:ARG:NH1	1:H:623:ILE:HA	2.18	0.58
1:C:415:ASN:ND2	1:C:420:ARG:HD2	2.17	0.58
1:B:369:LEU:HD23	1:B:372:MET:SD	2.44	0.58
1:I:434:THR:HG23	1:I:570:GLN:HB3	1.85	0.58
1:E:612:TYR:HA	1:E:615:MET:HE2	1.85	0.58
2:V:142:PRO:HA	2:V:232:ILE:O	2.04	0.58
1:B:435:LEU:HD23	1:B:547:PHE:HZ	1.68	0.58
1:K:512:LYS:HG3	1:K:513:HIS:N	2.18	0.58
1:L:583:ARG:HD3	1:L:587:GLU:OE1	2.04	0.58
1:A:439:LEU:O	1:A:442:LEU:HB3	2.04	0.58
2:P:158:ARG:HH11	2:P:158:ARG:HB2	1.67	0.58
1:K:454:LEU:CB	1:L:453:PRO:HG2	2.34	0.58
1:C:473:GLU:HG3	1:C:474:ASP:N	2.19	0.58
1:J:357:ARG:HA	1:J:360:MET:HE1	1.86	0.58
1:J:615:MET:O	1:J:619:VAL:HG23	2.04	0.58
1:D:466:ASP:H	1:D:519:GLN:HE22	1.52	0.58
1:D:268:VAL:HG11	1:D:327:PHE:HA	1.85	0.58
1:J:608:SER:OG	1:J:611:VAL:HG23	2.04	0.57
1:G:349:ARG:NH2	1:H:286:LEU:HD12	2.12	0.57
1:L:415:ASN:HD21	1:L:420:ARG:NH1	2.01	0.57
1:K:454:LEU:HD11	1:K:493:ASN:ND2	2.19	0.57
1:A:469:LEU:HD12	1:A:469:LEU:C	2.25	0.57
1:C:349:ARG:HD2	1:C:517:ARG:CZ	2.33	0.57
1:E:612:TYR:HA	1:E:615:MET:CE	2.34	0.57
2:S:175:ARG:HD3	2:S:191:PRO:O	2.04	0.57
2:R:158:ARG:HG3	2:R:217:VAL:HG22	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:451:ASN:HD21	1:K:476:LYS:H	1.51	0.57
1:K:369:LEU:HB2	1:K:595:ARG:HH11	1.69	0.57
2:N:118:THR:HG22	2:N:282:ARG:HD3	1.87	0.57
2:N:158:ARG:HH21	2:N:206:LEU:CD2	2.18	0.57
2:P:244:GLY:O	2:P:246:MET:N	2.37	0.57
1:J:383:ASP:HB3	1:J:386:GLU:HG3	1.87	0.57
1:I:608:SER:HB2	2:U:280:ARG:HH11	1.70	0.57
1:J:415:ASN:ND2	1:J:420:ARG:HH11	2.02	0.57
1:G:412:MET:HE1	1:G:524:GLY:N	2.19	0.57
1:I:420:ARG:HB3	1:I:523:PRO:HB3	1.85	0.57
1:L:514:LEU:HD12	1:L:515:ASN:H	1.69	0.57
1:L:409:LEU:O	1:L:413:VAL:HG23	2.05	0.57
1:L:420:ARG:HB2	1:L:523:PRO:HB3	1.86	0.57
1:B:306:ILE:HD12	1:B:307:LYS:N	2.20	0.57
2:N:193:HIS:CE1	2:N:214:HIS:HB3	2.39	0.57
1:H:581:TRP:HE1	2:T:246:MET:HE3	1.69	0.57
1:C:507:VAL:HG12	1:C:508:ASN:H	1.68	0.57
1:L:293:LEU:O	1:L:296:GLN:HG2	2.04	0.57
1:J:497:LEU:O	1:J:500:TYR:HB2	2.04	0.57
1:I:623:ILE:HG22	1:I:624:GLY:N	2.18	0.57
1:J:340:ALA:O	1:J:344:VAL:HG23	2.05	0.57
1:A:512:LYS:O	1:A:512:LYS:HG2	2.05	0.57
1:L:465:ILE:HG12	1:L:509:LEU:HD12	1.87	0.57
1:B:618:ASN:OD1	1:B:623:ILE:HD11	2.05	0.57
1:C:512:LYS:HG3	1:C:512:LYS:O	2.04	0.57
1:K:579:LEU:O	1:K:583:ARG:HB2	2.05	0.57
1:G:581:TRP:NE1	2:S:246:MET:HE3	2.16	0.57
1:B:449:ASN:ND2	1:B:451:ASN:H	2.03	0.57
1:K:346:ALA:HB1	1:L:290:GLY:H	1.70	0.57
1:H:303:LEU:HD23	1:H:306:ILE:HD11	1.87	0.56
1:A:270:TRP:CE2	1:A:336:ILE:HG12	2.40	0.56
1:F:371:ARG:O	1:F:375:MET:HG2	2.05	0.56
1:B:419:LYS:HD2	1:B:542:VAL:HG13	1.86	0.56
1:C:383:ASP:HB3	1:C:386:GLU:HG3	1.85	0.56
1:K:465:ILE:HD12	1:K:511:LYS:HG3	1.85	0.56
1:E:423:LEU:HD12	1:E:526:VAL:O	2.05	0.56
2:S:118:THR:HG22	2:S:282:ARG:HD3	1.87	0.56
2:M:158:ARG:HB2	2:M:158:ARG:HH11	1.70	0.56
1:H:349:ARG:NH2	1:H:515:ASN:HD21	1.97	0.56
1:I:357:ARG:HG2	1:I:357:ARG:NH1	2.19	0.56
1:H:402:ASP:CA	1:H:578:MET:HE3	2.34	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:282:ARG:O	2:P:286:GLU:HG3	2.05	0.56
2:U:254:ILE:HD13	2:U:269:SER:HB3	1.86	0.56
1:D:512:LYS:HG2	1:D:512:LYS:O	2.04	0.56
1:K:418:LYS:HG3	1:K:418:LYS:O	2.05	0.56
1:D:564:LEU:C	1:D:566:LYS:H	2.08	0.56
1:F:590:GLN:HA	1:F:593:GLN:CG	2.35	0.56
1:B:608:SER:HB3	1:B:611:VAL:HG23	1.87	0.56
2:R:136:GLN:HB2	2:R:139:LYS:HG3	1.87	0.56
1:G:417:PRO:HG3	1:H:567:ARG:NH2	2.20	0.56
1:H:387:TRP:O	1:H:391:VAL:HG23	2.05	0.56
2:P:257:LEU:O	2:P:265:LEU:HB2	2.05	0.56
2:V:132:LYS:HD3	2:V:134:PHE:CZ	2.41	0.56
1:A:303:LEU:HD11	1:A:307:LYS:HE3	1.86	0.56
2:W:118:THR:HG22	2:W:282:ARG:HD3	1.86	0.56
1:E:596:ILE:O	1:E:600:LYS:HG3	2.06	0.56
1:L:433:THR:HG23	1:L:473:GLU:OE2	2.06	0.56
1:J:268:VAL:HG11	1:J:327:PHE:HA	1.88	0.56
2:R:197:VAL:HG11	2:R:218:VAL:HG11	1.88	0.56
1:I:561:GLU:H	1:I:561:GLU:CD	2.09	0.56
1:G:498:ARG:HB3	1:G:540:ARG:NH2	2.21	0.56
1:H:559:ARG:HH11	1:H:623:ILE:HA	1.71	0.56
1:C:397:LEU:HB3	1:C:401:MET:HE3	1.87	0.56
1:B:581:TRP:HZ3	1:B:603:LEU:HB3	1.70	0.56
1:D:343:THR:HG23	1:E:293:LEU:HD13	1.88	0.56
1:B:456:ARG:HH21	1:B:512:LYS:NZ	2.04	0.56
1:J:500:TYR:CZ	1:J:507:VAL:HG11	2.41	0.56
1:F:480:GLY:HA2	1:F:483:ARG:NH2	2.20	0.56
1:H:460:GLU:O	1:H:463:VAL:HG22	2.06	0.56
1:H:481:GLU:H	1:H:481:GLU:CD	2.08	0.56
2:Q:190:PRO:HB3	2:Q:192:GLN:HE22	1.72	0.55
1:C:451:ASN:ND2	1:C:475:VAL:HA	2.20	0.55
1:K:369:LEU:HB2	1:K:595:ARG:NH1	2.21	0.55
1:D:416:ILE:HD12	1:E:565:GLU:HA	1.89	0.55
1:F:382:ALA:HB1	1:F:387:TRP:HE1	1.71	0.55
1:D:507:VAL:HG12	1:D:509:LEU:HD22	1.87	0.55
1:J:512:LYS:C	1:J:514:LEU:H	2.09	0.55
1:L:497:LEU:O	1:L:500:TYR:HB2	2.07	0.55
2:O:175:ARG:NH2	2:O:237:MET:HB3	2.19	0.55
1:A:514:LEU:HD23	1:A:515:ASN:N	2.21	0.55
1:L:416:ILE:O	1:L:420:ARG:HG2	2.07	0.55
1:H:412:MET:HE2	1:H:469:LEU:HD13	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:576:LEU:O	1:I:580:ILE:HG12	2.05	0.55
2:U:107:TYR:O	2:U:147:VAL:HG23	2.06	0.55
2:M:239:ASN:HA	2:M:274:VAL:HB	1.87	0.55
1:F:283:ASP:HA	1:F:341:VAL:HG13	1.89	0.55
2:N:110:ARG:NH2	2:N:146:TRP:HB3	2.21	0.55
2:O:245:GLY:O	2:O:247:ASN:N	2.39	0.55
1:G:421:TYR:CE1	1:G:523:PRO:HA	2.42	0.55
1:I:514:LEU:HD23	1:I:516:LYS:HE3	1.88	0.55
1:K:489:GLN:O	1:K:491:ILE:N	2.39	0.55
1:D:354:GLN:HE21	1:E:310:GLN:NE2	2.05	0.55
1:B:372:MET:CE	1:B:577:LEU:HG	2.35	0.55
1:J:289:LEU:HD11	1:J:333:GLN:HE21	1.72	0.55
1:D:349:ARG:HB2	1:D:349:ARG:HH11	1.72	0.55
1:E:357:ARG:HA	1:E:360:MET:CE	2.37	0.55
1:C:368:LEU:O	1:C:372:MET:HG3	2.06	0.55
1:C:369:LEU:HD13	1:C:595:ARG:HG2	1.88	0.55
1:L:356:THR:O	1:L:360:MET:HG3	2.06	0.55
2:P:107:TYR:O	2:P:147:VAL:HG23	2.06	0.55
1:C:451:ASN:HD21	1:C:476:LYS:H	1.53	0.55
1:D:354:GLN:NE2	1:E:310:GLN:HE21	2.05	0.55
1:E:386:GLU:O	1:E:389:ALA:HB3	2.05	0.55
1:A:473:GLU:HG3	1:F:505:VAL:HG21	1.88	0.55
1:I:424:PHE:HB2	1:I:527:THR:HG22	1.87	0.55
1:F:477:GLY:HA3	1:F:491:ILE:HD12	1.89	0.55
1:G:454:LEU:HA	1:G:457:LEU:CB	2.36	0.55
1:C:454:LEU:C	1:C:456:ARG:H	2.08	0.55
1:B:454:LEU:HD12	1:B:454:LEU:H	1.71	0.55
1:H:581:TRP:HZ3	1:H:603:LEU:HB3	1.71	0.55
1:L:475:VAL:HG22	1:L:528:MET:HB3	1.88	0.55
1:J:618:ASN:HB3	1:J:624:GLY:O	2.06	0.55
2:Q:160:MET:HG3	2:Q:214:HIS:O	2.07	0.55
1:K:419:LYS:HA	1:K:542:VAL:HG22	1.88	0.55
1:C:520:ILE:N	1:C:520:ILE:HD13	2.12	0.55
1:L:609:LEU:HD22	2:X:246:MET:HE1	1.88	0.55
1:G:427:PRO:HG3	1:G:530:GLU:OE1	2.06	0.55
1:A:456:ARG:HG3	1:F:458:ASN:HB2	1.87	0.55
2:P:191:PRO:HG2	2:P:192:GLN:HE21	1.71	0.55
1:L:450:VAL:HG12	1:L:457:LEU:HD11	1.89	0.55
1:C:465:ILE:HG21	1:C:517:ARG:HE	1.72	0.55
2:O:119:ALA:O	2:O:279:GLY:HA3	2.07	0.55
2:M:190:PRO:HB3	2:M:192:GLN:HE22	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:502:ASP:OD1	1:E:540:ARG:HD2	2.07	0.55
2:T:190:PRO:HB3	2:T:192:GLN:HE22	1.72	0.55
1:K:361:LEU:CD2	1:K:443:CYS:HB3	2.37	0.55
2:V:198:GLU:HB2	2:V:235:ASN:HD21	1.71	0.55
1:B:475:VAL:HG12	1:B:491:ILE:HD12	1.88	0.55
1:B:609:LEU:O	1:B:613:GLN:HG3	2.07	0.55
1:G:270:TRP:CE2	1:G:336:ILE:HG12	2.42	0.55
1:H:284:ASP:CG	1:H:287:LEU:HB2	2.27	0.55
1:L:425:LYS:O	1:L:546:ASP:HA	2.07	0.55
2:O:196:ARG:NH1	2:O:237:MET:CE	2.70	0.55
1:F:506:LYS:HG2	1:F:520:ILE:HG13	1.89	0.55
2:T:147:VAL:HG21	2:T:151:PRO:HD3	1.89	0.55
2:P:273:ARG:HG3	2:P:273:ARG:HH11	1.72	0.55
1:A:408:PHE:CD2	1:A:439:LEU:HD22	2.41	0.54
2:V:118:THR:HG22	2:V:282:ARG:HD3	1.88	0.54
1:I:583:ARG:HB3	1:I:587:GLU:OE1	2.06	0.54
1:I:500:TYR:CZ	1:I:507:VAL:HG11	2.41	0.54
1:K:269:SER:N	1:K:323:ASN:HD21	2.00	0.54
1:F:443:CYS:HB2	1:F:469:LEU:HD23	1.90	0.54
1:D:349:ARG:NE	1:D:517:ARG:HD2	2.21	0.54
1:C:395:HIS:HD2	1:C:616:LYS:NZ	2.04	0.54
2:O:244:GLY:HA3	2:O:248:ARG:HB2	1.89	0.54
1:B:299:PHE:HD2	1:B:299:PHE:H	1.55	0.54
1:G:291:MET:CG	1:G:291:MET:CE	2.86	0.54
1:C:454:LEU:CA	1:C:457:LEU:HB2	2.35	0.54
1:F:465:ILE:HG23	1:F:517:ARG:HD2	1.87	0.54
2:N:193:HIS:ND1	2:N:214:HIS:HB3	2.23	0.54
1:B:475:VAL:CG1	1:B:491:ILE:HD12	2.37	0.54
1:E:269:SER:OG	1:E:272:LEU:HB2	2.08	0.54
1:B:602:ARG:HE	1:B:606:GLU:HG3	1.72	0.54
2:R:196:ARG:O	2:R:234:TYR:HA	2.08	0.54
1:C:447:ALA:C	1:C:448:LEU:HD23	2.28	0.54
1:I:364:ARG:HG2	1:I:443:CYS:O	2.07	0.54
2:S:243:MET:CE	2:S:243:MET:CG	2.84	0.54
2:X:243:MET:CE	2:X:243:MET:CG	2.85	0.54
1:J:415:ASN:HD22	1:J:420:ARG:HG2	1.71	0.54
2:T:189:ALA:HB2	2:T:205:TYR:CZ	2.42	0.54
1:G:383:ASP:OD1	1:G:385:GLU:HB3	2.08	0.54
1:C:419:LYS:HA	1:C:542:VAL:HG22	1.89	0.54
1:G:311:PRO:C	1:G:313:HIS:H	2.10	0.54
2:P:224:GLU:H	2:P:224:GLU:CD	2.11	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:389:ALA:O	1:I:392:ALA:HB3	2.08	0.54
1:J:357:ARG:HB3	1:J:413:VAL:HG13	1.89	0.54
1:E:625:VAL:HG23	1:E:626:LEU:HG	1.89	0.54
1:G:372:MET:HA	1:G:375:MET:HG2	1.88	0.54
1:B:593:GLN:HE22	2:N:181:ARG:HH12	1.55	0.54
1:C:267:GLN:O	1:C:326:ILE:HG21	2.07	0.54
1:G:398:LEU:HB2	1:G:401:MET:CE	2.37	0.54
1:C:545:ILE:N	1:C:545:ILE:HD12	2.22	0.54
2:X:242:CYS:O	2:X:243:MET:HG3	2.07	0.54
1:H:581:TRP:HE3	1:H:603:LEU:HD23	1.73	0.54
1:E:556:CYS:SG	1:E:619:VAL:HA	2.48	0.54
2:P:158:ARG:HG3	2:P:217:VAL:HG22	1.89	0.54
1:F:497:LEU:O	1:F:500:TYR:HB2	2.08	0.54
1:K:561:GLU:O	1:K:565:GLU:HG3	2.07	0.54
2:M:175:ARG:HD3	2:M:191:PRO:O	2.08	0.54
1:E:585:VAL:HG23	2:Q:242:CYS:HA	1.89	0.54
2:Q:133:MET:HE3	2:Q:135:CYS:HB3	1.90	0.54
2:U:155:THR:HG23	2:U:258:GLU:O	2.08	0.54
1:H:454:LEU:HD21	1:H:493:ASN:ND2	2.23	0.54
1:E:556:CYS:SG	1:E:619:VAL:HG22	2.48	0.54
1:B:385:GLU:HA	1:B:607:PHE:CZ	2.43	0.54
1:L:470:VAL:O	1:L:524:GLY:HA3	2.08	0.54
2:O:158:ARG:CA	2:O:217:VAL:HG13	2.38	0.54
1:L:590:GLN:CD	1:L:590:GLN:H	2.10	0.54
1:H:612:TYR:CD2	2:T:246:MET:HE3	2.43	0.54
2:X:259:ASP:OD2	2:X:263:ASN:HB2	2.08	0.54
2:X:189:ALA:HB2	2:X:205:TYR:CZ	2.43	0.54
1:I:332:ASN:O	1:I:336:ILE:HG13	2.07	0.54
1:E:433:THR:HG23	1:E:473:GLU:CD	2.28	0.54
2:S:197:VAL:HG23	2:S:216:VAL:HG21	1.89	0.54
1:J:454:LEU:HD22	1:K:453:PRO:HG3	1.90	0.54
2:R:156:ARG:HB3	2:R:217:VAL:CG1	2.38	0.54
1:I:405:VAL:HG12	1:I:579:LEU:HD21	1.89	0.54
1:K:508:ASN:ND2	1:L:463:VAL:HG11	2.22	0.54
2:M:197:VAL:HG23	2:M:216:VAL:HG21	1.90	0.54
1:D:584:PRO:HG2	1:D:587:GLU:HG3	1.89	0.54
1:L:609:LEU:HD22	2:X:246:MET:CE	2.38	0.54
1:I:495:ASP:O	1:I:498:ARG:HG3	2.07	0.54
1:B:589:ALA:O	1:B:592:ILE:HG22	2.06	0.54
1:K:342:ASP:OD2	1:L:334:LYS:HD2	2.08	0.54
1:I:609:LEU:HD13	2:U:246:MET:HE1	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:485:LEU:CD2	1:A:529:ASN:HD22	2.21	0.54
1:C:410:LYS:HE2	1:C:410:LYS:HA	1.89	0.54
2:W:120:LYS:HD2	2:W:120:LYS:N	2.23	0.54
1:H:454:LEU:H	1:H:454:LEU:HD12	1.73	0.53
2:X:191:PRO:HG2	2:X:192:GLN:HE21	1.72	0.53
1:F:349:ARG:CZ	1:F:517:ARG:CD	2.86	0.53
1:A:454:LEU:HB3	1:B:453:PRO:HG2	1.90	0.53
1:J:357:ARG:HA	1:J:360:MET:CE	2.38	0.53
2:P:122:VAL:HG12	2:P:123:THR:N	2.23	0.53
1:E:397:LEU:HG	1:E:397:LEU:O	2.07	0.53
1:K:398:LEU:HB2	1:K:401:MET:CE	2.38	0.53
1:E:465:ILE:O	1:E:466:ASP:HB2	2.07	0.53
1:D:285:VAL:HG22	1:D:341:VAL:HG21	1.91	0.53
2:W:109:PHE:CD1	2:W:257:LEU:HD22	2.44	0.53
1:G:614:LYS:O	1:G:617:PHE:HB3	2.07	0.53
1:D:300:GLU:HB2	1:D:301:MET:SD	2.48	0.53
1:F:408:PHE:HE1	1:F:525:ILE:HD11	1.66	0.53
1:C:608:SER:HA	2:O:280:ARG:NH1	2.23	0.53
1:H:401:MET:HG3	1:H:578:MET:CE	2.39	0.53
2:O:245:GLY:C	2:O:247:ASN:H	2.10	0.53
2:W:175:ARG:HD3	2:W:191:PRO:O	2.08	0.53
1:L:372:MET:HA	1:L:375:MET:HG2	1.89	0.53
2:V:224:GLU:CD	2:V:224:GLU:H	2.11	0.53
1:K:454:LEU:HB3	1:L:453:PRO:HG2	1.88	0.53
1:H:506:LYS:HG2	1:H:519:GLN:HA	1.90	0.53
1:I:611:VAL:O	1:I:614:LYS:HB3	2.08	0.53
1:B:618:ASN:HB3	1:B:623:ILE:HG13	1.91	0.53
2:N:244:GLY:HA3	2:N:248:ARG:HB2	1.90	0.53
2:O:158:ARG:CZ	2:O:217:VAL:HG21	2.38	0.53
1:L:460:GLU:O	1:L:463:VAL:HB	2.09	0.53
2:M:176:CYS:SG	2:M:179:HIS:HB2	2.48	0.53
1:A:443:CYS:HB3	1:A:468:PHE:CD2	2.42	0.53
1:G:594:SER:O	1:G:597:VAL:HG12	2.07	0.53
1:J:417:PRO:HG3	1:K:567:ARG:NH1	2.24	0.53
1:F:452:LEU:HB3	1:F:453:PRO:CD	2.39	0.53
1:E:353:LEU:HD21	1:E:517:ARG:HH22	1.74	0.53
1:C:475:VAL:HG23	1:C:475:VAL:O	2.09	0.53
1:D:295:PHE:HB3	1:D:320:HIS:O	2.09	0.53
1:E:369:LEU:HD12	1:E:592:ILE:HD11	1.90	0.53
2:R:277:CYS:HB2	2:R:280:ARG:NH2	2.22	0.53
1:E:557:LEU:HD13	1:E:564:LEU:HD11	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:581:TRP:HZ3	1:E:603:LEU:HB3	1.73	0.53
1:J:621:MET:HB2	1:J:623:ILE:HG12	1.90	0.53
1:J:441:GLU:OE1	1:J:571:SER:HA	2.09	0.53
2:W:180:GLU:O	2:W:180:GLU:HG3	2.08	0.53
1:G:410:LYS:HA	1:G:410:LYS:HE2	1.91	0.53
2:N:101:LYS:HE2	2:N:101:LYS:N	2.24	0.53
1:H:454:LEU:HB2	1:I:453:PRO:HG2	1.90	0.53
1:F:608:SER:HB3	1:F:611:VAL:CG2	2.39	0.53
1:E:597:VAL:C	1:E:599:TRP:H	2.12	0.53
1:E:397:LEU:O	1:E:398:LEU:HD13	2.09	0.53
1:I:525:ILE:HG22	1:I:526:VAL:N	2.23	0.53
1:E:510:GLU:O	1:E:510:GLU:HG3	2.09	0.53
1:A:285:VAL:HG22	1:A:341:VAL:HG21	1.89	0.53
1:F:421:TYR:CE1	1:F:523:PRO:HA	2.43	0.53
1:C:389:ALA:HB1	1:C:625:VAL:HG11	1.89	0.53
2:T:107:TYR:CE1	2:T:151:PRO:HA	2.43	0.53
1:D:296:GLN:HG3	1:D:297:TYR:N	2.24	0.53
1:A:511:LYS:HB3	1:A:516:LYS:HG3	1.90	0.53
1:G:567:ARG:NH2	1:L:503:GLY:O	2.42	0.53
2:U:173:VAL:CG1	2:U:194:LEU:HD12	2.38	0.53
1:G:580:ILE:HD13	1:G:596:ILE:HG23	1.89	0.53
1:G:517:ARG:HG2	1:G:518:THR:N	2.24	0.53
1:I:458:ASN:HB2	1:J:456:ARG:HH21	1.74	0.53
1:J:579:LEU:C	1:J:581:TRP:N	2.62	0.53
1:C:386:GLU:O	1:C:389:ALA:HB3	2.09	0.53
1:D:402:ASP:HA	1:D:578:MET:HE3	1.91	0.53
1:G:351:ASP:O	1:G:355:LEU:HB2	2.08	0.53
1:F:389:ALA:HB1	1:F:625:VAL:HG21	1.89	0.53
1:H:559:ARG:HH11	1:H:559:ARG:HG3	1.74	0.53
1:J:403:SER:HA	1:J:583:ARG:NH2	2.22	0.53
2:T:179:HIS:HA	2:T:182:CYS:SG	2.48	0.53
2:V:251:ILE:HD12	2:V:251:ILE:H	1.73	0.53
1:A:520:ILE:CD1	1:A:520:ILE:H	2.18	0.53
2:N:112:GLY:HA3	2:N:146:TRP:HE1	1.74	0.53
1:I:472:PHE:HD2	1:I:526:VAL:HG22	1.74	0.53
2:O:176:CYS:SG	2:O:179:HIS:HB2	2.49	0.53
1:K:408:PHE:O	1:K:412:MET:HG2	2.08	0.53
2:R:175:ARG:HG3	2:R:192:GLN:O	2.09	0.52
1:K:454:LEU:HD22	1:K:454:LEU:N	2.22	0.52
1:E:287:LEU:O	1:E:291:MET:HG3	2.10	0.52
1:I:594:SER:O	1:I:598:GLU:HG3	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:425:LYS:NZ	1:I:530:GLU:HA	2.24	0.52
1:H:423:LEU:HD12	1:H:526:VAL:O	2.09	0.52
1:J:425:LYS:HE3	1:J:528:MET:HE3	1.92	0.52
2:U:196:ARG:HB2	2:U:235:ASN:HB2	1.89	0.52
2:V:159:ALA:HB3	2:V:216:VAL:HG13	1.90	0.52
1:B:614:LYS:O	1:B:617:PHE:HB3	2.09	0.52
2:Q:114:LEU:HD22	2:Q:142:PRO:HG3	1.91	0.52
1:E:424:PHE:O	1:E:527:THR:HA	2.09	0.52
1:L:514:LEU:HG	1:L:516:LYS:N	2.24	0.52
1:I:424:PHE:CE1	1:I:545:ILE:HD12	2.44	0.52
1:D:314:TYR:CE1	1:D:315:LYS:HG2	2.44	0.52
1:C:538:GLN:HE22	1:C:544:GLN:NE2	2.06	0.52
2:M:189:ALA:HB2	2:M:205:TYR:CZ	2.44	0.52
1:F:361:LEU:O	1:F:361:LEU:HD13	2.08	0.52
1:H:402:ASP:N	1:H:578:MET:HE3	2.24	0.52
1:B:346:ALA:O	1:B:350:VAL:HG23	2.09	0.52
1:G:388:MET:HG3	1:G:607:PHE:CE1	2.44	0.52
2:S:245:GLY:C	2:S:247:ASN:H	2.11	0.52
2:U:132:LYS:HE2	2:U:273:ARG:HB2	1.91	0.52
1:B:408:PHE:O	1:B:412:MET:HG2	2.09	0.52
1:E:580:ILE:HG21	1:E:599:TRP:HB3	1.91	0.52
2:O:244:GLY:O	2:O:246:MET:N	2.43	0.52
1:C:317:HIS:O	1:C:321:TYR:N	2.41	0.52
1:F:268:VAL:HG11	1:F:327:PHE:HA	1.91	0.52
1:L:299:PHE:CZ	1:L:318:GLU:HB2	2.44	0.52
2:T:264:LEU:HD11	2:T:267:ARG:HB2	1.91	0.52
1:C:568:ILE:O	1:C:570:GLN:N	2.43	0.52
1:J:420:ARG:CZ	1:J:503:GLY:HA3	2.40	0.52
1:J:421:TYR:CE1	1:J:523:PRO:HA	2.44	0.52
1:C:349:ARG:HD2	1:C:517:ARG:NH1	2.25	0.52
1:K:346:ALA:O	1:K:350:VAL:HG23	2.09	0.52
1:C:507:VAL:HG12	1:C:508:ASN:N	2.25	0.52
2:P:126:TYR:OH	2:P:131:ASN:ND2	2.42	0.52
1:E:307:LYS:HD2	1:E:309:GLU:HB3	1.92	0.52
1:I:512:LYS:O	1:I:512:LYS:HG3	2.09	0.52
1:J:415:ASN:HD21	1:J:420:ARG:NH1	2.05	0.52
1:C:498:ARG:CZ	1:D:476:LYS:HD3	2.40	0.52
1:A:512:LYS:HB2	1:F:514:LEU:HD13	1.92	0.52
2:N:147:VAL:HG21	2:N:151:PRO:HD3	1.91	0.52
2:Q:257:LEU:O	2:Q:265:LEU:HB2	2.09	0.52
2:O:189:ALA:HB2	2:O:205:TYR:CZ	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:289:LEU:O	1:B:293:LEU:HD12	2.09	0.52
1:I:454:LEU:HB2	1:J:453:PRO:CG	2.40	0.52
1:A:520:ILE:HD12	1:A:520:ILE:N	2.16	0.52
1:I:512:LYS:HD3	1:I:516:LYS:NZ	2.25	0.52
1:C:454:LEU:HD22	1:D:453:PRO:HG3	1.90	0.52
1:C:560:SER:OG	1:C:625:VAL:HG23	2.09	0.52
2:V:159:ALA:HB3	2:V:216:VAL:CG1	2.40	0.52
1:J:353:LEU:HD21	1:J:517:ARG:NH1	2.24	0.52
1:C:585:VAL:HG13	2:O:242:CYS:HA	1.91	0.52
1:I:445:GLY:O	1:I:446:LYS:HG2	2.10	0.52
2:N:105:GLY:HA3	2:N:265:LEU:O	2.10	0.52
2:Q:158:ARG:CZ	2:Q:217:VAL:HG21	2.40	0.52
1:G:470:VAL:O	1:G:524:GLY:HA3	2.08	0.52
1:K:287:LEU:O	1:K:291:MET:HG2	2.10	0.52
2:U:189:ALA:HB2	2:U:205:TYR:CZ	2.45	0.52
2:M:108:GLY:O	2:M:110:ARG:NH1	2.43	0.52
1:G:589:ALA:O	1:G:593:GLN:HG3	2.10	0.52
1:F:579:LEU:CD2	1:F:583:ARG:HG3	2.37	0.52
1:I:561:GLU:O	1:I:565:GLU:HG3	2.09	0.52
1:A:597:VAL:O	1:A:601:GLU:HG3	2.09	0.52
1:J:356:THR:OG1	1:J:359:GLN:HG3	2.09	0.51
1:A:609:LEU:HA	2:M:246:MET:HE1	1.91	0.51
1:J:560:SER:OG	1:J:624:GLY:HA2	2.09	0.51
2:T:264:LEU:O	2:T:265:LEU:HD23	2.09	0.51
1:G:274:THR:HA	1:G:340:ALA:HB1	1.92	0.51
2:W:158:ARG:HB2	2:W:217:VAL:HG13	1.93	0.51
2:N:203:VAL:HA	2:N:218:VAL:HG12	1.92	0.51
1:C:529:ASN:O	1:C:531:TYR:N	2.41	0.51
1:B:394:LEU:HD21	1:B:569:ILE:O	2.11	0.51
1:D:405:VAL:O	1:D:409:LEU:HG	2.09	0.51
2:T:132:LYS:HE3	2:T:271:GLU:OE2	2.10	0.51
1:I:405:VAL:CG1	1:I:579:LEU:HD21	2.40	0.51
1:F:550:LYS:HD3	1:F:552:TYR:OH	2.11	0.51
1:A:357:ARG:HA	1:A:360:MET:CE	2.40	0.51
1:F:584:PRO:HB3	2:R:243:MET:HA	1.92	0.51
1:E:451:ASN:HD22	1:E:490:GLY:HA3	1.76	0.51
1:L:583:ARG:HE	1:L:583:ARG:HA	1.75	0.51
1:F:510:GLU:HG3	1:F:514:LEU:O	2.10	0.51
1:K:368:LEU:O	1:K:372:MET:HG3	2.11	0.51
1:L:351:ASP:O	1:L:355:LEU:HB2	2.11	0.51
2:W:251:ILE:HG22	2:W:252:LEU:N	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:132:LYS:HD3	2:W:134:PHE:CZ	2.46	0.51
1:I:385:GLU:HA	1:I:607:PHE:CZ	2.45	0.51
2:U:249:ARG:HG3	2:U:249:ARG:HH11	1.76	0.51
1:G:458:ASN:OD1	1:G:510:GLU:HG2	2.10	0.51
1:H:454:LEU:HD11	1:H:493:ASN:HD21	1.76	0.51
1:C:454:LEU:HD12	1:C:454:LEU:H	1.75	0.51
1:F:349:ARG:NH1	1:F:517:ARG:HD3	2.25	0.51
1:F:550:LYS:HB2	1:F:553:LEU:HD12	1.91	0.51
2:V:155:THR:HG23	2:V:258:GLU:O	2.10	0.51
1:D:585:VAL:HG23	2:P:242:CYS:HA	1.93	0.51
2:T:163:TYR:CZ	2:T:173:VAL:HG22	2.45	0.51
1:G:456:ARG:HH11	1:G:456:ARG:HG2	1.75	0.51
1:L:454:LEU:HA	1:L:457:LEU:CB	2.38	0.51
1:D:354:GLN:NE2	1:E:310:GLN:NE2	2.59	0.51
1:A:389:ALA:HB1	1:A:625:VAL:HG21	1.91	0.51
1:D:343:THR:HG23	1:E:293:LEU:CD1	2.40	0.51
2:V:241:SER:HA	2:V:245:GLY:H	1.76	0.51
2:M:242:CYS:O	2:M:243:MET:HG3	2.11	0.51
1:G:415:ASN:ND2	1:G:420:ARG:CD	2.59	0.51
1:F:349:ARG:HD3	1:F:517:ARG:NH1	2.25	0.51
1:I:580:ILE:HG22	1:I:600:LYS:HG3	1.92	0.51
1:C:597:VAL:HG21	2:O:178:HIS:ND1	2.25	0.51
1:F:514:LEU:HD23	1:F:516:LYS:HD3	1.92	0.51
1:B:385:GLU:HA	1:B:607:PHE:HZ	1.74	0.51
1:I:311:PRO:C	1:I:313:HIS:H	2.13	0.51
2:V:126:TYR:OH	2:V:131:ASN:HA	2.11	0.51
1:B:335:THR:O	1:B:338:GLN:HB2	2.11	0.51
2:M:118:THR:HG22	2:M:282:ARG:HD3	1.93	0.51
1:D:608:SER:HB3	2:P:280:ARG:HH11	1.75	0.51
1:L:599:TRP:O	1:L:603:LEU:HB2	2.10	0.51
2:P:175:ARG:HG3	2:P:192:GLN:O	2.11	0.51
2:S:244:GLY:O	2:S:246:MET:N	2.44	0.51
1:J:401:MET:HG3	1:J:578:MET:CE	2.41	0.51
2:N:158:ARG:HB2	2:N:158:ARG:HH11	1.76	0.51
1:A:295:PHE:HA	1:A:317:HIS:CE1	2.44	0.51
1:B:386:GLU:O	1:B:389:ALA:HB3	2.11	0.51
2:R:203:VAL:HG23	2:R:218:VAL:CG1	2.41	0.51
1:A:298:SER:HA	1:A:321:TYR:CE1	2.45	0.51
1:E:428:ILE:CD1	1:E:428:ILE:H	2.19	0.51
1:I:580:ILE:HG21	1:I:599:TRP:O	2.10	0.51
1:G:476:LYS:HE2	1:L:496:ASN:HD22	1.73	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:458:ASN:HB2	1:J:456:ARG:NH2	2.26	0.51
1:A:609:LEU:HD22	2:M:246:MET:HE2	1.93	0.51
1:I:386:GLU:O	1:I:389:ALA:HB3	2.10	0.51
1:G:592:ILE:O	1:G:596:ILE:HG12	2.11	0.51
2:P:197:VAL:HG23	2:P:216:VAL:HG21	1.91	0.51
1:B:517:ARG:CZ	1:B:519:GLN:HB3	2.41	0.51
1:F:446:LYS:HG3	1:F:463:VAL:HG12	1.92	0.51
1:D:387:TRP:CZ3	1:D:573:ILE:HB	2.45	0.51
1:A:435:LEU:HD23	1:A:547:PHE:HZ	1.76	0.51
1:K:589:ALA:O	1:K:592:ILE:HG22	2.11	0.51
1:G:579:LEU:O	1:G:583:ARG:HB2	2.11	0.51
1:A:583:ARG:HD3	1:A:587:GLU:OE1	2.10	0.51
1:H:415:ASN:ND2	1:H:420:ARG:HH11	2.01	0.51
1:A:428:ILE:H	1:A:428:ILE:CD1	2.21	0.51
1:E:357:ARG:HA	1:E:360:MET:HE3	1.92	0.51
1:G:608:SER:HB2	2:S:280:ARG:HH11	1.76	0.51
1:I:430:SER:HB3	1:I:547:PHE:HB3	1.93	0.51
2:O:114:LEU:N	2:O:114:LEU:HD12	2.26	0.51
1:H:412:MET:HE1	1:H:469:LEU:HB2	1.92	0.50
1:I:589:ALA:H	1:I:592:ILE:HD11	1.74	0.50
1:D:398:LEU:HD21	1:D:545:ILE:HG21	1.93	0.50
1:I:374:ILE:HD12	1:I:374:ILE:N	2.26	0.50
1:C:568:ILE:C	1:C:570:GLN:H	2.13	0.50
1:A:287:LEU:O	1:A:291:MET:HB2	2.11	0.50
1:J:433:THR:HG23	1:J:473:GLU:CD	2.31	0.50
2:R:245:GLY:C	2:R:247:ASN:H	2.15	0.50
1:G:602:ARG:HD3	1:G:602:ARG:C	2.31	0.50
2:W:224:GLU:H	2:W:224:GLU:CD	2.14	0.50
1:G:459:PHE:HZ	1:G:513:HIS:H	1.58	0.50
1:A:428:ILE:N	1:A:428:ILE:HD12	2.22	0.50
1:K:346:ALA:HB1	1:L:290:GLY:N	2.25	0.50
2:P:132:LYS:HE2	2:P:273:ARG:HB2	1.94	0.50
1:J:617:PHE:O	1:J:621:MET:HG2	2.11	0.50
1:J:293:LEU:O	1:J:296:GLN:HB3	2.10	0.50
1:L:502:ASP:OD1	1:L:540:ARG:HD2	2.12	0.50
2:S:257:LEU:O	2:S:265:LEU:HB2	2.12	0.50
1:A:469:LEU:HD12	1:A:470:VAL:N	2.27	0.50
1:I:383:ASP:HB3	1:I:386:GLU:HG3	1.94	0.50
1:D:585:VAL:HG12	1:D:585:VAL:O	2.12	0.50
1:D:368:LEU:HD22	1:D:573:ILE:HD13	1.93	0.50
1:E:470:VAL:O	1:E:524:GLY:HA3	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:349:ARG:HH11	1:A:349:ARG:HB2	1.76	0.50
1:L:421:TYR:CE1	1:L:523:PRO:HA	2.47	0.50
1:E:454:LEU:HD13	1:E:457:LEU:HD22	1.92	0.50
1:A:576:LEU:C	1:A:578:MET:H	2.15	0.50
1:J:483:ARG:HG3	1:J:483:ARG:HH11	1.77	0.50
1:D:424:PHE:HB2	1:D:527:THR:HG22	1.93	0.50
2:T:197:VAL:HG23	2:T:216:VAL:HG21	1.94	0.50
2:O:137:LEU:O	2:O:139:LYS:HG2	2.11	0.50
1:J:584:PRO:CG	1:J:587:GLU:HG3	2.41	0.50
1:G:299:PHE:HA	1:G:302:CYS:HB2	1.93	0.50
1:G:311:PRO:HA	1:G:314:TYR:CE2	2.47	0.50
2:O:203:VAL:HA	2:O:218:VAL:HG12	1.93	0.50
1:D:384:ILE:HG23	1:D:385:GLU:N	2.25	0.50
1:J:589:ALA:O	1:J:591:SER:N	2.45	0.50
1:F:314:TYR:CD1	1:F:315:LYS:HG3	2.47	0.50
1:E:341:VAL:O	1:E:344:VAL:N	2.45	0.50
1:I:458:ASN:HD22	1:J:456:ARG:HE	1.59	0.50
2:U:108:GLY:O	2:U:147:VAL:HA	2.11	0.50
2:M:197:VAL:HG11	2:M:218:VAL:HG11	1.93	0.50
1:I:422:TRP:HB2	1:I:525:ILE:HD13	1.94	0.50
1:D:597:VAL:HG21	2:P:178:HIS:ND1	2.27	0.50
1:J:481:GLU:H	1:J:481:GLU:CD	2.15	0.50
1:G:299:PHE:O	1:G:302:CYS:HB3	2.11	0.50
1:F:465:ILE:HD12	1:F:517:ARG:HB3	1.92	0.50
1:K:387:TRP:CE3	1:K:568:ILE:HG23	2.47	0.50
1:G:417:PRO:HG3	1:H:567:ARG:CZ	2.42	0.50
2:U:119:ALA:O	2:U:279:GLY:HA3	2.11	0.50
1:F:422:TRP:CE2	1:F:543:LYS:HD2	2.47	0.50
1:E:575:LEU:O	1:E:578:MET:HB3	2.12	0.50
2:S:132:LYS:HE2	2:S:273:ARG:HB2	1.93	0.50
2:U:102:THR:HG23	2:U:268:ASN:OD1	2.12	0.50
1:I:299:PHE:CZ	1:I:318:GLU:HB2	2.47	0.50
1:F:383:ASP:HB3	1:F:386:GLU:CG	2.37	0.49
1:B:369:LEU:CB	1:B:595:ARG:HH11	2.24	0.49
2:U:101:LYS:N	2:U:101:LYS:HE2	2.26	0.49
2:Q:101:LYS:HB2	2:Q:267:ARG:HH21	1.76	0.49
1:F:430:SER:OG	1:F:432:LYS:HG3	2.12	0.49
1:G:346:ALA:O	1:G:350:VAL:HG23	2.12	0.49
2:M:119:ALA:O	2:M:279:GLY:HA3	2.12	0.49
1:I:424:PHE:HE1	1:I:545:ILE:HD12	1.77	0.49
2:W:191:PRO:HG2	2:W:192:GLN:HE21	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:576:LEU:O	1:G:580:ILE:HG12	2.12	0.49
1:E:356:THR:OG1	1:E:359:GLN:HG3	2.11	0.49
1:L:265:THR:C	1:L:267:GLN:H	2.15	0.49
1:E:605:LYS:O	1:E:606:GLU:HG2	2.12	0.49
1:K:517:ARG:HG2	1:K:519:GLN:HG2	1.93	0.49
1:I:357:ARG:HA	1:I:360:MET:CE	2.41	0.49
1:G:470:VAL:HG23	1:G:522:PRO:HB2	1.94	0.49
1:B:384:ILE:HG21	1:B:606:GLU:OE2	2.12	0.49
1:G:608:SER:HB2	2:S:280:ARG:NH1	2.27	0.49
1:J:589:ALA:C	1:J:591:SER:H	2.16	0.49
2:M:287:GLU:C	2:M:289:LEU:H	2.15	0.49
2:P:175:ARG:HD2	2:P:193:HIS:O	2.12	0.49
1:K:440:LEU:HD22	1:K:471:VAL:CG2	2.42	0.49
1:K:618:ASN:ND2	1:K:627:ASP:HB2	2.27	0.49
1:K:511:LYS:HB2	1:K:514:LEU:HB2	1.94	0.49
2:O:158:ARG:HA	2:O:217:VAL:HG13	1.93	0.49
1:D:400:LYS:O	1:D:404:VAL:HG23	2.12	0.49
2:Q:197:VAL:HG11	2:Q:218:VAL:HG11	1.93	0.49
1:C:272:LEU:HD13	1:C:323:ASN:HB2	1.94	0.49
2:O:252:LEU:HD12	2:O:271:GLU:HA	1.93	0.49
2:O:257:LEU:O	2:O:265:LEU:HB2	2.12	0.49
1:L:520:ILE:CD1	1:L:520:ILE:H	2.18	0.49
2:U:193:HIS:CE1	2:U:214:HIS:HB3	2.47	0.49
1:A:625:VAL:HG23	1:A:626:LEU:H	1.77	0.49
2:W:252:LEU:HD12	2:W:270:PHE:O	2.12	0.49
2:W:147:VAL:HG21	2:W:151:PRO:HD3	1.94	0.49
1:H:443:CYS:HB3	1:H:468:PHE:CD2	2.47	0.49
2:S:158:ARG:HH21	2:S:206:LEU:HD23	1.77	0.49
1:B:583:ARG:HD2	1:B:587:GLU:OE1	2.13	0.49
1:B:581:TRP:CZ3	1:B:603:LEU:HB3	2.47	0.49
2:U:132:LYS:HG3	2:U:271:GLU:HB3	1.95	0.49
1:E:372:MET:HG3	1:E:573:ILE:HD12	1.94	0.49
1:I:353:LEU:HD12	1:J:287:LEU:HD13	1.94	0.49
1:B:282:CYS:SG	1:B:288:LEU:HB2	2.53	0.49
1:D:425:LYS:HE2	1:D:530:GLU:HA	1.94	0.49
1:L:506:LYS:HG2	1:L:520:ILE:HG13	1.95	0.49
1:I:469:LEU:HB2	1:I:523:PRO:O	2.12	0.49
1:F:446:LYS:HG2	1:F:467:GLN:OE1	2.13	0.49
1:D:564:LEU:C	1:D:566:LYS:N	2.66	0.49
2:T:107:TYR:O	2:T:147:VAL:HG23	2.12	0.49
2:M:251:ILE:HG22	2:M:252:LEU:N	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:280:ARG:HH11	2:Q:280:ARG:HG2	1.77	0.49
1:E:408:PHE:CD2	1:E:439:LEU:HD22	2.48	0.49
1:B:382:ALA:HB1	1:B:387:TRP:HE1	1.76	0.49
1:F:470:VAL:O	1:F:524:GLY:HA3	2.13	0.49
1:L:349:ARG:CZ	1:L:517:ARG:CD	2.90	0.49
1:F:454:LEU:N	1:F:454:LEU:HD12	2.28	0.49
1:L:590:GLN:CD	1:L:590:GLN:N	2.66	0.49
1:J:507:VAL:O	1:J:518:THR:HA	2.12	0.49
1:D:608:SER:HB3	2:P:280:ARG:HD2	1.95	0.49
1:B:295:PHE:HA	1:B:317:HIS:CD2	2.48	0.49
2:X:109:PHE:HE1	2:X:145:LEU:HG	1.76	0.49
1:G:469:LEU:C	1:G:469:LEU:CD1	2.81	0.49
1:K:361:LEU:HD23	1:K:443:CYS:HB3	1.95	0.49
1:F:424:PHE:HB2	1:F:527:THR:HG22	1.93	0.49
1:E:410:LYS:HA	1:E:410:LYS:HE3	1.93	0.49
1:F:409:LEU:O	1:F:413:VAL:HG23	2.13	0.49
1:C:397:LEU:HG	1:C:398:LEU:HG	1.94	0.49
1:D:415:ASN:ND2	1:D:420:ARG:HH11	2.02	0.49
1:C:525:ILE:CG2	1:C:526:VAL:N	2.75	0.49
2:X:147:VAL:HG21	2:X:151:PRO:HD3	1.95	0.49
1:A:451:ASN:HB3	1:F:496:ASN:HD22	1.78	0.49
1:F:268:VAL:HG13	1:F:326:ILE:HG22	1.94	0.49
2:S:160:MET:SD	2:S:213:ARG:HG2	2.53	0.49
2:W:122:VAL:HG11	2:W:125:THR:HB	1.95	0.49
1:I:557:LEU:HD22	1:I:564:LEU:HG	1.94	0.49
1:D:606:GLU:HB3	1:D:607:PHE:CE1	2.48	0.49
2:R:126:TYR:CE2	2:R:128:PRO:HG3	2.47	0.49
1:C:401:MET:HG3	1:C:578:MET:CE	2.43	0.48
1:D:283:ASP:HA	1:D:341:VAL:HG13	1.95	0.48
2:R:158:ARG:CB	2:R:158:ARG:HH11	2.26	0.48
1:I:608:SER:CB	2:U:280:ARG:NH1	2.76	0.48
2:M:175:ARG:NH2	2:M:237:MET:HB3	2.28	0.48
2:S:245:GLY:O	2:S:247:ASN:N	2.44	0.48
1:I:385:GLU:HA	1:I:607:PHE:HZ	1.76	0.48
1:C:581:TRP:CZ3	1:C:603:LEU:HB3	2.48	0.48
1:C:375:MET:HE1	1:C:387:TRP:CE2	2.47	0.48
1:C:346:ALA:C	1:C:348:LYS:H	2.15	0.48
1:A:391:VAL:HG13	1:A:578:MET:HB2	1.95	0.48
1:I:408:PHE:HB2	1:I:422:TRP:CH2	2.49	0.48
1:A:511:LYS:HB3	1:A:516:LYS:CG	2.43	0.48
1:K:556:CYS:SG	1:K:625:VAL:HG13	2.54	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:189:ALA:HB2	2:R:205:TYR:CZ	2.49	0.48
1:J:311:PRO:C	1:J:313:HIS:H	2.17	0.48
1:K:510:GLU:HA	1:K:516:LYS:HA	1.96	0.48
1:F:623:ILE:HG22	1:F:624:GLY:N	2.26	0.48
2:Q:259:ASP:OD2	2:Q:263:ASN:HB2	2.13	0.48
1:H:383:ASP:OD1	1:H:385:GLU:HB3	2.13	0.48
1:J:537:LEU:HG	1:J:541:PHE:CE1	2.48	0.48
2:Q:94:SER:HB3	2:Q:211:THR:O	2.14	0.48
1:K:456:ARG:HG3	1:K:456:ARG:HH11	1.77	0.48
1:J:525:ILE:HG22	1:J:526:VAL:N	2.28	0.48
2:T:280:ARG:HH11	2:T:280:ARG:HG2	1.78	0.48
2:Q:175:ARG:HD2	2:Q:193:HIS:O	2.13	0.48
1:A:453:PRO:HG2	1:F:454:LEU:O	2.13	0.48
1:A:375:MET:O	1:A:382:ALA:HB3	2.13	0.48
2:S:175:ARG:NH2	2:S:237:MET:HB3	2.28	0.48
1:H:581:TRP:HD1	1:H:582:TYR:CE1	2.32	0.48
1:C:497:LEU:O	1:C:500:TYR:HB2	2.13	0.48
1:G:520:ILE:HD12	1:G:520:ILE:N	2.28	0.48
1:K:592:ILE:O	1:K:596:ILE:HG12	2.12	0.48
2:S:132:LYS:HD3	2:S:134:PHE:CZ	2.49	0.48
1:K:617:PHE:O	1:K:621:MET:HG2	2.14	0.48
1:F:359:GLN:O	1:F:362:THR:HB	2.12	0.48
1:A:608:SER:OG	1:A:611:VAL:HG23	2.12	0.48
2:Q:126:TYR:OH	2:Q:131:ASN:HA	2.12	0.48
2:T:108:GLY:O	2:T:110:ARG:NH1	2.46	0.48
1:H:410:LYS:HA	1:H:410:LYS:HE2	1.94	0.48
2:Q:216:VAL:O	2:Q:216:VAL:HG13	2.13	0.48
1:G:445:GLY:HA3	1:G:469:LEU:O	2.13	0.48
1:C:593:GLN:HE22	2:O:177:PRO:HB2	1.79	0.48
1:K:425:LYS:HE2	1:K:530:GLU:HA	1.95	0.48
2:O:176:CYS:SG	2:O:179:HIS:N	2.73	0.48
1:I:592:ILE:O	1:I:595:ARG:N	2.43	0.48
1:I:322:ALA:O	1:I:326:ILE:HG12	2.12	0.48
1:L:428:ILE:O	1:L:429:ASP:HB2	2.13	0.48
2:O:197:VAL:HG22	2:O:234:TYR:CE1	2.48	0.48
2:U:244:GLY:O	2:U:246:MET:N	2.47	0.48
2:S:132:LYS:HE3	2:S:271:GLU:OE2	2.13	0.48
1:J:592:ILE:HG23	1:J:596:ILE:HD13	1.94	0.48
1:G:505:VAL:HG11	1:H:447:ALA:HB2	1.96	0.48
2:P:155:THR:HG23	2:P:258:GLU:O	2.13	0.48
1:F:583:ARG:HD3	1:F:587:GLU:OE1	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:349:ARG:HG2	1:B:349:ARG:NH1	2.28	0.48
1:E:293:LEU:HD21	1:E:333:GLN:NE2	2.29	0.48
2:S:197:VAL:HG11	2:S:218:VAL:HG11	1.96	0.48
2:U:245:GLY:C	2:U:247:ASN:H	2.17	0.48
1:D:269:SER:H	1:D:323:ASN:HD21	1.61	0.48
2:R:259:ASP:OD2	2:R:263:ASN:HB2	2.14	0.48
1:L:295:PHE:CD1	1:L:295:PHE:N	2.79	0.48
2:Q:244:GLY:O	2:Q:246:MET:N	2.46	0.48
1:B:419:LYS:HA	1:B:542:VAL:HG22	1.96	0.48
2:V:132:LYS:HE2	2:V:273:ARG:HB2	1.96	0.48
2:R:203:VAL:HG23	2:R:218:VAL:HG12	1.96	0.48
1:K:421:TYR:O	1:K:542:VAL:HG23	2.14	0.48
1:E:581:TRP:CZ3	1:E:603:LEU:HB3	2.49	0.48
2:V:245:GLY:C	2:V:247:ASN:H	2.17	0.48
2:N:245:GLY:C	2:N:247:ASN:H	2.16	0.48
1:A:538:GLN:HE22	1:A:544:GLN:NE2	2.12	0.48
1:E:583:ARG:HD3	1:E:587:GLU:OE1	2.13	0.48
1:C:532:SER:O	1:C:534:PRO:HD3	2.13	0.48
2:X:158:ARG:HH11	2:X:158:ARG:HB2	1.79	0.48
1:F:440:LEU:HD23	1:F:440:LEU:O	2.14	0.48
2:Q:224:GLU:H	2:Q:224:GLU:CD	2.16	0.48
1:D:415:ASN:HD21	1:D:420:ARG:NH1	2.03	0.48
1:C:451:ASN:HD21	1:C:476:LYS:N	2.12	0.48
1:L:465:ILE:O	1:L:466:ASP:HB2	2.12	0.48
1:K:511:LYS:HB3	1:K:514:LEU:HD12	1.94	0.48
1:L:357:ARG:HA	1:L:360:MET:HE3	1.96	0.48
1:F:550:LYS:HD3	1:F:552:TYR:CZ	2.49	0.48
2:P:197:VAL:HG11	2:P:218:VAL:HG11	1.96	0.48
1:F:270:TRP:CE2	1:F:336:ILE:HG12	2.48	0.48
2:W:259:ASP:OD2	2:W:263:ASN:HB2	2.12	0.48
1:I:327:PHE:C	1:I:329:ASP:H	2.15	0.48
2:R:125:THR:O	2:R:133:MET:HG3	2.14	0.48
1:D:481:GLU:H	1:D:481:GLU:CD	2.17	0.48
1:K:584:PRO:HD2	1:K:587:GLU:OE1	2.14	0.48
1:C:387:TRP:CE3	1:C:568:ILE:HG23	2.48	0.48
1:F:448:LEU:HD23	1:F:448:LEU:N	2.29	0.48
1:D:349:ARG:HE	1:D:517:ARG:HD2	1.79	0.48
2:R:197:VAL:HG23	2:R:216:VAL:HG21	1.94	0.48
1:D:308:LYS:HA	1:D:314:TYR:CD2	2.49	0.48
2:U:249:ARG:HG3	2:U:249:ARG:NH1	2.28	0.48
1:I:369:LEU:HD13	1:I:595:ARG:HD3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:295:PHE:HA	1:L:317:HIS:CD2	2.49	0.48
1:B:445:GLY:O	1:B:446:LYS:HG2	2.14	0.48
1:F:391:VAL:HG13	1:F:578:MET:HB2	1.96	0.48
2:P:198:GLU:HB2	2:P:235:ASN:ND2	2.29	0.47
1:L:423:LEU:HD12	1:L:526:VAL:O	2.13	0.47
1:K:596:ILE:HG22	1:K:600:LYS:HD2	1.95	0.47
1:I:588:PHE:HB3	1:I:592:ILE:CD1	2.43	0.47
1:J:554:LYS:O	1:J:558:GLU:HG3	2.14	0.47
1:F:435:LEU:HD23	1:F:547:PHE:HZ	1.79	0.47
1:F:462:GLY:C	1:F:464:ALA:H	2.18	0.47
1:D:336:ILE:O	1:D:337:CYS:C	2.50	0.47
1:L:469:LEU:C	1:L:469:LEU:HD12	2.34	0.47
1:H:500:TYR:O	1:H:521:PHE:HB3	2.14	0.47
1:C:454:LEU:C	1:C:456:ARG:N	2.68	0.47
1:I:415:ASN:HD21	1:I:420:ARG:HD2	1.76	0.47
1:C:473:GLU:CG	1:C:474:ASP:N	2.78	0.47
1:J:268:VAL:HG12	1:J:326:ILE:HB	1.96	0.47
1:L:356:THR:C	1:L:360:MET:HE2	2.35	0.47
1:E:464:ALA:HB2	1:E:470:VAL:HG11	1.95	0.47
2:R:186:ASP:OD1	2:R:189:ALA:HB3	2.14	0.47
2:P:164:LYS:HB3	2:P:250:PRO:HG2	1.96	0.47
1:K:344:VAL:HG12	1:K:344:VAL:O	2.13	0.47
1:B:269:SER:OG	1:B:272:LEU:HB2	2.13	0.47
1:F:452:LEU:HB3	1:F:453:PRO:HD2	1.95	0.47
1:A:398:LEU:HB2	1:A:401:MET:HE1	1.97	0.47
2:T:132:LYS:HD3	2:T:134:PHE:CZ	2.49	0.47
2:U:107:TYR:CE1	2:U:151:PRO:HA	2.50	0.47
1:I:497:LEU:O	1:I:500:TYR:HB2	2.14	0.47
1:H:588:PHE:CD2	1:H:596:ILE:HG12	2.49	0.47
1:K:270:TRP:CE2	1:L:331:LYS:HD3	2.49	0.47
1:K:317:HIS:O	1:K:320:HIS:N	2.46	0.47
1:C:445:GLY:HA3	1:C:469:LEU:HD23	1.97	0.47
1:C:270:TRP:CE2	1:C:336:ILE:HG12	2.50	0.47
1:E:267:GLN:CA	1:E:267:GLN:HE21	2.26	0.47
2:X:175:ARG:HD2	2:X:193:HIS:O	2.14	0.47
1:A:453:PRO:CG	1:F:454:LEU:HB3	2.41	0.47
1:L:583:ARG:NE	1:L:583:ARG:CA	2.75	0.47
1:C:500:TYR:O	1:C:521:PHE:HB3	2.14	0.47
2:U:173:VAL:HG11	2:U:194:LEU:HD12	1.97	0.47
1:E:402:ASP:N	1:E:578:MET:HE1	2.29	0.47
1:E:550:LYS:HD3	1:E:552:TYR:CE2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:136:GLN:CB	2:O:139:LYS:HG3	2.36	0.47
1:C:451:ASN:ND2	1:C:476:LYS:H	2.12	0.47
1:L:514:LEU:HD23	1:L:516:LYS:HG2	1.96	0.47
1:H:581:TRP:CZ3	1:H:603:LEU:HB3	2.49	0.47
1:K:529:ASN:O	1:K:530:GLU:CB	2.62	0.47
1:G:385:GLU:HA	1:G:607:PHE:CE2	2.49	0.47
1:B:497:LEU:O	1:B:500:TYR:HB2	2.14	0.47
1:G:462:GLY:HA3	1:G:510:GLU:O	2.14	0.47
2:Q:107:TYR:CE1	2:Q:151:PRO:HA	2.50	0.47
1:L:608:SER:HB3	2:X:280:ARG:NH1	2.30	0.47
2:X:252:LEU:HD12	2:X:270:PHE:O	2.14	0.47
1:D:317:HIS:HD2	1:D:317:HIS:O	1.97	0.47
1:B:272:LEU:HD23	1:B:323:ASN:HB2	1.97	0.47
2:N:156:ARG:HB3	2:N:217:VAL:HG12	1.97	0.47
1:G:469:LEU:O	1:G:469:LEU:HD12	2.14	0.47
2:X:203:VAL:HG22	2:X:204:GLU:N	2.30	0.47
2:R:156:ARG:HB3	2:R:217:VAL:HG12	1.96	0.47
1:C:584:PRO:C	1:C:586:ALA:H	2.18	0.47
1:B:356:THR:HG23	1:B:359:GLN:OE1	2.15	0.47
2:N:244:GLY:O	2:N:246:MET:N	2.47	0.47
1:I:401:MET:O	1:I:405:VAL:HG23	2.15	0.47
1:G:583:ARG:HD3	1:G:587:GLU:OE1	2.15	0.47
1:D:383:ASP:OD1	1:D:385:GLU:HB3	2.14	0.47
2:S:98:PRO:HD2	2:S:213:ARG:NH1	2.30	0.47
1:B:596:ILE:O	1:B:600:LYS:HG3	2.15	0.47
1:H:389:ALA:O	1:H:392:ALA:HB3	2.15	0.47
1:K:308:LYS:HA	1:K:314:TYR:CD2	2.50	0.47
2:S:112:GLY:HA3	2:S:146:TRP:HE1	1.80	0.47
1:F:594:SER:O	1:F:597:VAL:HB	2.13	0.47
1:B:270:TRP:H	1:B:270:TRP:HD1	1.60	0.47
1:E:314:TYR:CD1	1:E:314:TYR:C	2.88	0.47
1:A:311:PRO:O	1:A:315:LYS:HB2	2.14	0.47
1:C:391:VAL:HG22	1:C:574:ALA:O	2.15	0.47
1:G:525:ILE:HG22	1:G:526:VAL:N	2.29	0.47
1:C:299:PHE:CE1	1:C:318:GLU:HB2	2.49	0.47
1:A:561:GLU:O	1:A:563:LEU:N	2.47	0.47
1:D:513:HIS:ND1	1:E:512:LYS:HE2	2.30	0.47
1:H:415:ASN:HD21	1:H:420:ARG:HD2	1.79	0.47
1:H:450:VAL:HG23	1:H:457:LEU:HD11	1.96	0.47
1:H:288:LEU:O	1:H:289:LEU:C	2.53	0.47
2:Q:107:TYR:HD1	2:Q:149:SER:O	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:418:LYS:HE2	1:L:502:ASP:OD2	2.14	0.47
1:H:582:TYR:HD2	2:T:248:ARG:HH21	1.63	0.47
1:I:507:VAL:HG12	1:I:508:ASN:N	2.29	0.47
1:K:270:TRP:CE2	1:K:336:ILE:HG12	2.50	0.47
1:G:408:PHE:CD2	1:G:439:LEU:HD22	2.50	0.47
1:H:529:ASN:O	1:H:530:GLU:C	2.53	0.47
1:E:504:SER:OG	1:F:570:GLN:NE2	2.47	0.47
1:D:609:LEU:HD23	1:D:609:LEU:N	2.29	0.47
2:V:175:ARG:NH2	2:V:237:MET:HB3	2.30	0.47
1:A:408:PHE:CZ	1:A:525:ILE:HD11	2.50	0.47
1:D:517:ARG:HG3	1:D:517:ARG:HH11	1.79	0.47
1:F:602:ARG:HE	1:F:606:GLU:HG3	1.80	0.47
1:L:345:LEU:O	1:L:348:LYS:HB3	2.15	0.47
1:B:508:ASN:OD1	1:B:518:THR:HG23	2.15	0.47
2:W:189:ALA:HB2	2:W:205:TYR:CZ	2.50	0.47
1:J:308:LYS:HA	1:J:314:TYR:CD2	2.50	0.47
2:V:176:CYS:SG	2:V:178:HIS:HB3	2.55	0.47
2:U:120:LYS:HD2	2:U:120:LYS:N	2.30	0.47
1:G:287:LEU:O	1:G:291:MET:HG3	2.14	0.47
2:T:243:MET:CE	2:T:243:MET:CG	2.91	0.47
1:H:289:LEU:O	1:H:293:LEU:HG	2.15	0.47
1:L:270:TRP:CZ2	1:L:336:ILE:HG12	2.50	0.47
1:G:476:LYS:CE	1:L:496:ASN:ND2	2.77	0.47
2:S:158:ARG:NH1	2:S:217:VAL:HG21	2.30	0.47
2:U:134:PHE:N	2:U:134:PHE:CD1	2.83	0.47
1:F:324:ALA:O	1:F:327:PHE:HB3	2.15	0.47
1:K:282:CYS:SG	1:K:287:LEU:HD23	2.55	0.47
1:E:448:LEU:HD22	1:E:460:GLU:O	2.14	0.47
1:A:560:SER:OG	1:A:624:GLY:HA2	2.15	0.47
1:A:535:LYS:HG3	1:A:536:THR:N	2.30	0.47
1:G:440:LEU:HD12	1:G:471:VAL:CG2	2.45	0.47
1:J:513:HIS:O	1:K:512:LYS:HG2	2.15	0.46
1:K:386:GLU:OE1	1:K:566:LYS:HE3	2.15	0.46
1:K:456:ARG:HG3	1:K:456:ARG:NH1	2.30	0.46
1:H:495:ASP:OD1	1:I:486:PRO:HG2	2.15	0.46
1:B:405:VAL:HG21	1:B:575:LEU:HD22	1.95	0.46
1:H:445:GLY:O	1:H:446:LYS:HG2	2.15	0.46
1:I:503:GLY:HA2	1:I:520:ILE:HG23	1.96	0.46
1:C:614:LYS:O	1:C:617:PHE:HB3	2.14	0.46
1:B:393:TRP:CE2	1:B:553:LEU:HD22	2.50	0.46
1:G:475:VAL:CG1	1:G:491:ILE:HD12	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:372:MET:SD	1:A:576:LEU:HD23	2.55	0.46
1:I:581:TRP:O	2:U:245:GLY:HA3	2.16	0.46
1:K:412:MET:HE2	1:K:469:LEU:HD22	1.97	0.46
1:D:502:ASP:OD2	1:D:540:ARG:HD2	2.15	0.46
1:C:356:THR:OG1	1:C:359:GLN:HG3	2.15	0.46
1:B:459:PHE:C	1:B:461:LEU:H	2.17	0.46
1:E:493:ASN:HD22	1:E:493:ASN:N	2.13	0.46
1:I:361:LEU:HD11	1:I:409:LEU:HD22	1.98	0.46
2:T:191:PRO:HG2	2:T:192:GLN:HE21	1.80	0.46
1:E:333:GLN:HA	1:E:336:ILE:HD12	1.96	0.46
1:L:538:GLN:HE22	1:L:544:GLN:NE2	2.12	0.46
1:G:608:SER:CB	2:S:280:ARG:NH1	2.79	0.46
1:D:270:TRP:CE2	1:D:336:ILE:HG12	2.51	0.46
2:U:109:PHE:CE1	2:U:145:LEU:HG	2.51	0.46
2:N:98:PRO:HG2	2:N:162:ILE:HG21	1.96	0.46
1:B:418:LYS:HE3	1:B:540:ARG:HE	1.81	0.46
1:C:443:CYS:HB3	1:C:468:PHE:CD2	2.50	0.46
2:T:224:GLU:CD	2:T:224:GLU:H	2.19	0.46
1:G:280:THR:O	1:G:280:THR:HG22	2.15	0.46
1:H:280:THR:HG22	1:H:280:THR:O	2.16	0.46
1:K:266:LYS:O	1:K:326:ILE:HD12	2.15	0.46
1:B:449:ASN:HD21	1:B:451:ASN:CB	2.22	0.46
1:C:375:MET:O	1:C:382:ALA:HB3	2.15	0.46
1:J:375:MET:O	1:J:382:ALA:HB3	2.15	0.46
1:F:420:ARG:HD2	1:F:523:PRO:HB3	1.96	0.46
1:B:590:GLN:HA	1:B:593:GLN:NE2	2.31	0.46
1:B:508:ASN:ND2	1:C:463:VAL:HG11	2.30	0.46
2:O:236:TYR:CE2	2:O:272:VAL:HG11	2.51	0.46
1:B:430:SER:HB3	1:B:549:PRO:HG3	1.96	0.46
1:A:550:LYS:HB2	1:A:553:LEU:HD12	1.98	0.46
1:H:420:ARG:NH1	1:H:521:PHE:O	2.49	0.46
2:N:158:ARG:HH21	2:N:206:LEU:HD23	1.79	0.46
2:O:196:ARG:NH1	2:O:237:MET:HE1	2.30	0.46
2:P:109:PHE:CD1	2:P:257:LEU:HD22	2.50	0.46
2:V:134:PHE:O	2:V:278:PRO:HB3	2.16	0.46
2:O:285:GLU:HA	2:O:288:ASN:HD22	1.81	0.46
1:E:311:PRO:C	1:E:313:HIS:H	2.19	0.46
2:Q:97:VAL:CG1	2:Q:169:MET:HG2	2.45	0.46
1:H:295:PHE:HA	1:H:317:HIS:CD2	2.51	0.46
2:U:156:ARG:HH11	2:U:156:ARG:HG2	1.80	0.46
1:A:280:THR:O	1:A:280:THR:HG22	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:349:ARG:HD3	1:F:517:ARG:CZ	2.46	0.46
1:D:470:VAL:HG12	1:D:471:VAL:N	2.30	0.46
2:X:203:VAL:HA	2:X:218:VAL:HG12	1.98	0.46
1:E:269:SER:H	1:E:323:ASN:HD21	1.63	0.46
1:F:295:PHE:HE1	1:F:313:HIS:ND1	2.13	0.46
1:L:434:THR:HG23	1:L:570:GLN:HG2	1.97	0.46
1:J:298:SER:O	1:J:302:CYS:HB2	2.16	0.46
2:U:197:VAL:HG23	2:U:216:VAL:HG21	1.98	0.46
1:J:405:VAL:O	1:J:405:VAL:HG12	2.15	0.46
1:H:559:ARG:HG3	1:H:559:ARG:NH1	2.31	0.46
1:H:450:VAL:O	1:H:450:VAL:HG13	2.16	0.46
1:C:465:ILE:CG2	1:C:517:ARG:HE	2.28	0.46
2:X:132:LYS:HG3	2:X:271:GLU:HB3	1.97	0.46
1:L:423:LEU:HD11	1:L:528:MET:CE	2.45	0.46
2:M:190:PRO:HB2	2:M:193:HIS:HD2	1.80	0.46
2:V:198:GLU:HB2	2:V:235:ASN:ND2	2.30	0.46
2:P:196:ARG:NH1	2:P:237:MET:HE3	2.31	0.46
1:A:334:LYS:HD2	1:F:342:ASP:OD2	2.16	0.46
1:J:299:PHE:CE1	1:J:318:GLU:HG3	2.50	0.46
1:K:497:LEU:O	1:K:500:TYR:HB2	2.14	0.46
2:N:134:PHE:N	2:N:134:PHE:CD1	2.84	0.46
2:X:243:MET:CE	2:X:243:MET:CB	2.94	0.46
1:H:465:ILE:HD12	1:H:511:LYS:HB2	1.98	0.46
1:B:417:PRO:CG	1:C:567:ARG:HE	2.29	0.46
1:J:356:THR:HG23	1:J:359:GLN:OE1	2.16	0.46
2:S:191:PRO:HG2	2:S:192:GLN:HE21	1.79	0.46
2:V:134:PHE:CD1	2:V:134:PHE:N	2.84	0.46
2:T:186:ASP:OD1	2:T:189:ALA:HB3	2.16	0.46
1:F:308:LYS:HA	1:F:314:TYR:CD2	2.51	0.46
1:H:316:TYR:HB3	1:H:320:HIS:HD2	1.80	0.46
1:F:296:GLN:HG3	1:F:297:TYR:CD1	2.51	0.46
2:X:209:ARG:NH1	2:X:210:ASN:HD21	2.13	0.46
1:D:497:LEU:O	1:D:500:TYR:HB2	2.15	0.46
2:O:259:ASP:OD1	2:O:261:SER:N	2.47	0.46
1:I:475:VAL:O	1:I:475:VAL:HG23	2.15	0.46
1:H:608:SER:HA	2:T:280:ARG:NH1	2.30	0.46
2:U:282:ARG:O	2:U:286:GLU:HG3	2.16	0.46
1:K:283:ASP:CA	1:K:341:VAL:HG13	2.41	0.46
1:K:454:LEU:HA	1:K:457:LEU:HB2	1.98	0.46
1:G:476:LYS:HB3	1:G:488:GLY:HA3	1.98	0.46
1:D:414:TYR:HB3	1:D:416:ILE:HD11	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:583:ARG:HA	1:G:584:PRO:HD3	1.79	0.46
1:D:461:LEU:HD13	1:D:500:TYR:CE2	2.51	0.46
1:J:609:LEU:O	1:J:613:GLN:HB2	2.16	0.46
1:C:608:SER:HB3	1:C:611:VAL:HG23	1.98	0.46
1:C:349:ARG:O	1:C:353:LEU:HB2	2.15	0.46
1:C:349:ARG:CD	1:C:517:ARG:HD2	2.46	0.46
1:B:368:LEU:O	1:B:372:MET:HG3	2.15	0.46
2:U:136:GLN:HA	2:U:275:CYS:O	2.16	0.46
1:J:608:SER:C	1:J:610:SER:N	2.70	0.46
1:L:372:MET:SD	1:L:576:LEU:HD23	2.56	0.46
1:B:405:VAL:O	1:B:409:LEU:HG	2.16	0.46
1:L:276:TYR:HB2	1:L:320:HIS:CE1	2.51	0.46
2:W:97:VAL:HG13	2:W:169:MET:HG2	1.98	0.46
1:L:555:HIS:O	1:L:559:ARG:HD2	2.16	0.46
1:G:269:SER:HB3	1:G:323:ASN:OD1	2.16	0.46
1:I:344:VAL:O	1:I:348:LYS:HG3	2.15	0.46
2:U:287:GLU:C	2:U:289:LEU:H	2.19	0.46
2:T:180:GLU:O	2:T:180:GLU:HG3	2.14	0.46
2:U:158:ARG:HH12	2:U:217:VAL:HG11	1.80	0.45
1:C:349:ARG:CD	1:C:517:ARG:NH1	2.80	0.45
1:I:357:ARG:HA	1:I:360:MET:HE3	1.98	0.45
1:C:525:ILE:HG22	1:C:526:VAL:H	1.81	0.45
1:D:349:ARG:NH1	1:D:466:ASP:OD2	2.49	0.45
1:G:398:LEU:HB2	1:G:401:MET:HE2	1.98	0.45
2:N:147:VAL:HG22	2:N:149:SER:H	1.80	0.45
2:R:97:VAL:HG13	2:R:169:MET:HG2	1.98	0.45
1:H:311:PRO:HA	1:H:314:TYR:CE2	2.51	0.45
2:V:112:GLY:HA3	2:V:146:TRP:HE1	1.81	0.45
1:B:413:VAL:HG13	1:B:414:TYR:N	2.31	0.45
1:A:267:GLN:HG2	1:A:268:VAL:H	1.81	0.45
1:J:320:HIS:O	1:J:321:TYR:C	2.54	0.45
2:X:112:GLY:HA3	2:X:144:GLN:HB2	1.98	0.45
1:E:497:LEU:HB3	1:E:500:TYR:HB2	1.97	0.45
1:L:311:PRO:HA	1:L:314:TYR:CE2	2.51	0.45
2:O:180:GLU:HG3	2:O:180:GLU:O	2.16	0.45
1:B:353:LEU:HD12	1:C:287:LEU:HD13	1.97	0.45
2:Q:189:ALA:HA	2:Q:190:PRO:HD3	1.86	0.45
1:L:510:GLU:HG3	1:L:514:LEU:O	2.16	0.45
1:H:584:PRO:HD2	1:H:587:GLU:CG	2.44	0.45
1:A:454:LEU:N	1:A:454:LEU:HD12	2.32	0.45
1:I:570:GLN:HB3	1:I:570:GLN:HE21	1.62	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:432:LYS:HG3	1:E:433:THR:N	2.30	0.45
2:W:107:TYR:O	2:W:147:VAL:HG23	2.16	0.45
1:H:585:VAL:HG23	2:T:242:CYS:HA	1.98	0.45
2:R:112:GLY:HA3	2:R:144:GLN:HB2	1.98	0.45
2:T:145:LEU:HD21	2:T:157:VAL:HG21	1.97	0.45
1:H:430:SER:HB3	1:H:549:PRO:HG3	1.98	0.45
2:T:119:ALA:O	2:T:279:GLY:HA3	2.16	0.45
1:D:614:LYS:O	1:D:617:PHE:HB3	2.15	0.45
1:A:584:PRO:HB3	2:M:243:MET:HA	1.97	0.45
1:G:295:PHE:CD1	1:G:317:HIS:HA	2.51	0.45
1:J:353:LEU:HD12	1:K:287:LEU:HD13	1.98	0.45
1:D:608:SER:CB	2:P:280:ARG:HH11	2.29	0.45
1:A:268:VAL:HG12	1:A:269:SER:N	2.32	0.45
1:K:274:THR:O	1:K:277:ALA:HB3	2.17	0.45
1:G:537:LEU:HG	1:G:541:PHE:HE1	1.81	0.45
1:G:386:GLU:O	1:G:389:ALA:HB3	2.15	0.45
1:B:412:MET:HE1	1:B:523:PRO:C	2.36	0.45
1:E:351:ASP:HB3	1:E:355:LEU:CD1	2.38	0.45
1:E:351:ASP:OD1	1:E:355:LEU:HD11	2.17	0.45
1:B:474:ASP:HA	1:B:527:THR:O	2.17	0.45
1:H:432:LYS:HE3	1:H:433:THR:H	1.78	0.45
1:F:520:ILE:HD12	1:F:520:ILE:N	2.29	0.45
1:I:498:ARG:NH2	1:I:536:THR:HG21	2.32	0.45
2:X:217:VAL:HG12	2:X:218:VAL:N	2.30	0.45
1:B:585:VAL:HG12	1:B:593:GLN:HG2	1.97	0.45
1:F:372:MET:O	1:F:376:PHE:HB2	2.17	0.45
2:N:249:ARG:HG3	2:N:249:ARG:HH11	1.81	0.45
2:O:136:GLN:OE1	2:O:139:LYS:HE3	2.17	0.45
1:E:454:LEU:HD11	1:E:493:ASN:ND2	2.32	0.45
2:X:137:LEU:O	2:X:139:LYS:HG2	2.16	0.45
1:J:369:LEU:CB	1:J:595:ARG:HH11	2.28	0.45
1:C:497:LEU:HB3	1:C:500:TYR:HB2	1.99	0.45
1:E:418:LYS:HG2	1:E:502:ASP:OD1	2.16	0.45
2:P:252:LEU:HD12	2:P:271:GLU:HA	1.99	0.45
2:N:107:TYR:O	2:N:147:VAL:HG23	2.17	0.45
1:C:315:LYS:HB3	1:C:316:TYR:CE1	2.52	0.45
1:J:590:GLN:HA	1:J:593:GLN:OE1	2.16	0.45
1:E:419:LYS:HA	1:E:542:VAL:HG22	1.96	0.45
1:J:346:ALA:O	1:J:349:ARG:HB3	2.15	0.45
1:E:538:GLN:O	1:E:538:GLN:HG3	2.17	0.45
1:C:300:GLU:H	1:C:300:GLU:CD	2.20	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:446:LYS:CG	1:A:467:GLN:HE21	2.14	0.45
1:D:550:LYS:HD3	1:D:552:TYR:OH	2.16	0.45
1:F:514:LEU:HB3	1:F:516:LYS:HZ3	1.82	0.45
2:P:151:PRO:HB3	2:P:152:PRO:HD2	1.99	0.45
1:D:418:LYS:HE2	1:D:502:ASP:OD1	2.17	0.45
1:F:368:LEU:O	1:F:372:MET:HG3	2.17	0.45
1:F:288:LEU:HD23	1:F:337:CYS:HB3	1.98	0.45
1:H:425:LYS:HE2	1:H:528:MET:CE	2.47	0.45
2:W:211:THR:O	2:W:212:PHE:HB2	2.15	0.45
1:E:618:ASN:HA	1:E:623:ILE:HD11	1.98	0.45
1:F:583:ARG:HA	1:F:584:PRO:HD3	1.80	0.45
1:E:454:LEU:HD21	1:E:493:ASN:HD21	1.81	0.45
1:L:622:GLY:C	1:L:623:ILE:HD13	2.37	0.45
2:T:193:HIS:CE1	2:T:214:HIS:HB3	2.51	0.45
1:J:289:LEU:HD11	1:J:333:GLN:NE2	2.32	0.45
2:P:132:LYS:HG3	2:P:271:GLU:HB3	1.99	0.45
2:M:203:VAL:HA	2:M:218:VAL:HG12	1.98	0.45
1:H:423:LEU:HD23	1:H:544:GLN:HG3	1.99	0.45
1:K:295:PHE:HE1	1:K:313:HIS:ND1	2.15	0.45
1:G:441:GLU:HG2	1:G:572:GLY:H	1.82	0.45
2:N:166:SER:HA	2:N:169:MET:HB2	1.97	0.45
1:A:387:TRP:HZ3	1:A:571:SER:HG	1.62	0.45
2:S:224:GLU:CD	2:S:224:GLU:H	2.19	0.45
1:C:466:ASP:H	1:C:519:GLN:HE22	1.63	0.45
1:I:283:ASP:HA	1:I:341:VAL:HG13	1.98	0.45
1:F:497:LEU:HB3	1:F:500:TYR:HB2	1.99	0.45
2:P:287:GLU:C	2:P:289:LEU:H	2.20	0.45
1:J:470:VAL:O	1:J:524:GLY:HA3	2.16	0.45
1:L:515:ASN:O	1:L:517:ARG:N	2.50	0.45
1:C:381:SER:O	1:C:382:ALA:HB2	2.17	0.45
1:I:375:MET:O	1:I:382:ALA:HB3	2.17	0.45
1:H:432:LYS:HD2	1:H:433:THR:H	1.81	0.45
2:O:196:ARG:O	2:O:234:TYR:HA	2.17	0.45
1:A:368:LEU:O	1:A:372:MET:HG3	2.17	0.45
2:S:175:ARG:HD2	2:S:193:HIS:O	2.16	0.45
1:L:555:HIS:HA	1:L:558:GLU:OE1	2.17	0.45
1:G:271:LYS:HD2	1:H:329:ASP:OD1	2.16	0.45
1:F:433:THR:HG23	1:F:473:GLU:CD	2.37	0.45
2:X:126:TYR:O	2:X:282:ARG:CZ	2.65	0.45
2:W:98:PRO:HD2	2:W:213:ARG:NH1	2.32	0.45
1:E:469:LEU:HD12	1:E:469:LEU:C	2.37	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:410:LYS:HD3	1:I:410:LYS:HA	1.86	0.45
1:F:409:LEU:HD11	1:F:579:LEU:HD11	1.99	0.45
2:S:243:MET:HE3	2:S:243:MET:HB2	1.99	0.45
1:B:420:ARG:O	1:B:421:TYR:CD1	2.69	0.45
1:B:302:CYS:SG	1:B:305:CYS:N	2.90	0.45
1:D:498:ARG:NH2	1:E:476:LYS:HD3	2.32	0.45
1:J:398:LEU:HD21	1:J:545:ILE:HG21	1.99	0.45
1:D:470:VAL:O	1:D:524:GLY:HA3	2.17	0.45
1:G:412:MET:CE	1:G:524:GLY:HA2	2.47	0.45
1:C:581:TRP:HZ3	1:C:603:LEU:HB3	1.81	0.45
2:O:259:ASP:OD2	2:O:263:ASN:HB2	2.17	0.45
1:A:533:VAL:HG13	1:A:537:LEU:HD23	1.98	0.45
1:A:465:ILE:O	1:A:466:ASP:HB2	2.17	0.45
2:S:110:ARG:HA	2:S:268:ASN:HD21	1.82	0.45
1:B:470:VAL:O	1:B:524:GLY:HA3	2.17	0.44
1:A:388:MET:HA	1:A:391:VAL:HG23	1.98	0.44
2:U:151:PRO:HB3	2:U:152:PRO:HD2	1.99	0.44
1:I:435:LEU:HD23	1:I:547:PHE:HZ	1.82	0.44
1:J:562:PHE:N	1:J:562:PHE:CD2	2.86	0.44
2:R:282:ARG:O	2:R:286:GLU:HG3	2.17	0.44
1:B:443:CYS:HB3	1:B:468:PHE:CD2	2.51	0.44
1:F:348:LYS:NZ	1:F:348:LYS:HB2	2.33	0.44
2:P:190:PRO:HB2	2:P:193:HIS:CD2	2.53	0.44
1:E:493:ASN:N	1:E:493:ASN:ND2	2.64	0.44
1:L:608:SER:O	1:L:609:LEU:C	2.55	0.44
1:E:435:LEU:HD12	1:E:435:LEU:O	2.17	0.44
1:I:526:VAL:HG21	1:I:541:PHE:HE2	1.82	0.44
2:W:119:ALA:HB3	2:W:122:VAL:HG23	1.99	0.44
1:C:270:TRP:CD2	1:C:336:ILE:HG12	2.52	0.44
2:N:125:THR:OG1	2:N:126:TYR:N	2.49	0.44
1:C:580:ILE:HG21	1:C:599:TRP:HB3	1.99	0.44
1:A:288:LEU:HD23	1:A:288:LEU:O	2.16	0.44
1:H:288:LEU:HD23	1:H:337:CYS:HB3	1.99	0.44
1:L:268:VAL:HG12	1:L:326:ILE:HB	2.00	0.44
1:L:303:LEU:HD13	1:L:306:ILE:HD12	1.98	0.44
1:H:609:LEU:HD21	2:T:246:MET:HA	2.00	0.44
2:T:190:PRO:HB2	2:T:193:HIS:HD2	1.82	0.44
2:M:244:GLY:O	2:M:246:MET:N	2.50	0.44
2:S:280:ARG:HG2	2:S:280:ARG:HH11	1.81	0.44
1:D:270:TRP:HE3	1:D:339:GLN:HG2	1.82	0.44
2:N:160:MET:SD	2:N:213:ARG:HG2	2.57	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:211:THR:C	2:N:213:ARG:H	2.20	0.44
2:N:98:PRO:HD2	2:N:213:ARG:NH1	2.32	0.44
1:H:311:PRO:C	1:H:313:HIS:H	2.21	0.44
1:C:458:ASN:CG	1:D:456:ARG:HD3	2.38	0.44
1:F:338:GLN:HA	1:F:338:GLN:HE21	1.83	0.44
1:G:512:LYS:HD3	1:G:512:LYS:O	2.17	0.44
1:C:568:ILE:C	1:C:570:GLN:N	2.69	0.44
1:J:415:ASN:HD22	1:J:415:ASN:HA	1.59	0.44
1:B:283:ASP:CA	1:B:341:VAL:HG13	2.45	0.44
1:L:498:ARG:HB3	1:L:540:ARG:NH1	2.30	0.44
1:A:274:THR:HA	1:A:340:ALA:CB	2.47	0.44
2:Q:251:ILE:HG22	2:Q:252:LEU:N	2.32	0.44
1:H:615:MET:O	1:H:616:LYS:C	2.55	0.44
1:J:521:PHE:HA	1:J:522:PRO:HD3	1.89	0.44
1:F:456:ARG:HD2	1:F:456:ARG:N	2.32	0.44
1:I:469:LEU:HA	1:I:523:PRO:O	2.18	0.44
1:L:514:LEU:CG	1:L:516:LYS:HG2	2.47	0.44
1:C:421:TYR:CE1	1:C:523:PRO:HA	2.52	0.44
1:K:376:PHE:HE1	1:K:387:TRP:CD1	2.35	0.44
1:A:454:LEU:H	1:A:454:LEU:HD12	1.83	0.44
1:I:551:ASP:O	1:I:554:LYS:HB3	2.17	0.44
1:F:514:LEU:HD23	1:F:516:LYS:HZ2	1.82	0.44
2:O:158:ARG:HB3	2:O:256:THR:HB	1.99	0.44
1:B:270:TRP:N	1:B:270:TRP:CD1	2.85	0.44
1:C:576:LEU:O	1:C:580:ILE:HG12	2.18	0.44
1:E:388:MET:HG3	1:E:607:PHE:CE1	2.53	0.44
2:M:101:LYS:HB2	2:M:267:ARG:HH21	1.82	0.44
1:F:557:LEU:HD13	1:F:564:LEU:HD11	1.99	0.44
1:I:601:GLU:O	1:I:605:LYS:HB2	2.18	0.44
1:D:322:ALA:C	1:D:324:ALA:H	2.21	0.44
2:V:156:ARG:HB3	2:V:217:VAL:HG12	2.00	0.44
1:F:540:ARG:HG3	1:F:540:ARG:HH11	1.82	0.44
2:W:243:MET:CG	2:W:243:MET:CE	2.93	0.44
1:D:372:MET:HA	1:D:375:MET:HG2	1.99	0.44
2:P:158:ARG:CZ	2:P:217:VAL:HG21	2.47	0.44
1:D:314:TYR:CD1	1:D:315:LYS:HG2	2.53	0.44
2:N:103:TYR:CZ	2:N:105:GLY:HA2	2.52	0.44
2:W:107:TYR:OH	2:W:152:PRO:HD3	2.18	0.44
1:J:314:TYR:CD1	1:J:315:LYS:N	2.86	0.44
1:E:555:HIS:O	1:E:559:ARG:HD2	2.17	0.44
2:R:190:PRO:HB2	2:R:193:HIS:HD2	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:550:LYS:HD3	1:G:552:TYR:OH	2.18	0.44
1:K:406:TYR:CE1	1:K:587:GLU:HB3	2.53	0.44
2:U:161:ALA:HB2	2:U:195:ILE:CD1	2.41	0.44
1:J:402:ASP:CA	1:J:578:MET:HE3	2.44	0.44
1:J:508:ASN:ND2	1:K:463:VAL:HG11	2.33	0.44
1:D:402:ASP:HA	1:D:578:MET:CE	2.48	0.44
2:V:197:VAL:HG23	2:V:216:VAL:HG21	1.99	0.44
2:W:134:PHE:CD1	2:W:134:PHE:N	2.85	0.44
1:E:511:LYS:O	1:E:512:LYS:HB3	2.18	0.44
2:T:145:LEU:O	2:T:229:CYS:HB2	2.18	0.44
2:V:239:ASN:HA	2:V:274:VAL:HB	2.00	0.44
1:D:619:VAL:HG22	1:D:625:VAL:HG22	1.99	0.44
1:L:440:LEU:C	1:L:440:LEU:HD23	2.38	0.44
1:E:451:ASN:HD21	1:E:476:LYS:N	2.09	0.44
1:G:453:PRO:HD3	1:L:454:LEU:HD22	1.98	0.44
1:C:517:ARG:HH22	1:D:286:LEU:HD13	1.83	0.44
1:K:512:LYS:CG	1:K:513:HIS:H	2.21	0.44
1:K:566:LYS:HB2	1:K:568:ILE:HG13	1.98	0.44
1:F:303:LEU:O	1:F:306:ILE:HG22	2.17	0.44
1:D:593:GLN:O	1:D:596:ILE:HB	2.18	0.44
1:I:425:LYS:HZ3	1:I:530:GLU:HA	1.83	0.44
1:C:455:ASP:O	1:D:456:ARG:NH2	2.51	0.44
1:K:502:ASP:CG	1:K:540:ARG:HH11	2.21	0.44
2:U:98:PRO:HD2	2:U:213:ARG:NH1	2.33	0.44
2:Q:287:GLU:C	2:Q:289:LEU:H	2.22	0.44
1:F:535:LYS:HG3	1:F:536:THR:N	2.33	0.44
2:W:129:ALA:C	2:W:130:LEU:HD12	2.37	0.44
1:B:440:LEU:HD12	1:B:440:LEU:O	2.17	0.44
2:Q:158:ARG:NH1	2:Q:217:VAL:HG21	2.33	0.44
1:K:583:ARG:HA	1:K:584:PRO:HD3	1.83	0.44
1:J:420:ARG:HB3	1:J:523:PRO:CB	2.45	0.44
1:J:398:LEU:HB2	1:J:401:MET:CE	2.48	0.44
2:U:175:ARG:NH2	2:U:237:MET:HB3	2.33	0.44
1:L:583:ARG:HA	1:L:584:PRO:HD3	1.75	0.44
1:H:581:TRP:CE3	1:H:603:LEU:HD23	2.53	0.44
1:I:560:SER:OG	1:I:625:VAL:HG23	2.18	0.44
1:G:299:PHE:HA	1:G:317:HIS:CE1	2.53	0.44
1:A:581:TRP:O	1:A:581:TRP:CG	2.71	0.44
1:B:585:VAL:HG23	2:N:242:CYS:HA	2.00	0.44
2:N:177:PRO:O	2:N:181:ARG:HG3	2.18	0.44
1:D:608:SER:OG	1:D:611:VAL:HG23	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:269:SER:N	1:D:323:ASN:HD21	2.16	0.44
1:K:317:HIS:O	1:K:318:GLU:C	2.55	0.44
1:B:316:TYR:HB3	1:B:320:HIS:CD2	2.53	0.44
2:O:211:THR:C	2:O:213:ARG:H	2.22	0.44
1:J:394:LEU:O	1:J:397:LEU:HB3	2.17	0.44
2:W:203:VAL:HG22	2:W:204:GLU:N	2.33	0.44
2:N:93:LEU:HD22	2:N:171:GLU:HA	1.99	0.44
1:J:602:ARG:HD3	1:J:602:ARG:O	2.17	0.44
1:J:434:THR:HG23	1:J:570:GLN:CB	2.47	0.43
1:H:401:MET:HG3	1:H:578:MET:HE3	2.00	0.43
1:A:418:LYS:HZ3	1:A:540:ARG:HD3	1.80	0.43
1:K:284:ASP:HB3	1:K:287:LEU:HB3	2.00	0.43
1:C:295:PHE:HE1	1:C:313:HIS:ND1	2.15	0.43
2:O:282:ARG:O	2:O:286:GLU:HG3	2.18	0.43
1:J:469:LEU:C	1:J:469:LEU:HD12	2.38	0.43
1:D:469:LEU:C	1:D:469:LEU:HD12	2.39	0.43
1:B:495:ASP:HB3	1:C:476:LYS:NZ	2.33	0.43
1:G:288:LEU:HD13	1:G:337:CYS:SG	2.58	0.43
1:L:623:ILE:HG22	1:L:624:GLY:N	2.28	0.43
2:N:136:GLN:HB2	2:N:139:LYS:CG	2.45	0.43
1:H:583:ARG:HA	1:H:584:PRO:HD3	1.81	0.43
2:S:156:ARG:HH11	2:S:156:ARG:HG2	1.83	0.43
1:F:303:LEU:H	1:F:303:LEU:CD2	2.29	0.43
2:T:252:LEU:HD12	2:T:271:GLU:HA	2.00	0.43
1:F:302:CYS:SG	1:F:304:LYS:HB2	2.58	0.43
1:H:520:ILE:HD13	1:H:521:PHE:O	2.18	0.43
1:E:517:ARG:HG2	1:E:519:GLN:HG2	2.00	0.43
1:J:398:LEU:HA	1:J:399:PRO:HD3	1.90	0.43
1:C:424:PHE:O	1:C:527:THR:HA	2.18	0.43
1:A:369:LEU:HD23	1:A:372:MET:SD	2.57	0.43
1:B:386:GLU:HG2	1:B:562:PHE:CE1	2.53	0.43
1:F:412:MET:SD	1:F:523:PRO:HB2	2.59	0.43
1:E:581:TRP:CE3	1:E:603:LEU:HD23	2.53	0.43
1:L:295:PHE:HD1	1:L:295:PHE:N	2.17	0.43
1:C:557:LEU:HD23	1:C:563:LEU:HD12	2.00	0.43
1:I:400:LYS:O	1:I:403:SER:N	2.50	0.43
2:Q:110:ARG:HA	2:Q:268:ASN:ND2	2.32	0.43
2:S:222:PRO:HA	2:S:223:PRO:HD3	1.95	0.43
2:W:133:MET:HE1	2:W:141:CYS:HB3	1.99	0.43
1:D:588:PHE:CD1	1:D:588:PHE:N	2.86	0.43
1:G:513:HIS:O	1:G:514:LEU:HB2	2.16	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:349:ARG:NE	1:L:517:ARG:HD3	2.33	0.43
1:B:394:LEU:C	1:B:396:CYS:H	2.21	0.43
2:T:134:PHE:CD1	2:T:134:PHE:N	2.86	0.43
1:B:356:THR:HG23	1:B:359:GLN:CD	2.38	0.43
1:E:615:MET:O	1:E:619:VAL:HG23	2.18	0.43
1:F:514:LEU:HD12	1:F:515:ASN:H	1.84	0.43
1:E:588:PHE:CD2	1:E:596:ILE:HG12	2.53	0.43
1:I:500:TYR:CE1	1:I:507:VAL:HG11	2.53	0.43
1:K:398:LEU:HD21	1:K:545:ILE:HG21	2.00	0.43
1:F:313:HIS:C	1:F:315:LYS:H	2.22	0.43
2:W:98:PRO:HD2	2:W:213:ARG:HH12	1.82	0.43
1:A:521:PHE:HA	1:A:522:PRO:HD3	1.92	0.43
1:H:371:ARG:O	1:H:374:ILE:HG22	2.18	0.43
1:B:550:LYS:HD3	1:B:552:TYR:OH	2.18	0.43
1:B:452:LEU:HB3	1:B:453:PRO:CD	2.49	0.43
1:A:454:LEU:CB	1:B:453:PRO:HG2	2.49	0.43
2:T:132:LYS:HA	2:T:271:GLU:O	2.17	0.43
2:R:158:ARG:HG2	2:R:159:ALA:N	2.32	0.43
1:C:511:LYS:O	1:C:512:LYS:HG2	2.18	0.43
1:F:483:ARG:HG3	1:F:483:ARG:HH11	1.83	0.43
1:L:525:ILE:HG22	1:L:526:VAL:N	2.32	0.43
1:A:485:LEU:HD21	1:A:529:ASN:HD22	1.82	0.43
1:H:320:HIS:O	1:H:321:TYR:C	2.54	0.43
1:L:311:PRO:C	1:L:313:HIS:H	2.22	0.43
2:X:118:THR:HG22	2:X:282:ARG:HD3	2.00	0.43
1:H:269:SER:HB3	1:H:323:ASN:OD1	2.18	0.43
1:F:423:LEU:HD23	1:F:544:GLN:NE2	2.33	0.43
1:G:595:ARG:O	1:G:598:GLU:HB3	2.19	0.43
1:B:469:LEU:C	1:B:469:LEU:HD12	2.38	0.43
1:L:420:ARG:CB	1:L:523:PRO:HB3	2.49	0.43
1:G:285:VAL:O	1:G:288:LEU:N	2.52	0.43
1:C:346:ALA:HA	1:D:286:LEU:HD22	2.00	0.43
1:A:510:GLU:HB2	1:A:514:LEU:O	2.18	0.43
1:C:424:PHE:CZ	1:C:525:ILE:HD13	2.53	0.43
1:B:452:LEU:HB3	1:B:453:PRO:HD2	2.00	0.43
1:B:583:ARG:HA	1:B:584:PRO:HD3	1.78	0.43
1:E:408:PHE:O	1:E:412:MET:HG2	2.18	0.43
1:F:398:LEU:HB2	1:F:401:MET:CE	2.48	0.43
2:T:211:THR:C	2:T:213:ARG:H	2.21	0.43
1:E:339:GLN:HE22	1:F:331:LYS:HA	1.84	0.43
1:I:459:PHE:HZ	1:I:513:HIS:H	1.65	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:365:PHE:C	1:B:367:ASP:H	2.22	0.43
2:U:252:LEU:HD12	2:U:270:PHE:O	2.19	0.43
1:C:278:MET:C	1:C:280:THR:H	2.21	0.43
1:E:499:ASP:N	1:E:499:ASP:OD1	2.49	0.43
1:K:492:ASN:HD22	1:K:492:ASN:N	2.16	0.43
2:T:192:GLN:H	2:T:192:GLN:NE2	2.16	0.43
1:A:609:LEU:HD22	2:M:246:MET:CE	2.49	0.43
2:P:156:ARG:HB3	2:P:217:VAL:HG12	1.99	0.43
1:K:451:ASN:ND2	1:K:476:LYS:H	2.15	0.43
2:O:157:VAL:O	2:O:217:VAL:HA	2.19	0.43
1:I:351:ASP:C	1:I:353:LEU:H	2.21	0.43
1:K:510:GLU:HB3	1:K:516:LYS:HB3	1.99	0.43
1:E:512:LYS:HG3	1:E:513:HIS:N	2.34	0.43
2:U:109:PHE:HE1	2:U:145:LEU:HG	1.83	0.43
1:G:275:GLU:O	1:G:278:MET:HB2	2.18	0.43
1:F:291:MET:HE3	1:F:312:SER:HB2	2.00	0.43
1:L:391:VAL:HG13	1:L:578:MET:HB2	2.00	0.43
2:R:249:ARG:HG3	2:R:249:ARG:HH11	1.84	0.43
2:N:243:MET:CG	2:N:243:MET:CE	2.92	0.43
2:X:242:CYS:C	2:X:243:MET:HG3	2.39	0.43
1:B:517:ARG:HG2	1:B:517:ARG:HH11	1.83	0.43
1:B:311:PRO:C	1:B:313:HIS:H	2.22	0.43
1:J:454:LEU:HD22	1:K:453:PRO:CG	2.49	0.43
1:F:525:ILE:CG2	1:F:526:VAL:N	2.82	0.43
2:N:175:ARG:NH2	2:N:237:MET:HB3	2.33	0.43
1:D:350:VAL:O	1:D:354:GLN:HG3	2.18	0.43
1:L:608:SER:CB	2:X:280:ARG:NH1	2.82	0.43
1:A:581:TRP:HE1	2:M:246:MET:HE3	1.84	0.43
1:H:303:LEU:O	1:H:307:LYS:HG3	2.18	0.43
1:L:423:LEU:HD23	1:L:544:GLN:NE2	2.34	0.43
1:B:293:LEU:O	1:B:296:GLN:HG2	2.19	0.43
2:N:103:TYR:O	2:N:267:ARG:N	2.49	0.43
2:P:216:VAL:HG13	2:P:216:VAL:O	2.19	0.43
1:F:317:HIS:O	1:F:321:TYR:N	2.51	0.43
1:A:405:VAL:O	1:A:409:LEU:HG	2.19	0.43
1:H:270:TRP:CE2	1:H:336:ILE:HG12	2.54	0.43
1:D:435:LEU:HD23	1:D:547:PHE:HZ	1.84	0.43
2:S:243:MET:CE	2:S:243:MET:CB	2.95	0.43
1:D:393:TRP:NE1	1:D:557:LEU:HD13	2.33	0.43
1:I:409:LEU:HD23	1:I:409:LEU:HA	1.80	0.43
1:I:409:LEU:O	1:I:413:VAL:HG23	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:189:ALA:HA	2:N:190:PRO:HD3	1.91	0.43
2:T:258:GLU:HA	2:T:263:ASN:O	2.19	0.43
1:E:401:MET:HE1	1:E:435:LEU:HD22	2.01	0.43
1:C:395:HIS:HD2	1:C:616:LYS:HZ2	1.64	0.43
1:I:364:ARG:HG2	1:I:443:CYS:C	2.39	0.43
1:A:608:SER:C	1:A:610:SER:N	2.72	0.43
1:C:278:MET:O	1:C:280:THR:N	2.51	0.43
2:T:127:SER:O	2:T:131:ASN:N	2.49	0.43
2:P:99:SER:HB2	2:P:101:LYS:HG2	2.01	0.43
1:L:419:LYS:HA	1:L:542:VAL:HG13	2.00	0.43
1:H:424:PHE:O	1:H:527:THR:HA	2.18	0.43
1:C:357:ARG:NH1	1:C:357:ARG:HG2	2.34	0.43
1:F:477:GLY:O	1:F:487:SER:HA	2.18	0.43
1:J:502:ASP:CG	1:J:540:ARG:HD2	2.39	0.43
1:C:608:SER:HB2	2:O:280:ARG:HH11	1.84	0.43
2:N:158:ARG:HB3	2:N:256:THR:HB	2.01	0.43
1:D:559:ARG:HD3	1:D:623:ILE:HA	2.01	0.43
1:I:497:LEU:HB3	1:I:500:TYR:HB2	2.01	0.43
1:D:606:GLU:HB3	1:D:607:PHE:CD1	2.54	0.43
1:F:456:ARG:HG3	1:F:456:ARG:HH11	1.84	0.43
1:H:424:PHE:HB2	1:H:527:THR:HG22	2.01	0.43
1:G:473:GLU:HG3	1:L:505:VAL:HG21	2.00	0.43
2:V:102:THR:HG23	2:V:268:ASN:OD1	2.19	0.43
1:D:533:VAL:HA	1:D:534:PRO:HD3	1.92	0.43
1:E:456:ARG:HH11	1:E:456:ARG:HG3	1.84	0.43
1:H:547:PHE:N	1:H:547:PHE:CD1	2.87	0.43
1:B:280:THR:O	1:B:280:THR:HG22	2.19	0.43
1:B:272:LEU:HD12	1:B:272:LEU:HA	1.90	0.42
2:N:175:ARG:HD2	2:N:193:HIS:O	2.19	0.42
1:H:581:TRP:O	2:T:245:GLY:HA3	2.19	0.42
1:B:356:THR:OG1	1:B:359:GLN:HG3	2.19	0.42
2:R:241:SER:HA	2:R:245:GLY:H	1.83	0.42
2:O:109:PHE:CD1	2:O:257:LEU:HD22	2.54	0.42
1:B:410:LYS:HA	1:B:413:VAL:HG12	2.00	0.42
2:M:241:SER:HA	2:M:245:GLY:H	1.83	0.42
1:K:550:LYS:HD3	1:K:552:TYR:OH	2.18	0.42
1:C:591:SER:O	1:C:592:ILE:HG23	2.19	0.42
1:H:343:THR:O	1:H:346:ALA:HB3	2.19	0.42
1:L:395:HIS:CD2	1:L:582:TYR:OH	2.72	0.42
1:F:479:GLY:C	1:F:481:GLU:H	2.23	0.42
2:T:103:TYR:CZ	2:T:105:GLY:HA2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:583:ARG:H	1:F:583:ARG:HG2	1.62	0.42
1:C:454:LEU:HB2	1:D:453:PRO:CG	2.47	0.42
1:F:590:GLN:HA	1:F:593:GLN:CD	2.40	0.42
2:O:175:ARG:CZ	2:O:237:MET:HB3	2.49	0.42
1:K:440:LEU:HD13	1:K:471:VAL:HG23	2.01	0.42
1:C:584:PRO:C	1:C:586:ALA:N	2.71	0.42
1:D:564:LEU:O	1:D:566:LYS:N	2.52	0.42
1:I:609:LEU:O	1:I:613:GLN:HB2	2.18	0.42
1:G:351:ASP:HB3	1:G:355:LEU:HD12	2.00	0.42
2:N:151:PRO:HB3	2:N:152:PRO:HD2	2.01	0.42
1:C:529:ASN:HB2	1:C:531:TYR:CE1	2.54	0.42
1:B:445:GLY:C	1:B:446:LYS:HG2	2.39	0.42
1:D:538:GLN:C	1:D:540:ARG:H	2.22	0.42
1:A:484:ASP:O	1:F:535:LYS:HE2	2.20	0.42
2:X:177:PRO:O	2:X:181:ARG:HG3	2.19	0.42
1:I:289:LEU:HG	1:I:293:LEU:HD12	2.00	0.42
1:C:555:HIS:HB3	1:C:559:ARG:NH1	2.34	0.42
2:Q:119:ALA:O	2:Q:279:GLY:HA3	2.19	0.42
2:Q:122:VAL:HG12	2:Q:123:THR:N	2.35	0.42
2:U:166:SER:HA	2:U:169:MET:HB2	2.02	0.42
2:Q:222:PRO:HA	2:Q:223:PRO:HD3	1.95	0.42
1:G:455:ASP:O	1:H:456:ARG:HD2	2.19	0.42
1:G:387:TRP:CE3	1:G:568:ILE:HG23	2.53	0.42
2:V:103:TYR:O	2:V:266:GLY:HA2	2.19	0.42
1:C:499:ASP:N	1:C:499:ASP:OD2	2.49	0.42
1:F:582:TYR:O	1:F:583:ARG:C	2.58	0.42
1:H:511:LYS:HB3	1:H:515:ASN:HB3	2.02	0.42
1:B:311:PRO:HB3	1:B:315:LYS:HE2	2.01	0.42
1:K:394:LEU:HD21	1:K:569:ILE:O	2.19	0.42
2:N:158:ARG:HH21	2:N:206:LEU:HD22	1.84	0.42
1:D:371:ARG:O	1:D:375:MET:HG2	2.18	0.42
2:T:134:PHE:CD2	2:T:273:ARG:HD3	2.53	0.42
2:O:158:ARG:NH1	2:O:258:GLU:OE1	2.52	0.42
1:D:399:PRO:O	1:D:400:LYS:HB2	2.19	0.42
1:G:505:VAL:HG21	1:H:473:GLU:HG3	2.01	0.42
1:J:299:PHE:CD1	1:J:318:GLU:HG3	2.55	0.42
1:G:529:ASN:HB2	1:G:531:TYR:CE1	2.54	0.42
2:R:103:TYR:CZ	2:R:105:GLY:HA2	2.54	0.42
1:E:534:PRO:HB3	1:F:486:PRO:CG	2.48	0.42
1:D:537:LEU:HG	1:D:541:PHE:CE1	2.54	0.42
2:X:133:MET:CE	2:X:141:CYS:SG	3.07	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:424:PHE:O	1:L:527:THR:HA	2.18	0.42
1:F:542:VAL:HG22	1:F:542:VAL:O	2.19	0.42
1:I:510:GLU:HG2	1:I:511:LYS:N	2.35	0.42
1:I:512:LYS:HD3	1:I:516:LYS:HZ1	1.84	0.42
1:L:349:ARG:NH2	1:L:517:ARG:HG3	2.34	0.42
1:J:420:ARG:NE	1:J:503:GLY:HA3	2.35	0.42
1:D:305:CYS:SG	1:D:313:HIS:NE2	2.92	0.42
1:J:283:ASP:HA	1:J:341:VAL:HG13	2.02	0.42
2:R:216:VAL:O	2:R:216:VAL:HG13	2.19	0.42
2:R:185:SER:HA	2:R:196:ARG:HH22	1.84	0.42
1:I:525:ILE:CG2	1:I:526:VAL:N	2.83	0.42
2:P:239:ASN:HB2	2:P:242:CYS:SG	2.59	0.42
1:E:372:MET:CG	1:E:573:ILE:HD12	2.50	0.42
1:H:385:GLU:HA	1:H:607:PHE:CZ	2.54	0.42
2:O:249:ARG:O	2:O:251:ILE:HD12	2.20	0.42
2:N:176:CYS:SG	2:N:178:HIS:HB3	2.59	0.42
1:D:298:SER:HA	1:D:321:TYR:CE1	2.54	0.42
2:R:134:PHE:CD1	2:R:134:PHE:N	2.87	0.42
1:B:448:LEU:HG	1:B:470:VAL:HG13	2.01	0.42
1:E:520:ILE:HD12	1:F:567:ARG:NH1	2.28	0.42
1:L:514:LEU:HD12	1:L:515:ASN:N	2.31	0.42
1:L:268:VAL:HG21	1:L:336:ILE:HD13	2.01	0.42
1:F:590:GLN:H	1:F:590:GLN:CD	2.22	0.42
1:C:507:VAL:N	1:C:519:GLN:O	2.51	0.42
1:A:502:ASP:CG	1:A:540:ARG:HE	2.23	0.42
1:A:451:ASN:OD1	1:A:476:LYS:HB2	2.19	0.42
1:K:465:ILE:HD12	1:K:511:LYS:CG	2.49	0.42
2:P:107:TYR:CE1	2:P:151:PRO:HA	2.54	0.42
1:B:602:ARG:O	1:B:602:ARG:HD2	2.18	0.42
1:G:311:PRO:C	1:G:313:HIS:N	2.71	0.42
2:O:145:LEU:HD21	2:O:157:VAL:HG21	2.00	0.42
1:I:590:GLN:HA	1:I:593:GLN:HG3	2.01	0.42
1:J:562:PHE:CE2	1:J:563:LEU:HG	2.55	0.42
1:C:458:ASN:OD1	1:D:456:ARG:HD3	2.20	0.42
1:D:322:ALA:O	1:D:326:ILE:HG13	2.18	0.42
1:B:364:ARG:O	1:B:367:ASP:HB2	2.18	0.42
1:C:592:ILE:O	1:C:596:ILE:HG12	2.19	0.42
1:H:456:ARG:HG2	1:H:456:ARG:HH11	1.85	0.42
1:F:428:ILE:O	1:F:429:ASP:HB2	2.19	0.42
2:Q:236:TYR:CE2	2:Q:272:VAL:HG11	2.54	0.42
1:G:618:ASN:OD1	1:G:623:ILE:HD11	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:317:HIS:O	1:I:321:TYR:N	2.52	0.42
1:C:535:LYS:HD2	1:D:484:ASP:HB2	2.01	0.42
1:B:448:LEU:HD22	1:B:463:VAL:HG23	2.01	0.42
1:F:386:GLU:HB3	1:F:562:PHE:HE1	1.85	0.42
1:D:354:GLN:CB	1:E:310:GLN:HE21	2.31	0.42
2:O:107:TYR:O	2:O:147:VAL:HG23	2.19	0.42
1:J:389:ALA:HB1	1:J:625:VAL:CG2	2.45	0.42
2:S:158:ARG:HH21	2:S:206:LEU:CD2	2.32	0.42
2:S:122:VAL:CG1	2:S:123:THR:N	2.83	0.42
1:E:423:LEU:HD22	1:E:541:PHE:CD1	2.55	0.42
2:P:151:PRO:HD2	2:P:220:TYR:CE2	2.54	0.42
2:S:203:VAL:HA	2:S:218:VAL:HG12	2.01	0.42
2:T:173:VAL:CG1	2:T:194:LEU:HD12	2.49	0.42
1:F:302:CYS:SG	1:F:305:CYS:N	2.90	0.42
1:F:609:LEU:O	1:F:613:GLN:HG3	2.19	0.42
2:Q:168:HIS:O	2:Q:171:GLU:N	2.46	0.42
1:J:270:TRP:CE2	1:J:336:ILE:HG12	2.55	0.42
1:L:507:VAL:N	1:L:519:GLN:O	2.52	0.42
1:B:420:ARG:NH2	1:B:521:PHE:O	2.49	0.42
1:A:568:ILE:C	1:A:570:GLN:H	2.21	0.42
1:F:608:SER:O	1:F:611:VAL:HB	2.20	0.42
1:K:386:GLU:O	1:K:389:ALA:HB3	2.20	0.42
2:W:251:ILE:CG2	2:W:252:LEU:N	2.83	0.42
1:I:311:PRO:C	1:I:313:HIS:N	2.73	0.42
1:J:589:ALA:C	1:J:591:SER:N	2.72	0.42
1:F:401:MET:HG3	1:F:578:MET:HE3	2.01	0.42
1:B:422:TRP:O	1:B:525:ILE:HA	2.20	0.42
1:I:394:LEU:HD21	1:I:569:ILE:O	2.20	0.42
1:I:454:LEU:C	1:I:456:ARG:H	2.23	0.42
1:B:353:LEU:HD21	1:B:517:ARG:NH2	2.35	0.42
2:N:158:ARG:NH1	2:N:217:VAL:HG21	2.34	0.42
1:D:557:LEU:C	1:D:559:ARG:H	2.23	0.42
1:F:590:GLN:N	1:F:590:GLN:OE1	2.53	0.42
2:O:175:ARG:NE	2:O:237:MET:HB2	2.35	0.42
1:H:517:ARG:CG	1:H:519:GLN:HG2	2.48	0.42
1:B:625:VAL:HG23	1:B:626:LEU:N	2.34	0.42
1:C:584:PRO:HG3	2:O:243:MET:O	2.20	0.42
1:I:609:LEU:HD13	2:U:246:MET:SD	2.60	0.42
1:J:353:LEU:HD21	1:J:517:ARG:HH12	1.83	0.42
1:I:295:PHE:HA	1:I:317:HIS:CD2	2.55	0.42
1:B:521:PHE:HA	1:B:522:PRO:HD3	1.86	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:175:ARG:HG3	2:R:192:GLN:C	2.40	0.42
1:K:507:VAL:N	1:K:519:GLN:O	2.53	0.42
1:I:372:MET:SD	1:I:576:LEU:HD23	2.60	0.42
1:D:580:ILE:CD1	1:D:596:ILE:HG23	2.50	0.42
1:I:346:ALA:O	1:I:350:VAL:HG23	2.20	0.42
1:G:608:SER:CB	2:S:280:ARG:HH11	2.32	0.42
1:D:398:LEU:HA	1:D:399:PRO:HD3	1.94	0.42
2:Q:264:LEU:HD11	2:Q:267:ARG:HB2	2.02	0.42
1:I:615:MET:O	1:I:619:VAL:HG23	2.19	0.42
1:B:267:GLN:HG2	1:B:267:GLN:H	1.64	0.42
1:J:371:ARG:O	1:J:375:MET:HG2	2.20	0.42
1:J:372:MET:C	1:J:374:ILE:H	2.21	0.42
2:R:107:TYR:O	2:R:147:VAL:HG23	2.19	0.42
1:C:500:TYR:CE2	1:C:507:VAL:HG11	2.54	0.42
2:T:160:MET:HG3	2:T:214:HIS:O	2.20	0.42
1:E:561:GLU:O	1:E:565:GLU:HG3	2.20	0.42
1:I:609:LEU:HD13	2:U:246:MET:CE	2.50	0.42
2:T:216:VAL:O	2:T:216:VAL:HG13	2.20	0.42
1:F:295:PHE:HA	1:F:317:HIS:CE1	2.55	0.42
1:I:299:PHE:CE1	1:I:318:GLU:HB2	2.55	0.42
1:D:386:GLU:O	1:D:389:ALA:HB3	2.20	0.42
1:A:599:TRP:O	1:A:603:LEU:HB2	2.20	0.42
2:W:104:GLN:HB3	2:W:108:GLY:HA2	2.02	0.42
1:K:495:ASP:O	1:K:498:ARG:HG3	2.20	0.42
2:O:276:ALA:C	2:O:278:PRO:HD3	2.40	0.42
1:J:605:LYS:O	1:J:605:LYS:HG2	2.20	0.42
1:C:520:ILE:CD1	1:C:520:ILE:N	2.79	0.41
1:D:454:LEU:HA	1:D:457:LEU:HB2	2.01	0.41
2:V:236:TYR:CZ	2:V:272:VAL:HG11	2.55	0.41
1:A:385:GLU:HA	1:A:607:PHE:HZ	1.85	0.41
1:C:389:ALA:HA	1:C:615:MET:SD	2.60	0.41
1:B:590:GLN:C	1:B:592:ILE:H	2.23	0.41
1:D:608:SER:HB3	2:P:280:ARG:NH1	2.35	0.41
2:O:114:LEU:N	2:O:114:LEU:CD1	2.83	0.41
2:M:251:ILE:N	2:M:251:ILE:HD12	2.35	0.41
1:J:562:PHE:N	1:J:562:PHE:HD2	2.18	0.41
1:A:409:LEU:O	1:A:413:VAL:HG23	2.19	0.41
1:L:424:PHE:HB2	1:L:527:THR:HG22	2.02	0.41
2:N:145:LEU:HD21	2:N:157:VAL:HG21	2.02	0.41
2:W:126:TYR:OH	2:W:131:ASN:HA	2.20	0.41
1:C:449:ASN:ND2	1:C:452:LEU:HG	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:592:ILE:O	1:L:593:GLN:C	2.58	0.41
2:R:120:LYS:N	2:R:120:LYS:HD2	2.35	0.41
1:C:517:ARG:HH22	1:D:286:LEU:CD1	2.32	0.41
1:D:520:ILE:O	1:D:521:PHE:C	2.58	0.41
1:C:439:LEU:HD13	1:C:525:ILE:HD11	2.02	0.41
1:B:569:ILE:HD13	1:B:570:GLN:OE1	2.20	0.41
1:J:579:LEU:O	1:J:581:TRP:N	2.53	0.41
1:C:590:GLN:HA	1:C:593:GLN:CG	2.50	0.41
1:J:507:VAL:HG12	1:J:508:ASN:N	2.35	0.41
1:H:303:LEU:C	1:H:305:CYS:H	2.23	0.41
1:L:356:THR:O	1:L:357:ARG:C	2.59	0.41
1:I:508:ASN:OD1	1:I:518:THR:HG23	2.20	0.41
1:G:594:SER:HA	2:S:178:HIS:CD2	2.55	0.41
1:E:303:LEU:O	1:E:307:LYS:HB2	2.20	0.41
2:V:127:SER:O	2:V:131:ASN:N	2.52	0.41
2:Q:97:VAL:HG13	2:Q:169:MET:HG2	2.02	0.41
2:X:112:GLY:CA	2:X:144:GLN:HB2	2.50	0.41
2:U:211:THR:OG1	2:U:213:ARG:HB2	2.19	0.41
1:F:612:TYR:HA	1:F:615:MET:HE3	2.01	0.41
1:C:394:LEU:HD21	1:C:569:ILE:O	2.21	0.41
1:C:408:PHE:HA	1:C:422:TRP:CZ2	2.55	0.41
1:C:288:LEU:HG	1:C:337:CYS:SG	2.61	0.41
1:H:368:LEU:HD22	1:H:573:ILE:HD13	2.02	0.41
1:H:394:LEU:HD21	1:H:569:ILE:O	2.20	0.41
2:N:120:LYS:HD2	2:N:120:LYS:N	2.35	0.41
1:E:415:ASN:HD22	1:E:420:ARG:HD2	1.80	0.41
1:B:311:PRO:C	1:B:313:HIS:N	2.73	0.41
1:G:510:GLU:O	1:G:511:LYS:HB3	2.21	0.41
1:E:349:ARG:HG2	1:E:349:ARG:HH11	1.85	0.41
1:I:597:VAL:O	1:I:600:LYS:HB2	2.20	0.41
1:J:568:ILE:C	1:J:570:GLN:N	2.73	0.41
1:J:360:MET:HB2	1:J:360:MET:HE2	1.97	0.41
1:A:418:LYS:HZ2	1:A:540:ARG:HD3	1.82	0.41
1:A:625:VAL:HG23	1:A:626:LEU:N	2.35	0.41
1:D:512:LYS:HD3	1:D:514:LEU:HD21	2.02	0.41
1:F:382:ALA:HB1	1:F:387:TRP:NE1	2.35	0.41
2:Q:218:VAL:HA	2:Q:219:PRO:HD3	1.92	0.41
1:J:590:GLN:HA	1:J:593:GLN:CD	2.40	0.41
1:H:299:PHE:CZ	1:H:318:GLU:HG3	2.55	0.41
1:H:614:LYS:O	1:H:617:PHE:HB3	2.20	0.41
1:L:387:TRP:CE3	1:L:568:ILE:HG23	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:283:ASP:HA	1:G:341:VAL:HG13	2.02	0.41
1:F:465:ILE:HD11	1:F:509:LEU:HB2	2.03	0.41
1:J:568:ILE:O	1:J:570:GLN:N	2.54	0.41
2:O:151:PRO:HB3	2:O:152:PRO:HD2	2.02	0.41
1:L:498:ARG:O	1:L:502:ASP:HB2	2.20	0.41
1:H:356:THR:O	1:H:359:GLN:N	2.51	0.41
2:S:192:GLN:HB2	2:S:214:HIS:HE1	1.86	0.41
1:B:581:TRP:HE1	2:N:246:MET:HE3	1.84	0.41
2:U:132:LYS:HB3	2:U:134:PHE:HE1	1.85	0.41
1:K:291:MET:HG2	1:K:291:MET:H	1.65	0.41
2:M:110:ARG:HH11	2:M:110:ARG:HG3	1.86	0.41
1:K:502:ASP:OD1	1:K:540:ARG:NH1	2.52	0.41
2:P:189:ALA:HB2	2:P:205:TYR:CZ	2.56	0.41
2:P:211:THR:OG1	2:P:213:ARG:HB2	2.21	0.41
2:S:242:CYS:O	2:S:243:MET:HG3	2.20	0.41
1:E:417:PRO:HG3	1:F:567:ARG:CZ	2.50	0.41
1:F:349:ARG:NE	1:F:517:ARG:NE	2.69	0.41
1:K:489:GLN:O	1:K:490:GLY:C	2.58	0.41
1:D:521:PHE:HA	1:D:522:PRO:HD3	1.94	0.41
1:D:295:PHE:HE1	1:D:313:HIS:ND1	2.18	0.41
1:J:369:LEU:HD23	1:J:372:MET:SD	2.60	0.41
2:X:280:ARG:HG2	2:X:280:ARG:HH11	1.85	0.41
1:B:369:LEU:HB2	1:B:595:ARG:NH1	2.32	0.41
1:L:540:ARG:HA	1:L:540:ARG:HD3	1.89	0.41
1:D:589:ALA:O	1:D:590:GLN:C	2.58	0.41
1:K:623:ILE:HG12	1:K:624:GLY:N	2.34	0.41
1:J:493:ASN:O	1:J:497:LEU:HG	2.20	0.41
1:E:357:ARG:HA	1:E:360:MET:HE2	2.02	0.41
1:C:369:LEU:O	1:C:372:MET:HB2	2.19	0.41
1:I:567:ARG:HG2	1:I:567:ARG:HH11	1.85	0.41
2:U:158:ARG:NH1	2:U:217:VAL:HG11	2.35	0.41
1:D:285:VAL:HG21	1:D:338:GLN:HE21	1.82	0.41
1:H:296:GLN:HG3	1:H:297:TYR:N	2.36	0.41
1:J:557:LEU:HD21	1:J:564:LEU:HD21	2.01	0.41
2:S:105:GLY:HA3	2:S:265:LEU:O	2.20	0.41
1:F:420:ARG:NH1	1:F:521:PHE:O	2.52	0.41
1:B:593:GLN:HE21	2:N:181:ARG:HH22	1.69	0.41
1:A:485:LEU:HD22	1:A:529:ASN:HD22	1.84	0.41
2:N:245:GLY:O	2:N:247:ASN:N	2.50	0.41
1:K:271:LYS:O	1:K:274:THR:HB	2.21	0.41
1:E:623:ILE:HD13	1:E:623:ILE:H	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:500:TYR:O	1:A:521:PHE:HB3	2.20	0.41
2:R:236:TYR:CE2	2:R:272:VAL:HG11	2.55	0.41
2:R:239:ASN:HA	2:R:274:VAL:HB	2.02	0.41
2:W:145:LEU:HD21	2:W:157:VAL:HG11	2.01	0.41
2:W:111:LEU:CD1	2:W:268:ASN:HB3	2.51	0.41
2:M:134:PHE:N	2:M:134:PHE:CD1	2.88	0.41
1:G:465:ILE:O	1:G:466:ASP:HB2	2.20	0.41
1:B:503:GLY:O	1:C:567:ARG:NH2	2.53	0.41
1:H:356:THR:O	1:H:357:ARG:C	2.59	0.41
2:S:264:LEU:O	2:S:265:LEU:HD23	2.21	0.41
1:A:448:LEU:HG	1:A:470:VAL:HG22	2.00	0.41
1:C:448:LEU:HD23	1:C:448:LEU:N	2.33	0.41
2:R:277:CYS:HB3	2:R:280:ARG:HB3	2.03	0.41
1:J:425:LYS:HE2	1:J:530:GLU:HA	2.03	0.41
1:F:314:TYR:CD1	1:F:314:TYR:C	2.94	0.41
1:F:372:MET:C	1:F:374:ILE:H	2.23	0.41
2:S:189:ALA:HB2	2:S:205:TYR:CZ	2.56	0.41
1:K:399:PRO:O	1:K:400:LYS:HB2	2.21	0.41
1:A:290:GLY:CA	1:F:346:ALA:HB1	2.51	0.41
1:K:297:TYR:O	1:K:321:TYR:CD1	2.74	0.41
1:K:604:ASP:C	1:K:606:GLU:N	2.74	0.41
1:L:520:ILE:CD1	1:L:520:ILE:N	2.80	0.41
1:B:306:ILE:HD12	1:B:306:ILE:C	2.41	0.41
1:B:311:PRO:O	1:B:315:LYS:HB2	2.21	0.41
1:C:465:ILE:HD13	1:C:517:ARG:HB2	2.02	0.41
1:C:583:ARG:HA	1:C:584:PRO:HD3	1.77	0.41
1:A:417:PRO:O	1:A:418:LYS:HB3	2.20	0.41
1:K:369:LEU:O	1:K:370:ASP:C	2.58	0.41
1:C:383:ASP:HB3	1:C:386:GLU:CG	2.48	0.41
2:M:197:VAL:HB	2:M:203:VAL:HG21	2.02	0.41
2:U:156:ARG:NH1	2:U:156:ARG:HG2	2.36	0.41
1:G:369:LEU:HB3	1:G:595:ARG:HH21	1.86	0.41
1:B:597:VAL:C	1:B:599:TRP:N	2.74	0.41
1:E:452:LEU:HB3	1:E:453:PRO:CD	2.51	0.41
1:E:375:MET:O	1:E:380:GLY:HA3	2.20	0.41
2:V:207:ASP:O	2:V:208:ASP:C	2.59	0.41
1:A:618:ASN:O	1:A:622:GLY:N	2.53	0.41
1:L:397:LEU:HB3	1:L:401:MET:CE	2.51	0.41
1:H:449:ASN:HD22	1:H:451:ASN:H	1.68	0.41
1:A:399:PRO:O	1:A:400:LYS:HB2	2.21	0.41
1:C:332:ASN:ND2	1:C:332:ASN:N	2.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:242:CYS:C	2:S:243:MET:HG3	2.41	0.41
1:H:520:ILE:HD13	1:H:520:ILE:C	2.41	0.41
1:B:311:PRO:HA	1:B:314:TYR:CE2	2.56	0.41
1:B:305:CYS:HA	1:B:314:TYR:HB3	2.01	0.41
1:L:462:GLY:HA3	1:L:510:GLU:O	2.21	0.41
1:G:286:LEU:HB2	1:L:517:ARG:HH22	1.86	0.41
1:L:496:ASN:HD22	1:L:496:ASN:N	2.19	0.41
1:J:375:MET:HG3	1:J:376:PHE:CD2	2.56	0.41
2:O:190:PRO:HD2	2:O:193:HIS:CD2	2.56	0.41
1:I:306:ILE:HG23	1:I:307:LYS:N	2.34	0.41
1:J:458:ASN:HA	1:J:458:ASN:HD22	1.61	0.41
2:R:160:MET:CE	2:R:213:ARG:HB3	2.50	0.41
1:E:525:ILE:HG22	1:E:526:VAL:N	2.36	0.41
2:W:282:ARG:HE	2:W:286:GLU:CD	2.24	0.41
2:P:272:VAL:HG12	2:P:273:ARG:N	2.35	0.41
1:I:583:ARG:HA	1:I:584:PRO:HD3	1.78	0.41
1:C:609:LEU:HA	2:O:246:MET:HE1	2.02	0.41
1:E:625:VAL:HG23	1:E:626:LEU:N	2.35	0.41
1:J:416:ILE:CD1	1:K:565:GLU:HA	2.51	0.41
2:O:145:LEU:HD12	2:O:145:LEU:N	2.36	0.41
1:G:589:ALA:C	1:G:591:SER:H	2.24	0.41
1:I:589:ALA:O	1:I:593:GLN:HG3	2.21	0.41
1:E:608:SER:OG	1:E:611:VAL:HG23	2.21	0.41
1:H:385:GLU:HA	1:H:607:PHE:HZ	1.85	0.41
1:E:583:ARG:HA	1:E:584:PRO:HD3	1.87	0.41
2:R:166:SER:HA	2:R:169:MET:HB2	2.02	0.41
1:J:349:ARG:NH2	1:J:516:LYS:HE3	2.36	0.41
1:H:528:MET:CE	1:H:531:TYR:H	2.34	0.41
1:C:455:ASP:HA	1:D:456:ARG:NH1	2.35	0.41
1:D:289:LEU:HD11	1:D:333:GLN:HE21	1.86	0.41
1:E:461:LEU:C	1:E:463:VAL:H	2.24	0.41
1:K:375:MET:O	1:K:380:GLY:HA3	2.21	0.41
1:G:354:GLN:HE22	1:H:291:MET:CE	2.34	0.41
1:H:592:ILE:HA	1:H:592:ILE:HD12	1.84	0.41
2:X:198:GLU:HB2	2:X:235:ASN:ND2	2.36	0.41
1:G:434:THR:HG22	1:G:569:ILE:O	2.21	0.41
2:N:284:THR:O	2:N:287:GLU:HB3	2.21	0.41
1:E:465:ILE:HD13	1:E:509:LEU:HD12	2.03	0.41
1:H:506:LYS:HG2	1:H:519:GLN:CA	2.51	0.41
2:X:107:TYR:CE1	2:X:151:PRO:HA	2.56	0.41
2:X:147:VAL:HG22	2:X:149:SER:H	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:593:GLN:NE2	2:O:177:PRO:HB2	2.36	0.41
1:H:388:MET:O	1:H:391:VAL:HB	2.21	0.41
2:M:197:VAL:HG22	2:M:234:TYR:CE1	2.56	0.41
1:C:423:LEU:HB3	1:C:544:GLN:HG3	2.03	0.41
2:P:126:TYR:OH	2:P:131:ASN:HA	2.21	0.41
1:D:387:TRP:HZ3	1:D:573:ILE:HB	1.86	0.41
1:E:608:SER:CB	2:Q:280:ARG:NH1	2.84	0.41
2:X:145:LEU:HD21	2:X:157:VAL:HG11	2.03	0.41
1:H:427:PRO:HG3	1:H:530:GLU:OE1	2.21	0.41
1:L:292:TYR:HE1	1:L:320:HIS:ND1	2.19	0.41
1:L:304:LYS:HB3	1:L:313:HIS:CD2	2.56	0.41
2:R:112:GLY:CA	2:R:144:GLN:HB2	2.50	0.41
1:H:548:ARG:HA	1:H:549:PRO:HD3	1.96	0.41
1:F:374:ILE:C	1:F:376:PHE:N	2.75	0.41
1:D:615:MET:O	1:D:619:VAL:HG23	2.20	0.41
1:E:445:GLY:O	1:E:446:LYS:HG2	2.21	0.41
2:N:197:VAL:HG23	2:N:216:VAL:HG21	2.03	0.41
1:F:533:VAL:HA	1:F:534:PRO:HD3	1.91	0.41
2:S:94:SER:HB3	2:S:211:THR:O	2.21	0.41
2:X:243:MET:HE2	2:X:243:MET:HB2	1.98	0.40
1:F:408:PHE:HE1	1:F:525:ILE:CD1	2.32	0.40
1:K:459:PHE:CZ	1:K:512:LYS:HD3	2.56	0.40
2:T:175:ARG:NH2	2:T:237:MET:HB3	2.36	0.40
1:D:443:CYS:HB3	1:D:468:PHE:HD2	1.84	0.40
1:E:592:ILE:O	1:E:596:ILE:HD13	2.20	0.40
1:F:619:VAL:HG22	1:F:625:VAL:HG12	2.03	0.40
1:G:441:GLU:OE1	1:G:571:SER:HA	2.21	0.40
1:E:594:SER:HA	2:Q:178:HIS:CD2	2.56	0.40
2:X:257:LEU:O	2:X:265:LEU:HB2	2.21	0.40
2:V:119:ALA:O	2:V:122:VAL:HG23	2.21	0.40
1:J:368:LEU:HD23	1:J:368:LEU:HA	1.91	0.40
2:U:224:GLU:H	2:U:224:GLU:CD	2.23	0.40
2:P:134:PHE:CD1	2:P:134:PHE:N	2.89	0.40
1:D:602:ARG:HD3	1:D:602:ARG:C	2.42	0.40
1:F:469:LEU:HD13	1:F:524:GLY:HA2	2.03	0.40
2:U:158:ARG:HA	2:U:217:VAL:HG13	2.03	0.40
1:I:356:THR:O	1:I:360:MET:HG3	2.21	0.40
1:H:432:LYS:HE2	1:H:432:LYS:N	2.36	0.40
2:T:190:PRO:HD2	2:T:193:HIS:CD2	2.56	0.40
1:I:408:PHE:HB2	1:I:422:TRP:CZ3	2.56	0.40
1:K:469:LEU:HD12	1:K:469:LEU:C	2.42	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:387:TRP:CE3	1:D:568:ILE:HG23	2.56	0.40
1:K:305:CYS:O	1:K:308:LYS:HG3	2.21	0.40
1:C:357:ARG:HH11	1:C:357:ARG:HG2	1.86	0.40
2:P:96:SER:OG	2:P:211:THR:HB	2.20	0.40
2:O:103:TYR:O	2:O:266:GLY:HA2	2.21	0.40
1:J:440:LEU:HD12	1:J:471:VAL:CG2	2.51	0.40
1:A:423:LEU:HD12	1:A:526:VAL:O	2.21	0.40
1:A:534:PRO:HB3	1:B:486:PRO:HG2	2.02	0.40
2:O:159:ALA:HB3	2:O:216:VAL:CG1	2.52	0.40
1:D:506:LYS:HB3	1:D:518:THR:HG22	2.03	0.40
2:V:164:LYS:HB3	2:V:250:PRO:HG2	2.04	0.40
2:M:224:GLU:O	2:M:225:VAL:C	2.59	0.40
1:H:561:GLU:O	1:H:565:GLU:HG3	2.21	0.40
1:I:512:LYS:HB2	1:I:512:LYS:HE3	1.89	0.40
1:D:393:TRP:CZ2	1:D:553:LEU:HD22	2.56	0.40
1:D:369:LEU:HD23	1:D:372:MET:SD	2.61	0.40
1:J:608:SER:C	1:J:610:SER:H	2.24	0.40
2:R:196:ARG:HD2	2:R:237:MET:SD	2.61	0.40
2:U:246:MET:O	2:U:247:ASN:HB3	2.22	0.40
2:O:189:ALA:HA	2:O:205:TYR:CD2	2.56	0.40
1:A:287:LEU:HD12	1:F:350:VAL:HG22	2.02	0.40
1:J:296:GLN:NE2	1:J:328:ALA:HB1	2.36	0.40
1:G:440:LEU:HD23	1:G:440:LEU:C	2.42	0.40
1:A:268:VAL:HG22	1:A:326:ILE:HG22	2.02	0.40
1:D:441:GLU:HG2	1:D:572:GLY:HA3	2.03	0.40
1:F:273:VAL:HG22	1:F:292:TYR:CE2	2.57	0.40
2:T:109:PHE:CE2	2:T:257:LEU:HB2	2.57	0.40
1:I:439:LEU:HD23	1:I:575:LEU:CD1	2.52	0.40
1:A:548:ARG:HD3	1:A:548:ARG:N	2.36	0.40
1:I:452:LEU:HB3	1:I:453:PRO:CD	2.51	0.40
1:A:433:THR:O	1:A:434:THR:C	2.60	0.40
1:J:583:ARG:HA	1:J:583:ARG:HD3	1.92	0.40
1:F:349:ARG:CD	1:F:517:ARG:CZ	2.99	0.40
1:G:285:VAL:O	1:G:286:LEU:C	2.58	0.40
1:G:327:PHE:CE2	1:G:333:GLN:HB3	2.56	0.40
1:D:439:LEU:HD23	1:D:575:LEU:HD13	2.03	0.40
2:U:193:HIS:ND1	2:U:214:HIS:HB3	2.36	0.40
1:K:289:LEU:CD1	1:K:333:GLN:HB3	2.49	0.40
2:P:150:THR:HA	2:P:151:PRO:HD3	1.91	0.40
1:D:424:PHE:O	1:D:527:THR:HA	2.21	0.40
1:F:594:SER:OG	1:F:595:ARG:N	2.53	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:414:TYR:HB3	1:A:416:ILE:HG13	2.03	0.40
2:R:127:SER:O	2:R:131:ASN:N	2.55	0.40
1:C:397:LEU:HB3	1:C:401:MET:CE	2.49	0.40
1:H:454:LEU:N	1:H:454:LEU:HD12	2.36	0.40
1:I:415:ASN:HB3	1:J:567:ARG:NH2	2.36	0.40
1:H:405:VAL:HG21	1:H:578:MET:HE1	2.04	0.40
1:C:583:ARG:HB3	1:C:587:GLU:OE1	2.21	0.40
1:B:366:ASN:HD21	1:B:592:ILE:HD13	1.87	0.40
1:D:402:ASP:CA	1:D:578:MET:HE3	2.52	0.40
1:D:568:ILE:C	1:D:570:GLN:N	2.74	0.40
2:W:151:PRO:HD2	2:W:220:TYR:CE2	2.56	0.40
1:B:387:TRP:O	1:B:390:GLY:N	2.54	0.40
1:H:311:PRO:HA	1:H:314:TYR:CZ	2.57	0.40
2:N:159:ALA:HB3	2:N:216:VAL:HG13	2.02	0.40
1:C:440:LEU:HD13	1:C:471:VAL:HG23	2.04	0.40
1:F:367:ASP:C	1:F:369:LEU:N	2.74	0.40
1:K:423:LEU:HD11	1:K:528:MET:SD	2.62	0.40
2:V:186:ASP:OD1	2:V:189:ALA:HB3	2.22	0.40
2:Q:203:VAL:HG22	2:Q:204:GLU:N	2.36	0.40
2:V:222:PRO:HA	2:V:223:PRO:HD3	1.97	0.40
1:A:590:GLN:HG3	2:M:181:ARG:NH1	2.36	0.40
1:F:299:PHE:CZ	1:F:318:GLU:HB2	2.57	0.40
2:M:156:ARG:HG2	2:M:156:ARG:HH11	1.87	0.40
1:L:456:ARG:HG3	1:L:456:ARG:HH11	1.86	0.40
1:B:516:LYS:N	1:B:516:LYS:HD3	2.36	0.40
1:B:548:ARG:O	1:B:548:ARG:HG3	2.21	0.40
2:W:237:MET:SD	2:W:237:MET:N	2.93	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	360/370 (97%)	320 (89%)	35 (10%)	5 (1%)	14	55
1	B	360/370 (97%)	310 (86%)	44 (12%)	6 (2%)	11	50
1	C	361/370 (98%)	306 (85%)	44 (12%)	11 (3%)	5	34
1	D	360/370 (97%)	312 (87%)	43 (12%)	5 (1%)	14	55
1	E	360/370 (97%)	316 (88%)	38 (11%)	6 (2%)	11	50
1	F	361/370 (98%)	309 (86%)	46 (13%)	6 (2%)	11	50
1	G	360/370 (97%)	326 (91%)	29 (8%)	5 (1%)	14	55
1	H	360/370 (97%)	317 (88%)	39 (11%)	4 (1%)	17	61
1	I	361/370 (98%)	321 (89%)	36 (10%)	4 (1%)	17	61
1	J	360/370 (97%)	319 (89%)	37 (10%)	4 (1%)	17	61
1	K	360/370 (97%)	329 (91%)	26 (7%)	5 (1%)	14	55
1	L	361/370 (98%)	330 (91%)	29 (8%)	2 (1%)	30	74
2	M	197/203 (97%)	174 (88%)	19 (10%)	4 (2%)	9	46
2	N	197/203 (97%)	175 (89%)	17 (9%)	5 (2%)	7	39
2	O	197/203 (97%)	177 (90%)	15 (8%)	5 (2%)	7	39
2	P	197/203 (97%)	174 (88%)	20 (10%)	3 (2%)	13	53
2	Q	197/203 (97%)	172 (87%)	22 (11%)	3 (2%)	13	53
2	R	197/203 (97%)	172 (87%)	21 (11%)	4 (2%)	9	46
2	S	197/203 (97%)	173 (88%)	20 (10%)	4 (2%)	9	46
2	T	197/203 (97%)	178 (90%)	15 (8%)	4 (2%)	9	46
2	U	197/203 (97%)	172 (87%)	22 (11%)	3 (2%)	13	53
2	V	197/203 (97%)	180 (91%)	14 (7%)	3 (2%)	13	53
2	W	197/203 (97%)	180 (91%)	16 (8%)	1 (0%)	34	76
2	X	197/203 (97%)	176 (89%)	19 (10%)	2 (1%)	19	63
All	All	6688/6876 (97%)	5918 (88%)	666 (10%)	104 (2%)	12	52

All (104) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	473	GLU
1	C	475	VAL
1	D	530	GLU
1	E	514	LEU
1	H	530	GLU
1	J	512	LYS

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Mol	Chain	Res	Type
1	K	490	GLY
1	K	514	LEU
2	T	245	GLY
2	X	119	ALA
1	A	297	TYR
1	A	562	PHE
1	B	474	ASP
1	C	530	GLU
1	C	625	VAL
1	L	516	LYS
2	M	245	GLY
2	N	115	HIS
2	N	119	ALA
2	N	246	MET
2	O	245	GLY
2	O	246	MET
2	P	245	GLY
2	R	245	GLY
2	S	245	GLY
2	S	246	MET
2	T	119	ALA
2	U	245	GLY
2	V	245	GLY
2	X	245	GLY
1	A	480	GLY
1	B	308	LYS
1	B	513	HIS
1	C	382	ALA
1	C	569	ILE
1	E	300	GLU
1	E	598	GLU
1	F	530	GLU
1	I	486	PRO
1	I	513	HIS
1	I	514	LEU
1	J	312	SER
1	J	590	GLN
1	K	427	PRO
1	K	530	GLU
2	N	245	GLY
2	O	244	GLY
2	Q	244	GLY

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Mol	Chain	Res	Type
2	R	244	GLY
2	R	246	MET
2	U	244	GLY
2	U	246	MET
2	V	244	GLY
2	V	246	MET
2	W	244	GLY
1	A	310	GLN
1	B	395	HIS
1	C	266	LYS
1	C	279	GLU
1	C	592	ILE
1	D	515	ASN
1	E	512	LYS
1	F	314	TYR
1	G	285	VAL
1	G	561	GLU
1	K	308	LYS
2	M	246	MET
2	N	244	GLY
2	O	119	ALA
2	O	194	LEU
2	P	119	ALA
2	P	244	GLY
2	Q	119	ALA
2	S	119	ALA
2	T	244	GLY
2	T	259	ASP
1	A	300	GLU
1	B	515	ASN
1	B	591	SER
1	C	308	LYS
1	D	330	SER
1	E	606	GLU
1	F	427	PRO
1	F	583	ARG
1	G	511	LYS
1	H	505	VAL
1	H	583	ARG
1	I	427	PRO
2	M	244	GLY
1	D	427	PRO

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Mol	Chain	Res	Type
1	F	502	ASP
1	J	480	GLY
2	M	259	ASP
2	R	208	ASP
1	D	268	VAL
1	H	569	ILE
2	S	244	GLY
1	C	490	GLY
1	E	465	ILE
1	L	427	PRO
2	Q	245	GLY
1	F	569	ILE
1	G	592	ILE
1	G	480	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	323/329 (98%)	305 (94%)	18 (6%)	26	66
1	B	323/329 (98%)	297 (92%)	26 (8%)	15	50
1	C	324/329 (98%)	308 (95%)	16 (5%)	31	71
1	D	323/329 (98%)	307 (95%)	16 (5%)	30	70
1	E	323/329 (98%)	298 (92%)	25 (8%)	16	52
1	F	324/329 (98%)	307 (95%)	17 (5%)	29	68
1	G	323/329 (98%)	307 (95%)	16 (5%)	30	70
1	H	323/329 (98%)	305 (94%)	18 (6%)	26	66
1	I	324/329 (98%)	305 (94%)	19 (6%)	24	63
1	J	323/329 (98%)	307 (95%)	16 (5%)	30	70
1	K	323/329 (98%)	301 (93%)	22 (7%)	20	57
1	L	324/329 (98%)	300 (93%)	24 (7%)	17	54
2	M	179/182 (98%)	168 (94%)	11 (6%)	23	62

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	N	179/182 (98%)	172 (96%)	7 (4%)	39	76
2	O	179/182 (98%)	171 (96%)	8 (4%)	34	73
2	P	179/182 (98%)	169 (94%)	10 (6%)	26	66
2	Q	179/182 (98%)	171 (96%)	8 (4%)	34	73
2	R	179/182 (98%)	173 (97%)	6 (3%)	44	80
2	S	179/182 (98%)	172 (96%)	7 (4%)	39	76
2	T	179/182 (98%)	171 (96%)	8 (4%)	34	73
2	U	179/182 (98%)	168 (94%)	11 (6%)	23	62
2	V	179/182 (98%)	174 (97%)	5 (3%)	51	83
2	W	179/182 (98%)	171 (96%)	8 (4%)	34	73
2	X	179/182 (98%)	171 (96%)	8 (4%)	34	73
All	All	6028/6132 (98%)	5698 (94%)	330 (6%)	27	66

All (330) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	302	CYS
1	A	338	GLN
1	A	349	ARG
1	A	398	LEU
1	A	415	ASN
1	A	420	ARG
1	A	470	VAL
1	A	476	LYS
1	A	492	ASN
1	A	504	SER
1	A	508	ASN
1	A	520	ILE
1	A	528	MET
1	A	536	THR
1	A	548	ARG
1	A	594	SER
1	A	602	ARG
1	A	610	SER
1	B	267	GLN
1	B	287	LEU
1	B	299	PHE
1	B	303	LEU

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Mol	Chain	Res	Type
1	B	356	THR
1	B	357	ARG
1	B	363	ASN
1	B	370	ASP
1	B	398	LEU
1	B	415	ASN
1	B	420	ARG
1	B	454	LEU
1	B	457	LEU
1	B	463	VAL
1	B	478	THR
1	B	504	SER
1	B	515	ASN
1	B	516	LYS
1	B	525	ILE
1	B	542	VAL
1	B	569	ILE
1	B	570	GLN
1	B	595	ARG
1	B	608	SER
1	B	610	SER
1	B	627	ASP
1	C	307	LYS
1	C	316	TYR
1	C	329	ASP
1	C	332	ASN
1	C	353	LEU
1	C	361	LEU
1	C	368	LEU
1	C	375	MET
1	C	415	ASN
1	C	417	PRO
1	C	454	LEU
1	C	457	LEU
1	C	474	ASP
1	C	520	ILE
1	C	608	SER
1	C	617	PHE
1	D	286	LEU
1	D	292	TYR
1	D	302	CYS
1	D	309	GLU

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Mol	Chain	Res	Type
1	D	339	GLN
1	D	349	ARG
1	D	361	LEU
1	D	388	MET
1	D	456	ARG
1	D	481	GLU
1	D	492	ASN
1	D	508	ASN
1	D	513	HIS
1	D	570	GLN
1	D	602	ARG
1	D	627	ASP
1	E	267	GLN
1	E	282	CYS
1	E	285	VAL
1	E	302	CYS
1	E	316	TYR
1	E	323	ASN
1	E	331	LYS
1	E	338	GLN
1	E	357	ARG
1	E	361	LEU
1	E	410	LYS
1	E	415	ASN
1	E	420	ARG
1	E	455	ASP
1	E	456	ARG
1	E	473	GLU
1	E	474	ASP
1	E	491	ILE
1	E	504	SER
1	E	512	LYS
1	E	520	ILE
1	E	551	ASP
1	E	591	SER
1	E	610	SER
1	E	623	ILE
1	F	278	MET
1	F	291	MET
1	F	302	CYS
1	F	319	LYS
1	F	348	LYS

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Mol	Chain	Res	Type
1	F	353	LEU
1	F	357	ARG
1	F	358	GLU
1	F	415	ASN
1	F	455	ASP
1	F	456	ARG
1	F	469	LEU
1	F	499	ASP
1	F	583	ARG
1	F	590	GLN
1	F	603	LEU
1	F	606	GLU
1	G	288	LEU
1	G	338	GLN
1	G	339	GLN
1	G	361	LEU
1	G	398	LEU
1	G	415	ASN
1	G	429	ASP
1	G	454	LEU
1	G	459	PHE
1	G	481	GLU
1	G	500	TYR
1	G	513	HIS
1	G	530	GLU
1	G	591	SER
1	G	602	ARG
1	G	603	LEU
1	H	296	GLN
1	H	302	CYS
1	H	323	ASN
1	H	432	LYS
1	H	449	ASN
1	H	469	LEU
1	H	474	ASP
1	H	492	ASN
1	H	515	ASN
1	H	516	LYS
1	H	519	GLN
1	H	520	ILE
1	H	532	SER
1	H	542	VAL

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Mol	Chain	Res	Type
1	H	551	ASP
1	H	559	ARG
1	H	603	LEU
1	H	609	LEU
1	I	281	LYS
1	I	291	MET
1	I	303	LEU
1	I	329	ASP
1	I	361	LEU
1	I	370	ASP
1	I	415	ASN
1	I	454	LEU
1	I	502	ASP
1	I	513	HIS
1	I	542	VAL
1	I	551	ASP
1	I	567	ARG
1	I	570	GLN
1	I	590	GLN
1	I	602	ARG
1	I	608	SER
1	I	609	LEU
1	I	613	GLN
1	J	309	GLU
1	J	315	LYS
1	J	361	LEU
1	J	367	ASP
1	J	379	THR
1	J	388	MET
1	J	415	ASN
1	J	454	LEU
1	J	458	ASN
1	J	474	ASP
1	J	508	ASN
1	J	520	ILE
1	J	551	ASP
1	J	562	PHE
1	J	592	ILE
1	J	602	ARG
1	K	272	LEU
1	K	291	MET
1	K	302	CYS

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Mol	Chain	Res	Type
1	K	338	GLN
1	K	410	LYS
1	K	443	CYS
1	K	455	ASP
1	K	474	ASP
1	K	491	ILE
1	K	492	ASN
1	K	513	HIS
1	K	516	LYS
1	K	519	GLN
1	K	520	ILE
1	K	527	THR
1	K	529	ASN
1	K	542	VAL
1	K	551	ASP
1	K	569	ILE
1	K	594	SER
1	K	608	SER
1	K	627	ASP
1	L	278	MET
1	L	329	ASP
1	L	338	GLN
1	L	361	LEU
1	L	420	ARG
1	L	429	ASP
1	L	433	THR
1	L	448	LEU
1	L	454	LEU
1	L	455	ASP
1	L	456	ARG
1	L	463	VAL
1	L	469	LEU
1	L	502	ASP
1	L	505	VAL
1	L	520	ILE
1	L	528	MET
1	L	532	SER
1	L	542	VAL
1	L	561	GLU
1	L	590	GLN
1	L	591	SER
1	L	603	LEU

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Mol	Chain	Res	Type
1	L	611	VAL
2	M	120	LYS
2	M	149	SER
2	M	156	ARG
2	M	168	HIS
2	M	180	GLU
2	M	192	GLN
2	M	194	LEU
2	M	207	ASP
2	M	213	ARG
2	M	228	ASP
2	M	238	CYS
2	N	120	LYS
2	N	156	ARG
2	N	158	ARG
2	N	167	GLN
2	N	192	GLN
2	N	194	LEU
2	N	213	ARG
2	O	120	LYS
2	O	131	ASN
2	O	180	GLU
2	O	192	GLN
2	O	194	LEU
2	O	207	ASP
2	O	213	ARG
2	O	217	VAL
2	P	120	LYS
2	P	156	ARG
2	P	158	ARG
2	P	167	GLN
2	P	170	THR
2	P	192	GLN
2	P	194	LEU
2	P	213	ARG
2	P	217	VAL
2	P	238	CYS
2	Q	120	LYS
2	Q	131	ASN
2	Q	156	ARG
2	Q	167	GLN
2	Q	176	CYS

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Mol	Chain	Res	Type
2	Q	192	GLN
2	Q	194	LEU
2	Q	213	ARG
2	R	120	LYS
2	R	131	ASN
2	R	156	ARG
2	R	158	ARG
2	R	194	LEU
2	R	213	ARG
2	S	120	LYS
2	S	156	ARG
2	S	158	ARG
2	S	192	GLN
2	S	194	LEU
2	S	213	ARG
2	S	217	VAL
2	T	120	LYS
2	T	158	ARG
2	T	176	CYS
2	T	180	GLU
2	T	192	GLN
2	T	194	LEU
2	T	213	ARG
2	T	238	CYS
2	U	120	LYS
2	U	156	ARG
2	U	158	ARG
2	U	167	GLN
2	U	170	THR
2	U	192	GLN
2	U	194	LEU
2	U	207	ASP
2	U	213	ARG
2	U	217	VAL
2	U	240	SER
2	V	156	ARG
2	V	158	ARG
2	V	192	GLN
2	V	194	LEU
2	V	213	ARG
2	W	120	LYS
2	W	180	GLU

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Mol	Chain	Res	Type
2	W	192	GLN
2	W	194	LEU
2	W	207	ASP
2	W	213	ARG
2	W	217	VAL
2	W	238	CYS
2	X	120	LYS
2	X	123	THR
2	X	145	LEU
2	X	192	GLN
2	X	194	LEU
2	X	213	ARG
2	X	228	ASP
2	X	238	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (203) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	333	GLN
1	A	338	GLN
1	A	354	GLN
1	A	415	ASN
1	A	467	GLN
1	A	508	ASN
1	A	513	HIS
1	A	529	ASN
1	A	544	GLN
1	B	267	GLN
1	B	320	HIS
1	B	323	ASN
1	B	332	ASN
1	B	333	GLN
1	B	415	ASN
1	B	449	ASN
1	B	458	ASN
1	B	493	ASN
1	B	529	ASN
1	B	593	GLN
1	B	613	GLN
1	C	310	GLN
1	C	320	HIS
1	C	332	ASN

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Mol	Chain	Res	Type
1	C	333	GLN
1	C	339	GLN
1	C	395	HIS
1	C	415	ASN
1	C	449	ASN
1	C	451	ASN
1	C	458	ASN
1	C	529	ASN
1	C	544	GLN
1	C	613	GLN
1	D	320	HIS
1	D	333	GLN
1	D	338	GLN
1	D	415	ASN
1	D	458	ASN
1	D	467	GLN
1	D	508	ASN
1	D	519	GLN
1	D	529	ASN
1	D	544	GLN
1	D	570	GLN
1	E	267	GLN
1	E	310	GLN
1	E	339	GLN
1	E	415	ASN
1	E	451	ASN
1	E	489	GLN
1	E	492	ASN
1	E	493	ASN
1	E	515	ASN
1	E	519	GLN
1	E	529	ASN
1	F	310	GLN
1	F	333	GLN
1	F	338	GLN
1	F	354	GLN
1	F	395	HIS
1	F	415	ASN
1	F	496	ASN
1	F	544	GLN
1	F	570	GLN
1	F	613	GLN

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Mol	Chain	Res	Type
1	G	296	GLN
1	G	339	GLN
1	G	354	GLN
1	G	415	ASN
1	G	508	ASN
1	G	529	ASN
1	G	538	GLN
1	G	544	GLN
1	G	613	GLN
1	H	296	GLN
1	H	320	HIS
1	H	323	ASN
1	H	333	GLN
1	H	338	GLN
1	H	415	ASN
1	H	449	ASN
1	H	493	ASN
1	H	515	ASN
1	H	529	ASN
1	H	590	GLN
1	I	310	GLN
1	I	320	HIS
1	I	333	GLN
1	I	395	HIS
1	I	415	ASN
1	I	449	ASN
1	I	458	ASN
1	I	492	ASN
1	I	529	ASN
1	I	544	GLN
1	I	570	GLN
1	I	613	GLN
1	J	296	GLN
1	J	320	HIS
1	J	333	GLN
1	J	338	GLN
1	J	415	ASN
1	J	458	ASN
1	J	467	GLN
1	J	508	ASN
1	J	529	ASN
1	J	544	GLN

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Mol	Chain	Res	Type
1	K	267	GLN
1	K	323	ASN
1	K	333	GLN
1	K	339	GLN
1	K	415	ASN
1	K	451	ASN
1	K	492	ASN
1	K	493	ASN
1	K	519	GLN
1	K	529	ASN
1	K	590	GLN
1	L	310	GLN
1	L	333	GLN
1	L	354	GLN
1	L	395	HIS
1	L	415	ASN
1	L	496	ASN
1	L	544	GLN
1	L	570	GLN
1	L	590	GLN
1	L	613	GLN
2	M	131	ASN
2	M	168	HIS
2	M	192	GLN
2	M	193	HIS
2	M	210	ASN
2	M	214	HIS
2	M	235	ASN
2	N	131	ASN
2	N	179	HIS
2	N	192	GLN
2	N	193	HIS
2	N	210	ASN
2	N	214	HIS
2	O	131	ASN
2	O	192	GLN
2	O	193	HIS
2	O	210	ASN
2	O	235	ASN
2	O	288	ASN
2	P	131	ASN
2	P	192	GLN

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Mol	Chain	Res	Type
2	P	193	HIS
2	P	210	ASN
2	P	235	ASN
2	P	239	ASN
2	P	247	ASN
2	Q	100	GLN
2	Q	131	ASN
2	Q	179	HIS
2	Q	192	GLN
2	Q	193	HIS
2	Q	210	ASN
2	Q	268	ASN
2	R	100	GLN
2	R	131	ASN
2	R	192	GLN
2	R	193	HIS
2	R	210	ASN
2	R	214	HIS
2	R	247	ASN
2	R	288	ASN
2	S	131	ASN
2	S	192	GLN
2	S	210	ASN
2	S	214	HIS
2	S	233	HIS
2	S	268	ASN
2	T	131	ASN
2	T	179	HIS
2	T	192	GLN
2	T	193	HIS
2	T	210	ASN
2	U	131	ASN
2	U	192	GLN
2	U	193	HIS
2	U	210	ASN
2	U	214	HIS
2	U	235	ASN
2	V	131	ASN
2	V	192	GLN
2	V	193	HIS
2	V	210	ASN
2	V	235	ASN

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Mol	Chain	Res	Type
2	V	288	ASN
2	W	192	GLN
2	W	193	HIS
2	W	210	ASN
2	W	263	ASN
2	X	100	GLN
2	X	131	ASN
2	X	192	GLN
2	X	210	ASN
2	X	247	ASN
2	X	288	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 24 ligands modelled in this entry, 24 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	362/370 (97%)	-0.31	7 (1%) 70 54	38, 60, 99, 131	0
1	B	362/370 (97%)	-0.29	1 (0%) 94 92	43, 70, 103, 139	0
1	C	363/370 (98%)	-0.15	6 (1%) 73 59	40, 74, 110, 136	0
1	D	362/370 (97%)	-0.29	3 (0%) 87 79	39, 62, 102, 148	0
1	E	362/370 (97%)	-0.33	3 (0%) 87 79	35, 61, 97, 124	0
1	F	363/370 (98%)	-0.22	6 (1%) 73 59	36, 66, 110, 133	0
1	G	362/370 (97%)	-0.45	4 (1%) 82 71	28, 52, 91, 129	0
1	H	362/370 (97%)	-0.34	3 (0%) 87 79	33, 57, 98, 133	0
1	I	363/370 (98%)	-0.25	5 (1%) 78 64	41, 68, 103, 135	0
1	J	362/370 (97%)	-0.21	6 (1%) 73 59	44, 74, 106, 123	0
1	K	362/370 (97%)	-0.39	5 (1%) 78 64	32, 56, 91, 127	0
1	L	363/370 (98%)	-0.42	6 (1%) 73 59	28, 48, 97, 134	0
2	M	199/203 (98%)	-0.01	4 (2%) 68 52	50, 75, 120, 137	0
2	N	199/203 (98%)	0.70	23 (11%) 6 3	80, 110, 144, 151	0
2	O	199/203 (98%)	0.39	14 (7%) 19 10	67, 96, 134, 147	0
2	P	199/203 (98%)	0.15	8 (4%) 42 26	55, 87, 131, 144	0
2	Q	199/203 (98%)	0.18	10 (5%) 32 17	64, 94, 126, 137	0
2	R	199/203 (98%)	0.51	20 (10%) 9 4	69, 104, 142, 152	0
2	S	199/203 (98%)	0.21	9 (4%) 37 21	53, 88, 129, 143	0
2	T	199/203 (98%)	0.26	8 (4%) 42 26	60, 91, 128, 138	0
2	U	199/203 (98%)	0.65	21 (10%) 8 4	72, 103, 138, 147	0
2	V	199/203 (98%)	1.17	49 (24%) 1 1	85, 123, 147, 154	0
2	W	199/203 (98%)	-0.11	1 (0%) 91 87	41, 70, 109, 123	0
2	X	199/203 (98%)	-0.14	6 (3%) 54 37	35, 65, 112, 136	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
All	All	6736/6876 (97%)	-0.08	228 (3%)	49	32	28, 71, 126, 154	0

All (228) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	N	119	ALA	8.9
2	S	119	ALA	8.6
2	P	120	LYS	8.2
2	S	118	THR	7.6
1	C	513	HIS	7.5
2	T	120	LYS	7.1
2	N	118	THR	6.8
2	X	119	ALA	6.5
2	N	117	GLY	6.1
1	A	513	HIS	5.8
1	F	513	HIS	5.7
1	I	513	HIS	5.6
2	P	119	ALA	5.6
2	V	153	PRO	5.3
2	U	118	THR	5.2
2	T	119	ALA	5.2
2	N	225	VAL	5.2
1	L	513	HIS	5.1
2	U	119	ALA	5.0
2	V	115	HIS	4.9
2	R	118	THR	4.9
1	D	513	HIS	4.8
2	R	119	ALA	4.7
2	X	226	GLY	4.7
2	V	149	SER	4.6
2	R	120	LYS	4.5
2	N	115	HIS	4.5
2	V	94	SER	4.5
2	T	118	THR	4.4
2	O	120	LYS	4.4
2	U	117	GLY	4.4
2	X	120	LYS	4.4
2	S	120	LYS	4.3
1	F	627	ASP	4.3
2	V	102	THR	4.3
2	X	118	THR	4.2
2	M	120	LYS	4.2

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Mol	Chain	Res	Type	RSRZ
2	S	115	HIS	4.2
2	U	95	SER	4.2
2	N	120	LYS	4.1
2	S	225	VAL	4.1
1	C	265	THR	4.0
2	N	94	SER	4.0
2	M	119	ALA	4.0
2	U	186	ASP	4.0
2	U	120	LYS	3.9
1	J	301	MET	3.9
2	U	188	LEU	3.9
2	N	184	ASP	3.9
1	F	265	THR	3.9
2	R	115	HIS	3.8
1	B	515	ASN	3.8
2	V	228	ASP	3.8
1	J	513	HIS	3.8
2	V	268	ASN	3.7
2	P	184	ASP	3.7
2	V	184	ASP	3.7
2	V	199	GLY	3.7
2	P	118	THR	3.7
2	R	185	SER	3.6
2	U	187	GLY	3.6
1	A	301	MET	3.5
1	K	515	ASN	3.5
2	P	183	SER	3.5
1	A	515	ASN	3.5
2	V	185	SER	3.5
2	M	183	SER	3.5
1	K	298	SER	3.4
2	R	183	SER	3.4
2	R	117	GLY	3.4
1	I	265	THR	3.4
2	S	117	GLY	3.4
2	N	261	SER	3.4
2	S	183	SER	3.3
2	R	114	LEU	3.3
1	E	515	ASN	3.3
1	F	514	LEU	3.3
1	H	515	ASN	3.3
2	R	146	TRP	3.3

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Mol	Chain	Res	Type	RSRZ
2	Q	118	THR	3.3
2	R	202	ARG	3.2
2	U	153	PRO	3.2
2	V	146	TRP	3.2
2	V	93	LEU	3.2
1	C	514	LEU	3.2
2	Q	119	ALA	3.2
2	U	228	ASP	3.2
2	V	229	CYS	3.2
2	O	248	ARG	3.2
2	V	203	VAL	3.2
2	O	118	THR	3.1
2	R	198	GLU	3.1
1	L	514	LEU	3.1
2	O	185	SER	3.1
2	V	186	ASP	3.1
2	O	226	GLY	3.1
2	N	202	ARG	3.1
2	U	185	SER	3.1
2	R	186	ASP	3.1
2	N	188	LEU	3.1
2	U	184	ASP	3.1
1	C	266	LYS	3.0
2	O	119	ALA	3.0
2	V	226	GLY	3.0
1	G	515	ASN	3.0
1	C	516	LYS	3.0
2	Q	115	HIS	3.0
1	L	515	ASN	3.0
2	V	100	GLN	2.9
2	M	115	HIS	2.9
2	V	148	ASP	2.9
2	V	156	ARG	2.9
2	P	95	SER	2.9
2	V	225	VAL	2.8
2	V	248	ARG	2.8
2	N	183	SER	2.8
1	L	265	THR	2.8
1	A	379	THR	2.7
1	I	514	LEU	2.7
2	U	202	ARG	2.7
2	N	185	SER	2.7

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Mol	Chain	Res	Type	RSRZ
2	V	200	ASN	2.7
2	N	186	ASP	2.7
2	V	120	LYS	2.7
2	V	227	SER	2.7
2	V	95	SER	2.7
2	U	93	LEU	2.7
2	V	129	ALA	2.7
2	V	106	SER	2.6
2	X	225	VAL	2.6
2	V	104	GLN	2.6
2	N	228	ASP	2.6
2	Q	121	SER	2.6
2	U	115	HIS	2.6
2	U	96	SER	2.6
2	Q	207	ASP	2.6
1	J	627	ASP	2.5
1	L	301	MET	2.5
2	R	116	SER	2.5
1	G	306	ILE	2.5
2	T	227	SER	2.5
2	P	115	HIS	2.5
1	G	514	LEU	2.5
2	V	197	VAL	2.5
2	Q	225	VAL	2.5
2	V	103	TYR	2.5
2	N	100	GLN	2.5
2	X	183	SER	2.5
2	T	121	SER	2.5
2	O	184	ASP	2.4
2	R	184	ASP	2.4
1	D	514	LEU	2.4
2	N	226	GLY	2.4
1	K	483	ARG	2.4
2	U	212	PHE	2.4
2	V	91	SER	2.4
2	T	183	SER	2.4
2	V	155	THR	2.4
2	V	188	LEU	2.4
2	V	152	PRO	2.4
2	R	224	GLU	2.4
1	C	306	ILE	2.4
2	O	227	SER	2.3

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Mol	Chain	Res	Type	RSRZ
2	V	209	ARG	2.3
2	U	91	SER	2.3
1	H	300	GLU	2.3
2	W	225	VAL	2.3
1	K	513	HIS	2.3
2	V	252	LEU	2.3
1	F	378	SER	2.3
2	V	204	GLU	2.3
1	E	300	GLU	2.3
2	N	260	SER	2.3
2	N	264	LEU	2.3
1	G	513	HIS	2.3
2	N	146	TRP	2.3
2	O	104	GLN	2.3
2	Q	101	LYS	2.3
2	V	264	LEU	2.3
2	Q	224	GLU	2.2
2	V	154	GLY	2.2
2	V	263	ASN	2.2
1	J	453	PRO	2.2
1	L	306	ILE	2.2
2	V	189	ALA	2.2
2	O	228	ASP	2.2
1	H	514	LEU	2.2
2	R	91	SER	2.2
2	O	209	ARG	2.2
1	I	267	GLN	2.2
2	U	227	SER	2.2
1	D	515	ASN	2.2
2	N	153	PRO	2.2
2	V	118	THR	2.1
2	O	204	GLU	2.1
2	N	103	TYR	2.1
1	A	303	LEU	2.1
1	A	514	LEU	2.1
2	V	202	ARG	2.1
2	V	147	VAL	2.1
1	F	515	ASN	2.1
2	U	262	GLY	2.1
2	R	180	GLU	2.1
1	J	266	LYS	2.1
1	I	453	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
2	S	227	SER	2.1
2	R	225	VAL	2.1
1	E	299	PHE	2.1
2	R	124	CYS	2.1
1	J	455	ASP	2.1
2	V	201	LEU	2.1
2	S	226	GLY	2.1
2	V	238	CYS	2.1
1	K	484	ASP	2.1
2	N	210	ASN	2.1
2	O	117	GLY	2.1
2	V	101	LYS	2.1
2	U	264	LEU	2.0
2	P	228	ASP	2.0
2	Q	116	SER	2.0
2	Q	120	LYS	2.0
2	T	226	GLY	2.0
2	R	210	ASN	2.0
1	A	306	ILE	2.0
2	V	222	PRO	2.0
2	O	108	GLY	2.0
2	T	91	SER	2.0
2	V	196	ARG	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	ZN	C	6	1/1	0.96	0.15	-0.66	79,79,79,79	0
3	ZN	B	2	1/1	0.99	0.12	-0.81	71,71,71,71	0
3	ZN	K	11	1/1	0.98	0.09	-0.98	59,59,59,59	0
3	ZN	E	4	1/1	0.95	0.13	-1.06	57,57,57,57	0
3	ZN	A	1	1/1	0.95	0.12	-1.06	66,66,66,66	0
3	ZN	H	9	1/1	0.98	0.13	-1.07	60,60,60,60	0
3	ZN	D	3	1/1	0.95	0.13	-1.09	84,84,84,84	0
3	ZN	N	14	1/1	0.98	0.13	-1.12	81,81,81,81	0
3	ZN	I	8	1/1	0.98	0.13	-1.18	60,60,60,60	0
3	ZN	G	7	1/1	0.98	0.09	-1.27	66,66,66,66	0
3	ZN	V	22	1/1	0.94	0.15	-1.27	85,85,85,85	0
3	ZN	U	21	1/1	0.98	0.13	-1.29	78,78,78,78	0
3	ZN	R	18	1/1	0.98	0.12	-1.33	74,74,74,74	0
3	ZN	X	24	1/1	0.99	0.12	-1.39	38,38,38,38	0
3	ZN	S	19	1/1	0.99	0.11	-1.73	45,45,45,45	0
3	ZN	W	23	1/1	0.98	0.10	-1.81	45,45,45,45	0
3	ZN	L	12	1/1	0.99	0.13	-1.85	57,57,57,57	0
3	ZN	Q	17	1/1	0.98	0.11	-1.99	44,44,44,44	0
3	ZN	J	10	1/1	0.98	0.10	-2.12	76,76,76,76	0
3	ZN	T	20	1/1	0.99	0.09	-2.14	51,51,51,51	0
3	ZN	M	13	1/1	0.95	0.12	-2.33	55,55,55,55	0
3	ZN	O	15	1/1	0.99	0.11	-2.50	61,61,61,61	0
3	ZN	P	16	1/1	0.97	0.12	-	58,58,58,58	0
3	ZN	F	5	1/1	0.98	0.12	-	68,68,68,68	0

6.5 Other polymers [i](#)

There are no such residues in this entry.