



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 03:31 AM GMT

PDB ID : 1X0U  
Title : Crystal Structure of the carboxyl transferase subunit of putative PCC of *Sulfolobus tokodaii*  
Authors : Kakuta, Y.; Sueda, S.; Kondo, H.  
Deposited on : 2005-03-29  
Resolution : 2.20 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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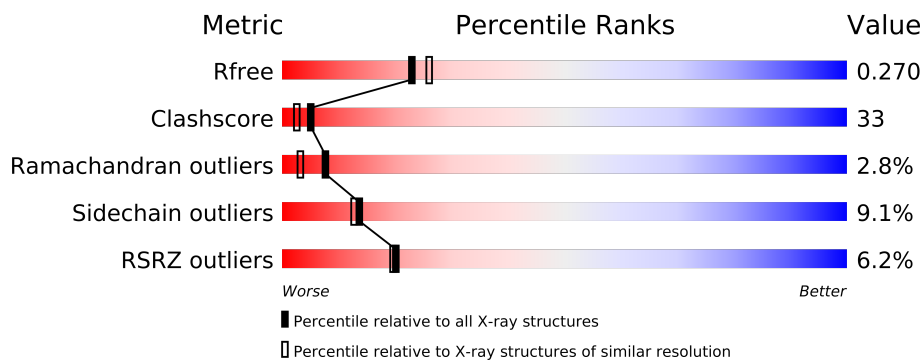
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.20 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))
$R_{free}$	66092	2938 (2.20-2.20)
Clashscore	79885	3751 (2.20-2.20)
Ramachandran outliers	78287	3681 (2.20-2.20)
Sidechain outliers	78261	3682 (2.20-2.20)
RSRZ outliers	66119	2939 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	522	
1	B	522	
1	C	522	
1	D	522	
1	E	522	
1	F	522	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 25335 atoms, of which 0 are hydrogen and 0 are deuterium.

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 hypothetical methylmalonyl-CoA decarboxylase alpha subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	518	Total	C	N	O	S	0	0	0
			4002	2560	683	746	13			
1	B	518	Total	C	N	O	S	0	0	0
			4002	2560	683	746	13			
1	C	518	Total	C	N	O	S	0	0	0
			4002	2560	683	746	13			
1	D	518	Total	C	N	O	S	0	0	0
			4002	2560	683	746	13			
1	E	518	Total	C	N	O	S	0	0	0
			4002	2560	683	746	13			
1	F	518	Total	C	N	O	S	0	0	0
			4002	2560	683	746	13			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	ALA	SER	CONFLICT	UNP Q974R9
B	2	ALA	SER	CONFLICT	UNP Q974R9
C	2	ALA	SER	CONFLICT	UNP Q974R9
D	2	ALA	SER	CONFLICT	UNP Q974R9
E	2	ALA	SER	CONFLICT	UNP Q974R9
F	2	ALA	SER	CONFLICT	UNP Q974R9

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	216	Total	O	0	0
			216	216		
2	B	214	Total	O	0	0
			214	214		
2	C	205	Total	O	0	0
			205	205		

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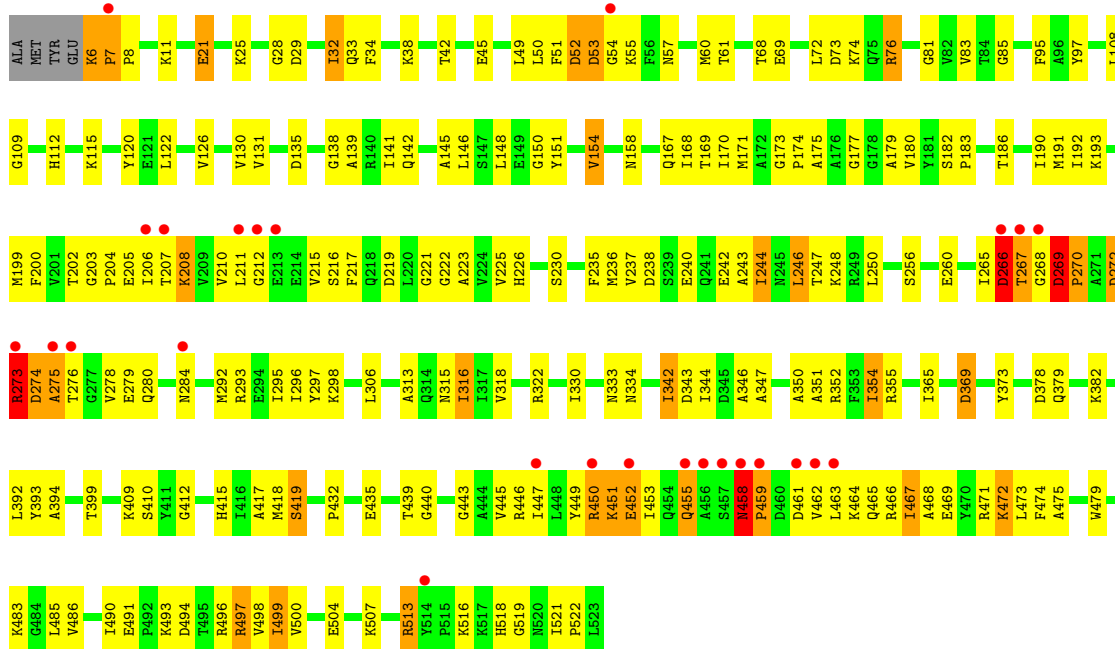
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	235	Total 235	O 235	0	0
2	E	230	Total 230	O 230	0	0
2	F	223	Total 223	O 223	0	0

### 3 Residue-property plots

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

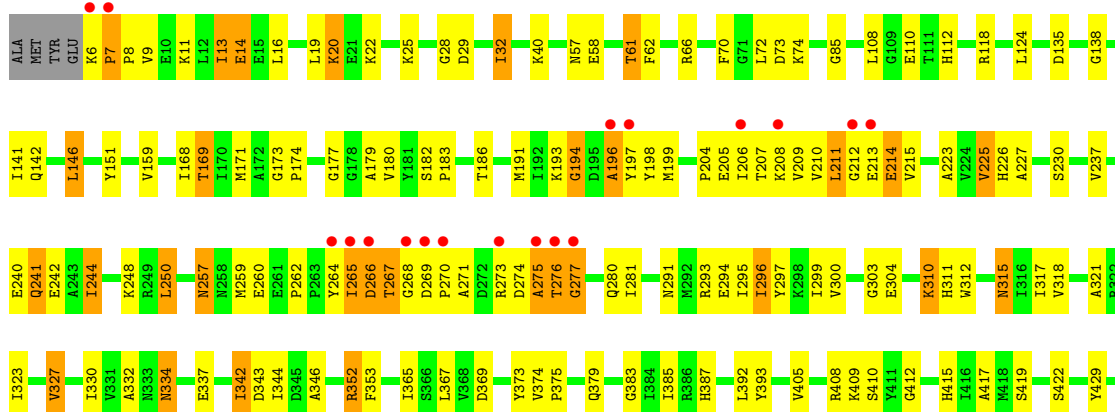
- Molecule 1: hypothetical methylmalonyl-CoA decarboxylase alpha subunit

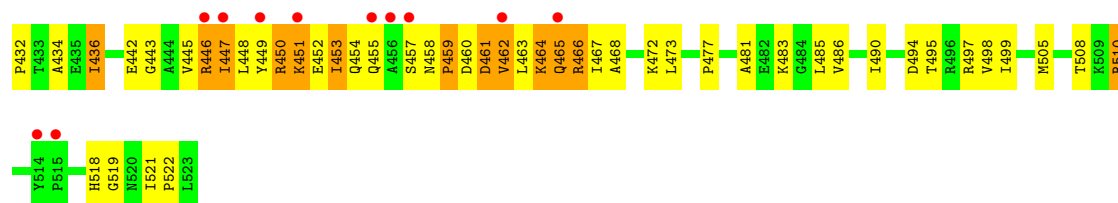
Chain A: 



- Molecule 1: hypothetical methylmalonyl-CoA decarboxylase alpha subunit

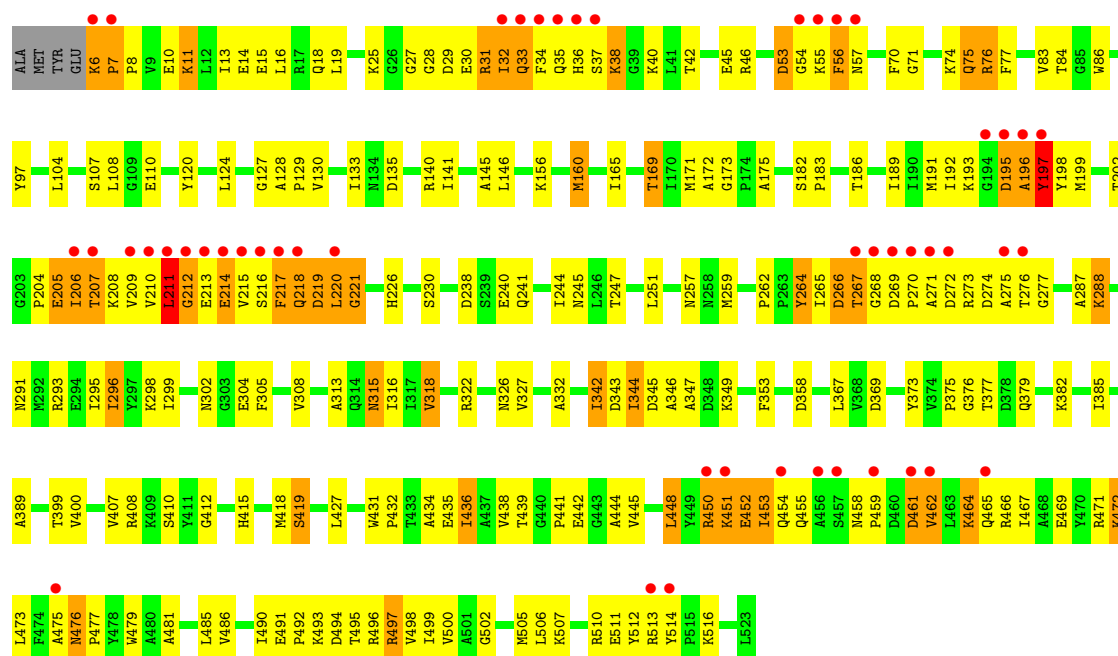
Chain B: 





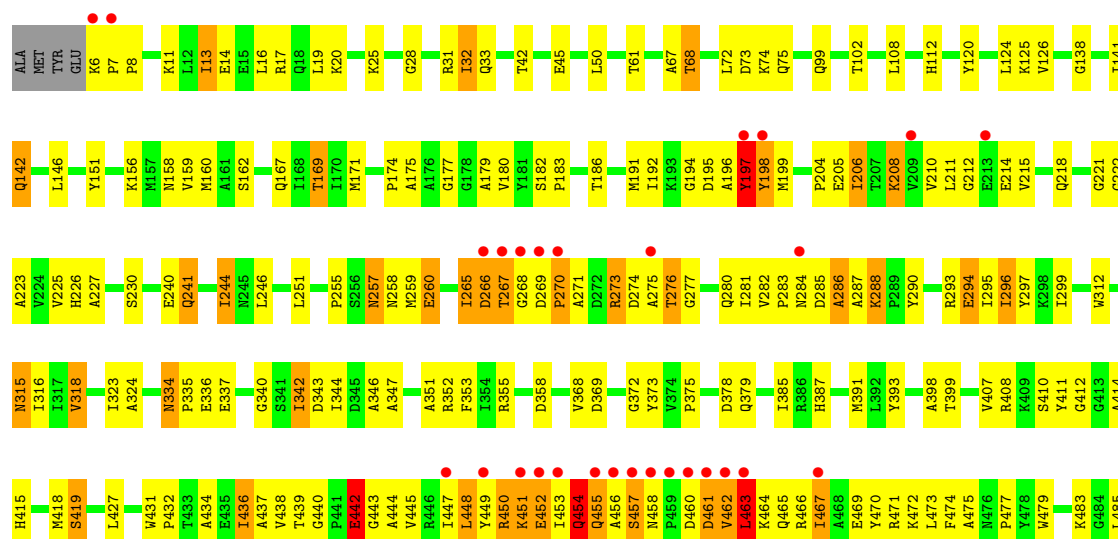
● Molecule 1: hypothetical methylmalonyl-CoA decarboxylase alpha subunit

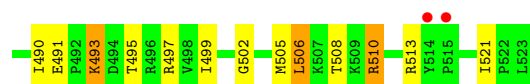
Chain C:



● Molecule 1: hypothetical methylmalonyl-CoA decarboxylase alpha subunit

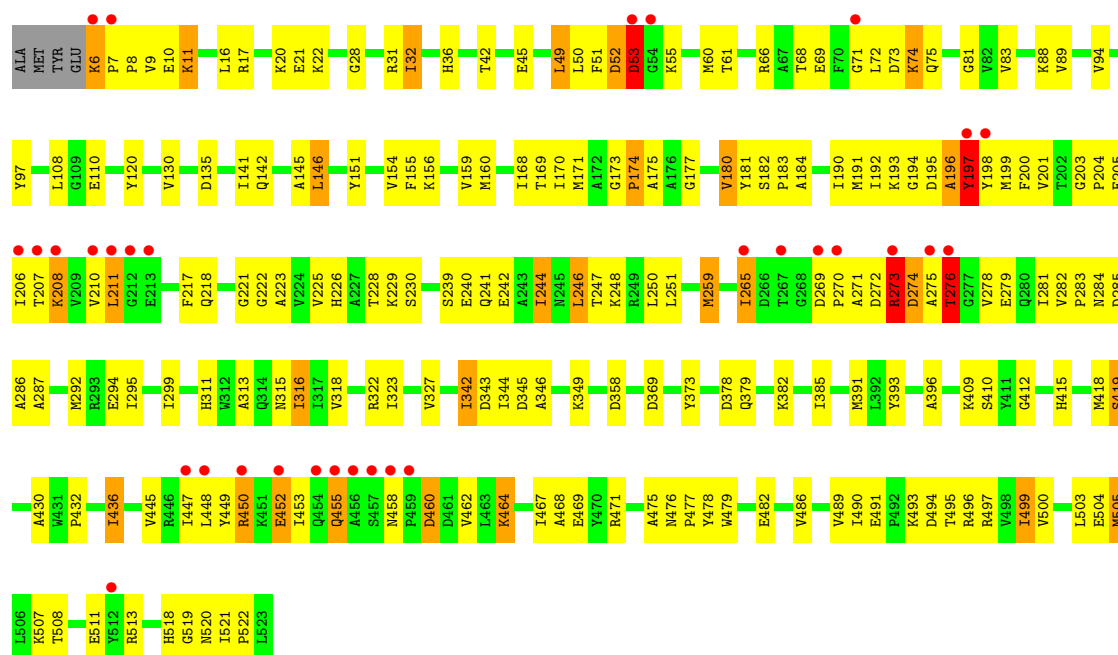
Chain D:





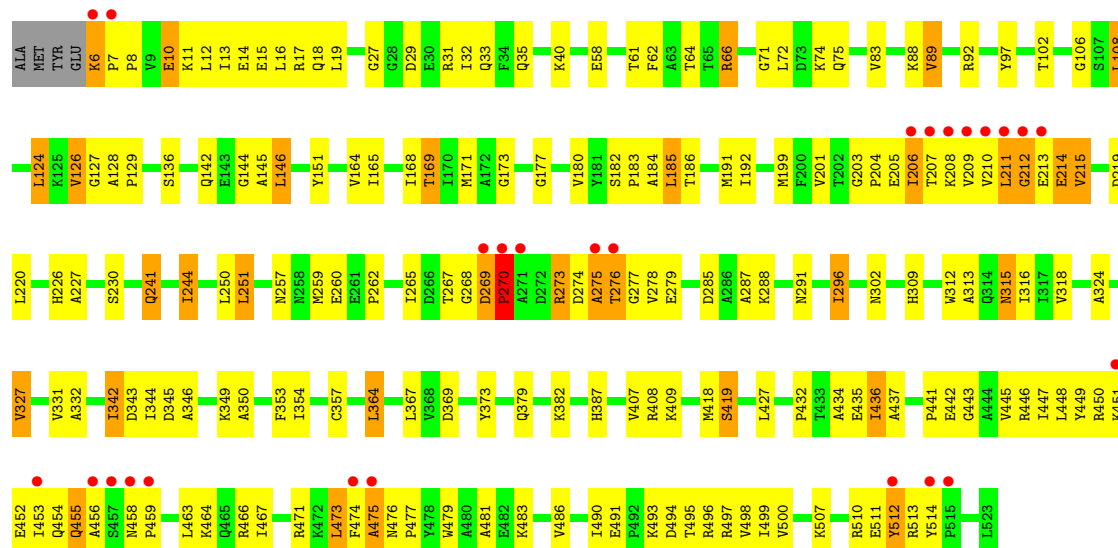
- Molecule 1: hypothetical methylmalonyl-CoA decarboxylase alpha subunit

Chain E:



- Molecule 1: hypothetical methylmalonyl-CoA decarboxylase alpha subunit

Chain F:



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	99.61Å 181.47Å 112.70Å 90.00° 116.21° 90.00°	Depositor
Resolution (Å)	48.03 – 2.20 48.03 – 2.20	Depositor EDS
% Data completeness (in resolution range)	92.4 (48.03-2.20) 92.4 (48.03-2.20)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	0.10	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.61 (at 2.20Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.228 , 0.271 0.227 , 0.270	Depositor DCC
$R_{free}$ test set	8420 reflections (5.02%)	DCC
Wilson B-factor (Å <sup>2</sup> )	16.7	Xtriage
Anisotropy	1.205	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 19.9	EDS
Estimated twinning fraction	0.479 for h,-k,-h-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	1 of 180457 reflections (0.001%)	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	25335	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.73% of the height of the origin peak. No significant pseudotranslation is detected.*

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



## 5 Model quality

### 5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.39	0/4086	0.67	2/5531 (0.0%)
1	B	0.37	0/4086	0.64	0/5531
1	C	0.38	0/4086	0.66	4/5531 (0.1%)
1	D	0.37	0/4086	0.65	2/5531 (0.0%)
1	E	0.38	0/4086	0.66	0/5531
1	F	0.36	0/4086	0.63	0/5531
All	All	0.38	0/24516	0.65	8/33186 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	463	LEU	CA-CB-CG	6.71	130.73	115.30
1	C	53	ASP	N-CA-C	6.57	128.74	111.00
1	C	197	TYR	N-CA-C	5.92	126.97	111.00
1	D	454	GLN	N-CA-C	-5.37	96.51	111.00
1	A	269	ASP	CB-CG-OD2	5.24	123.01	118.30
1	A	272	ASP	CB-CG-OD2	5.20	122.98	118.30
1	C	196	ALA	N-CA-C	-5.16	97.08	111.00
1	C	221	GLY	N-CA-C	-5.08	100.41	113.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	269	ASP	Peptide

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4002	0	4019	302	0
1	B	4002	0	4019	274	0
1	C	4002	0	4019	339	0
1	D	4002	0	4019	286	0
1	E	4002	0	4019	268	0
1	F	4002	0	4019	246	0
2	A	216	0	0	5	0
2	B	214	0	0	4	0
2	C	205	0	0	7	0
2	D	235	0	0	9	0
2	E	230	0	0	9	0
2	F	223	0	0	7	0
All	All	25335	0	24114	1609	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 33.

All (1609) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:273:ARG:HB3	1:E:497:ARG:HG3	1.21	1.18
1:A:275:ALA:HA	1:A:493:LYS:HD2	1.25	1.16
1:B:466:ARG:NH2	1:B:468:ALA:H	1.46	1.12
1:F:273:ARG:HD3	1:F:493:LYS:HD2	1.32	1.11
1:B:466:ARG:HG2	1:B:467:ILE:H	1.13	1.09
1:A:273:ARG:HG3	1:A:497:ARG:HG3	1.13	1.07
1:E:198:TYR:HD2	1:E:222:GLY:HA2	1.17	1.06
1:E:74:LYS:HE3	1:E:75:GLN:H	1.19	1.06
1:B:273:ARG:HG3	1:B:497:ARG:HH22	1.15	1.06
1:B:463:LEU:HD12	1:B:466:ARG:HE	1.16	1.05
1:A:284:ASN:HD21	1:B:7:PRO:HB2	1.16	1.05

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:273:ARG:HB3	1:F:497:ARG:HH12	1.19	1.04
1:E:198:TYR:CD2	1:E:222:GLY:HA2	1.92	1.04
1:A:273:ARG:NE	1:A:497:ARG:HD3	1.73	1.03
1:F:490:ILE:HD12	1:F:498:VAL:HG21	1.40	1.03
1:F:205:GLU:HA	1:F:208:LYS:HE2	1.39	1.01
1:A:205:GLU:HG2	1:A:206:ILE:HD12	1.39	1.01
1:B:458:ASN:HD22	1:B:462:VAL:HG21	1.24	1.01
1:F:6:LYS:HD2	1:F:8:PRO:HD2	1.43	1.01
1:C:453:ILE:HA	1:C:462:VAL:HG11	1.42	1.00
1:E:191:MET:HE1	1:E:198:TYR:HB3	1.41	0.99
1:F:455:GLN:HE21	1:F:455:GLN:HA	1.27	0.99
1:D:315:ASN:H	1:D:315:ASN:HD22	1.01	0.97
1:D:50:LEU:HA	1:D:244:ILE:HD11	1.45	0.97
1:D:198:TYR:CD2	1:D:222:GLY:HA2	1.99	0.97
1:F:315:ASN:HD21	1:F:343:ASP:HB2	1.28	0.97
1:D:142:GLN:HE21	1:D:142:GLN:H	1.13	0.96
1:C:344:ILE:HD12	1:C:379:GLN:HE22	1.28	0.96
1:A:284:ASN:ND2	1:B:7:PRO:HB2	1.79	0.96
1:D:521:ILE:HD12	1:D:521:ILE:H	1.31	0.95
1:D:265:ILE:HG22	1:D:266:ASP:N	1.81	0.95
1:D:208:LYS:HE3	1:D:208:LYS:HA	1.48	0.94
1:B:451:LYS:HZ3	1:B:451:LYS:HA	1.29	0.94
1:B:451:LYS:NZ	1:B:451:LYS:HA	1.82	0.94
1:E:292:MET:HE3	1:E:295:ILE:HB	1.50	0.94
1:E:494:ASP:HB3	1:E:497:ARG:HH11	1.30	0.94
1:A:207:THR:HG22	1:D:375:PRO:HB2	1.50	0.93
1:C:192:ILE:HG21	1:C:195:ASP:HB2	1.47	0.93
1:F:434:ALA:HB3	1:F:477:PRO:HG3	1.51	0.93
1:D:493:LYS:H	1:D:493:LYS:CD	1.83	0.92
1:D:273:ARG:HG3	1:D:497:ARG:CZ	1.99	0.92
1:E:171:MET:HG2	1:E:191:MET:HE3	1.49	0.92
1:C:375:PRO:HB2	1:F:207:THR:HG22	1.50	0.92
1:F:445:VAL:HG21	1:F:467:ILE:HA	1.50	0.92
1:E:6:LYS:HD2	1:E:7:PRO:HD3	1.49	0.92
1:A:273:ARG:CZ	1:A:497:ARG:HD3	1.99	0.92
1:D:142:GLN:NE2	1:D:142:GLN:H	1.67	0.92
1:C:315:ASN:HD21	1:C:343:ASP:HB2	1.31	0.92
1:C:273:ARG:HH21	1:C:274:ASP:H	1.01	0.92
1:B:375:PRO:HB2	1:E:207:THR:HG22	1.51	0.91
1:F:257:ASN:HD22	1:F:259:MET:H	1.17	0.91
1:A:211:LEU:HD23	1:D:375:PRO:HG2	1.52	0.91
1:B:210:VAL:HG12	1:B:211:LEU:HD13	1.50	0.91

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:273:ARG:HG3	1:A:497:ARG:CG	1.99	0.91
1:C:215:VAL:HG21	1:C:220:LEU:HD21	1.50	0.90
1:D:315:ASN:H	1:D:315:ASN:ND2	1.68	0.90
1:C:32:ILE:O	1:C:35:GLN:HB3	1.69	0.90
1:E:194:GLY:N	1:E:198:TYR:OH	2.05	0.90
1:D:276:THR:HG22	1:D:277:GLY:H	1.35	0.90
1:B:466:ARG:HG2	1:B:467:ILE:N	1.87	0.89
1:A:451:LYS:H	1:A:451:LYS:HD2	1.35	0.88
1:C:451:LYS:HE3	1:C:452:GLU:HG3	1.54	0.88
1:A:494:ASP:HB3	1:A:497:ARG:HH12	1.39	0.88
1:C:257:ASN:HD22	1:C:259:MET:H	1.19	0.87
1:A:273:ARG:HB3	1:A:496:ARG:HB3	1.53	0.87
1:F:331:VAL:HG21	1:F:354:ILE:HD11	1.57	0.87
1:B:463:LEU:HB3	1:B:466:ARG:CZ	2.04	0.87
1:E:273:ARG:HG3	1:E:494:ASP:HA	1.57	0.87
1:C:265:ILE:HG22	1:C:322:ARG:NH2	1.89	0.87
1:B:466:ARG:HH22	1:B:468:ALA:H	1.15	0.87
1:E:273:ARG:HH21	1:E:497:ARG:HD2	1.41	0.86
1:B:273:ARG:HG3	1:B:497:ARG:NH2	1.90	0.86
1:D:265:ILE:HG22	1:D:266:ASP:H	1.37	0.86
1:C:30:GLU:HG2	1:C:31:ARG:HH11	1.40	0.86
1:C:273:ARG:NH1	1:C:494:ASP:OD2	2.08	0.85
1:A:50:LEU:HA	1:A:244:ILE:HD13	1.58	0.85
1:A:51:PHE:O	1:A:53:ASP:N	2.09	0.85
1:C:441:PRO:HG3	1:C:471:ARG:NH2	1.91	0.85
1:F:273:ARG:HD2	1:F:275:ALA:H	1.42	0.85
1:C:490:ILE:HD11	1:C:494:ASP:OD1	1.77	0.85
1:C:458:ASN:HB3	1:C:461:ASP:HB3	1.58	0.84
1:D:171:MET:HG2	1:D:191:MET:HE2	1.58	0.84
1:B:171:MET:HG2	1:B:191:MET:HE3	1.59	0.84
1:B:385:ILE:HG23	1:E:180:VAL:HG13	1.57	0.84
1:B:466:ARG:CG	1:B:467:ILE:H	1.89	0.84
1:E:494:ASP:HB3	1:E:497:ARG:NH1	1.92	0.84
1:A:275:ALA:HA	1:A:493:LYS:CD	2.08	0.84
1:E:191:MET:CE	1:E:198:TYR:HB3	2.08	0.84
1:E:17:ARG:O	1:E:21:GLU:HG2	1.78	0.83
1:D:73:ASP:OD1	1:D:74:LYS:HG3	1.78	0.83
1:F:269:ASP:H	1:F:270:PRO:HD2	1.42	0.83
1:C:128:ALA:O	1:C:165:ILE:HD13	1.77	0.83
1:F:435:GLU:HG3	1:F:475:ALA:HB1	1.61	0.83
1:C:342:ILE:HD11	1:C:347:ALA:HB2	1.61	0.83
1:E:197:TYR:H	1:E:197:TYR:HD1	1.24	0.82

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:264:TYR:HD2	1:C:326:ASN:ND2	1.77	0.82
1:C:31:ARG:CZ	1:C:31:ARG:HA	2.09	0.82
1:A:180:VAL:HG13	1:D:385:ILE:HG23	1.60	0.82
1:C:195:ASP:HB3	1:C:240:GLU:HG3	1.60	0.82
1:B:445:VAL:HG21	1:B:467:ILE:HG23	1.62	0.82
1:C:74:LYS:HD3	1:C:75:GLN:N	1.94	0.82
1:C:29:ASP:HA	1:C:32:ILE:HD11	1.60	0.82
1:E:259:MET:HA	1:E:259:MET:HE2	1.62	0.82
1:A:273:ARG:HG2	1:A:494:ASP:HA	1.62	0.81
1:D:273:ARG:HG3	1:D:497:ARG:NH2	1.95	0.81
1:A:316:ILE:HD12	1:A:346:ALA:HB1	1.63	0.81
1:A:141:ILE:HD12	1:A:141:ILE:H	1.46	0.81
1:E:74:LYS:CE	1:E:75:GLN:H	1.93	0.81
1:A:265:ILE:HG23	1:A:266:ASP:N	1.93	0.81
1:E:449:TYR:H	1:E:450:ARG:HH11	1.28	0.81
1:E:449:TYR:N	1:E:450:ARG:HH11	1.79	0.81
1:D:466:ARG:HH11	1:D:469:GLU:CG	1.95	0.80
1:D:241:GLN:H	1:D:241:GLN:NE2	1.79	0.80
1:F:315:ASN:ND2	1:F:343:ASP:HB2	1.96	0.80
1:A:490:ILE:HD12	1:A:491:GLU:H	1.46	0.80
1:A:497:ARG:NH1	1:A:497:ARG:HB2	1.96	0.80
1:B:454:GLN:HE21	1:B:455:GLN:HG3	1.46	0.80
1:B:463:LEU:O	1:B:466:ARG:NH2	2.15	0.79
1:F:490:ILE:CD1	1:F:498:VAL:HG21	2.13	0.79
1:A:451:LYS:C	1:A:453:ILE:H	1.84	0.79
1:D:393:TYR:CZ	1:D:521:ILE:HG13	2.18	0.79
1:C:445:VAL:HG21	1:C:467:ILE:HA	1.65	0.79
1:E:74:LYS:HZ1	1:E:75:GLN:HB3	1.48	0.78
1:C:29:ASP:O	1:C:33:GLN:HB2	1.81	0.78
1:C:171:MET:HE2	1:C:173:GLY:H	1.48	0.78
1:E:378:ASP:O	1:E:382:LYS:HG2	1.84	0.78
1:D:436:ILE:O	1:D:436:ILE:HG13	1.83	0.78
1:B:463:LEU:CD1	1:B:466:ARG:HE	1.94	0.78
1:B:458:ASN:ND2	1:B:462:VAL:HG21	1.98	0.78
1:B:210:VAL:CG1	1:B:211:LEU:HD13	2.14	0.78
1:A:146:LEU:HD22	1:D:485:LEU:HD11	1.64	0.78
1:B:262:PRO:HB2	1:B:327:VAL:HG11	1.66	0.78
1:C:273:ARG:HH12	1:C:493:LYS:HG3	1.49	0.78
1:E:74:LYS:HE3	1:E:75:GLN:N	1.96	0.77
1:C:28:GLY:O	1:C:32:ILE:HD13	1.83	0.77
1:C:382:LYS:HE3	1:F:382:LYS:NZ	1.99	0.77
1:B:352:ARG:HD3	1:E:520:ASN:HD21	1.47	0.77

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:450:ARG:O	1:E:453:ILE:HG12	1.84	0.77
1:C:192:ILE:HB	1:C:196:ALA:HB3	1.66	0.77
1:E:198:TYR:HB2	1:E:221:GLY:O	1.84	0.77
1:B:450:ARG:HH12	1:B:453:ILE:HD13	1.50	0.77
1:B:174:PRO:HB3	1:B:197:TYR:CD1	2.19	0.77
1:E:51:PHE:O	1:E:53:ASP:N	2.17	0.77
1:F:455:GLN:NE2	1:F:455:GLN:HA	2.00	0.76
1:C:54:GLY:O	1:C:55:LYS:HG2	1.84	0.76
1:D:198:TYR:HE2	1:D:218:GLN:NE2	1.83	0.76
1:C:273:ARG:NH2	1:C:274:ASP:H	1.81	0.76
1:B:463:LEU:HD12	1:B:466:ARG:NE	1.98	0.76
1:E:196:ALA:O	1:E:197:TYR:O	2.03	0.76
1:B:466:ARG:H	1:B:466:ARG:HD3	1.50	0.76
1:C:192:ILE:HB	1:C:196:ALA:CB	2.16	0.76
1:D:466:ARG:HH11	1:D:469:GLU:HG3	1.50	0.76
1:B:241:GLN:HE21	1:B:241:GLN:H	1.34	0.76
1:D:241:GLN:H	1:D:241:GLN:HE21	1.29	0.75
1:A:351:ALA:HA	1:A:354:ILE:CD1	2.15	0.75
1:C:434:ALA:HB3	1:C:477:PRO:HG3	1.68	0.75
1:C:410:SER:OG	1:C:415:HIS:HD2	1.69	0.75
1:C:211:LEU:HG	1:C:212:GLY:H	1.51	0.75
1:A:267:THR:HG22	1:A:268:GLY:H	1.52	0.75
1:F:171:MET:HG2	1:F:191:MET:HE2	1.66	0.75
1:E:69:GLU:O	1:E:72:LEU:HD23	1.87	0.75
1:B:463:LEU:HB3	1:B:466:ARG:NH1	1.99	0.75
1:C:315:ASN:ND2	1:C:343:ASP:HB2	2.02	0.75
1:D:315:ASN:N	1:D:315:ASN:HD22	1.82	0.74
1:F:463:LEU:O	1:F:467:ILE:HB	1.86	0.74
1:C:29:ASP:HA	1:C:32:ILE:CD1	2.16	0.74
1:B:269:ASP:N	1:B:270:PRO:HD2	2.02	0.74
1:D:495:THR:O	1:D:499:ILE:HG12	1.88	0.74
1:F:171:MET:HE2	1:F:173:GLY:H	1.52	0.74
1:A:292:MET:HE3	1:A:295:ILE:HB	1.70	0.74
1:B:463:LEU:O	1:B:465:GLN:N	2.20	0.74
1:C:197:TYR:CZ	1:C:218:GLN:HB2	2.22	0.74
1:A:485:LEU:HD11	1:D:146:LEU:HD22	1.69	0.74
1:C:441:PRO:HG3	1:C:471:ARG:HH21	1.50	0.73
1:A:445:VAL:HG21	1:A:467:ILE:HG22	1.69	0.73
1:F:269:ASP:HB2	1:F:496:ARG:NH2	2.03	0.73
1:C:264:TYR:CD2	1:C:326:ASN:ND2	2.56	0.73
1:B:40:LYS:CE	1:B:197:TYR:HE2	2.01	0.73
1:E:315:ASN:HD21	1:E:343:ASP:HB2	1.52	0.73

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:273:ARG:HH21	1:C:274:ASP:N	1.83	0.73
1:B:466:ARG:NH1	1:B:467:ILE:HG13	2.03	0.73
1:E:259:MET:HA	1:E:259:MET:CE	2.17	0.73
1:C:492:PRO:O	1:C:495:THR:HG23	1.88	0.73
1:B:374:VAL:HG13	1:B:379:GLN:HG3	1.70	0.73
1:D:464:LYS:HA	1:D:467:ILE:CG1	2.19	0.73
1:C:269:ASP:C	1:C:271:ALA:H	1.92	0.73
1:A:237:VAL:HG21	1:A:242:GLU:HB3	1.71	0.73
1:B:466:ARG:HH22	1:B:468:ALA:N	1.86	0.72
1:F:74:LYS:C	1:F:74:LYS:HD3	2.10	0.72
1:E:50:LEU:HA	1:E:244:ILE:HD13	1.71	0.72
1:A:342:ILE:HD12	1:A:343:ASP:H	1.51	0.72
1:D:174:PRO:HB3	1:D:197:TYR:CD2	2.24	0.72
1:D:198:TYR:CE2	1:D:222:GLY:HA2	2.24	0.72
1:D:393:TYR:CE2	1:D:521:ILE:HG13	2.24	0.72
1:A:265:ILE:HG12	1:A:266:ASP:H	1.54	0.72
1:F:127:GLY:HA2	1:F:165:ILE:HD11	1.70	0.72
1:A:458:ASN:HD22	1:A:458:ASN:N	1.87	0.72
1:A:69:GLU:O	1:A:72:LEU:HD23	1.88	0.72
1:F:209:VAL:HG12	1:F:210:VAL:HG23	1.72	0.72
1:A:351:ALA:HA	1:A:354:ILE:HD11	1.71	0.72
1:A:450:ARG:CZ	1:A:450:ARG:HA	2.20	0.71
1:B:28:GLY:O	1:B:32:ILE:HG23	1.89	0.71
1:B:450:ARG:CZ	1:B:453:ILE:HG21	2.20	0.71
1:B:257:ASN:ND2	1:B:260:GLU:HG3	2.06	0.71
1:D:222:GLY:O	1:D:225:VAL:HG22	1.91	0.71
1:E:342:ILE:HD12	1:E:343:ASP:H	1.55	0.71
1:C:192:ILE:HD13	1:C:196:ALA:HB2	1.72	0.71
1:C:274:ASP:OD2	1:C:276:THR:HG22	1.90	0.71
1:A:451:LYS:HZ3	1:A:451:LYS:N	1.88	0.71
1:B:262:PRO:HB2	1:B:327:VAL:CG1	2.20	0.71
1:B:466:ARG:NH2	1:B:468:ALA:N	2.31	0.71
1:E:455:GLN:O	1:E:455:GLN:HG2	1.89	0.71
1:A:496:ARG:O	1:A:499:ILE:HG22	1.90	0.71
1:A:145:ALA:HB1	1:D:436:ILE:HD11	1.71	0.71
1:D:493:LYS:HD2	1:D:493:LYS:H	1.56	0.71
1:C:74:LYS:HD3	1:C:74:LYS:C	2.11	0.71
1:A:399:THR:HG23	1:A:513:ARG:HE	1.54	0.71
1:D:472:LYS:HD3	1:D:472:LYS:O	1.91	0.71
1:A:293:ARG:O	1:A:296:ILE:HG12	1.91	0.70
1:D:521:ILE:CD1	1:D:521:ILE:H	2.03	0.70
1:E:6:LYS:HA	1:E:11:LYS:HG2	1.73	0.70

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:191:MET:HE3	1:B:199:MET:HG3	1.73	0.70
1:B:466:ARG:CZ	1:B:468:ALA:H	2.04	0.70
1:C:490:ILE:HD12	1:C:491:GLU:H	1.56	0.70
1:B:241:GLN:O	1:B:244:ILE:HD13	1.92	0.70
1:B:257:ASN:HD22	1:B:259:MET:H	1.40	0.70
1:D:142:GLN:HE21	1:D:142:GLN:N	1.89	0.70
1:C:127:GLY:HA2	1:C:165:ILE:HD11	1.73	0.70
1:B:25:LYS:HE3	1:B:29:ASP:OD2	1.91	0.70
1:A:7:PRO:HG2	1:A:8:PRO:CD	2.22	0.70
1:A:494:ASP:HB3	1:A:497:ARG:NH1	2.06	0.70
1:C:343:ASP:H	1:C:346:ALA:HB3	1.56	0.70
1:C:399:THR:HG21	1:C:513:ARG:HD3	1.73	0.70
1:A:206:ILE:HD12	1:A:206:ILE:H	1.56	0.70
1:D:286:ALA:HA	1:D:408:ARG:NH2	2.07	0.70
1:E:273:ARG:HH21	1:E:497:ARG:CD	2.05	0.70
1:D:192:ILE:O	1:D:198:TYR:HE1	1.75	0.69
1:E:315:ASN:ND2	1:E:343:ASP:HB2	2.06	0.69
1:E:490:ILE:HD12	1:E:491:GLU:H	1.55	0.69
1:A:469:GLU:HA	1:A:472:LYS:HE3	1.72	0.69
1:D:505:MET:O	1:F:126:VAL:HG21	1.93	0.69
1:D:169:THR:HG21	1:D:183:PRO:HA	1.73	0.69
1:F:490:ILE:HG12	1:F:491:GLU:N	2.07	0.69
1:C:375:PRO:HB3	1:F:206:ILE:HD11	1.73	0.69
1:A:462:VAL:HA	1:A:465:GLN:CD	2.12	0.69
1:D:210:VAL:HG12	1:D:211:LEU:HD22	1.74	0.69
1:D:50:LEU:HA	1:D:244:ILE:CD1	2.20	0.69
1:E:450:ARG:HB2	1:E:450:ARG:NH2	2.07	0.69
1:F:58:GLU:HG2	1:F:61:THR:HG22	1.74	0.69
1:B:385:ILE:HD12	1:E:180:VAL:HG11	1.75	0.69
1:B:450:ARG:NH1	1:B:453:ILE:HG21	2.07	0.69
1:C:265:ILE:HG22	1:C:322:ARG:CZ	2.22	0.69
1:C:207:THR:O	1:C:211:LEU:HD22	1.93	0.69
1:F:106:GLY:O	1:F:136:SER:HB2	1.92	0.69
1:C:28:GLY:C	1:C:30:GLU:H	1.96	0.69
1:A:141:ILE:N	1:A:141:ILE:HD12	2.06	0.69
1:B:385:ILE:HG23	1:E:180:VAL:CG1	2.23	0.69
1:B:180:VAL:HG23	1:B:199:MET:CE	2.22	0.69
1:A:169:THR:HG21	1:A:183:PRO:HA	1.73	0.69
1:D:368:VAL:O	1:D:407:VAL:HG12	1.91	0.69
1:A:273:ARG:CG	1:A:497:ARG:HG3	2.08	0.69
1:E:199:MET:O	1:E:226:HIS:HE1	1.76	0.68
1:F:203:GLY:HA3	1:F:205:GLU:OE2	1.93	0.68

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:273:ARG:H	1:D:497:ARG:CG	2.06	0.68
1:E:74:LYS:NZ	1:E:75:GLN:HB3	2.07	0.68
1:D:483:LYS:HD2	1:F:66:ARG:HH21	1.56	0.68
1:D:269:ASP:N	1:D:270:PRO:HD2	2.08	0.68
1:E:222:GLY:O	1:E:225:VAL:HG22	1.92	0.68
1:B:180:VAL:HG23	1:B:199:MET:HE3	1.75	0.68
1:A:469:GLU:HA	1:A:472:LYS:CE	2.22	0.68
1:B:495:THR:O	1:B:499:ILE:HG12	1.92	0.68
1:A:222:GLY:O	1:A:225:VAL:HG22	1.94	0.68
1:A:273:ARG:HE	1:A:497:ARG:HD3	1.56	0.68
1:E:410:SER:OG	1:E:415:HIS:HD2	1.76	0.68
1:B:450:ARG:NH1	1:B:453:ILE:HD13	2.09	0.68
1:C:104:LEU:O	1:C:107:SER:HB2	1.94	0.68
1:F:490:ILE:HD11	1:F:494:ASP:CB	2.23	0.68
1:A:354:ILE:CG1	1:A:394:ALA:HB1	2.24	0.68
1:D:126:VAL:HG11	1:E:505:MET:HE1	1.75	0.68
1:C:6:LYS:HA	1:C:6:LYS:HE3	1.76	0.68
1:A:497:ARG:CZ	1:A:497:ARG:HB2	2.24	0.67
1:E:198:TYR:HE2	1:E:218:GLN:OE1	1.76	0.67
1:F:441:PRO:HG3	1:F:471:ARG:NH2	2.10	0.67
1:D:449:TYR:O	1:D:450:ARG:HG3	1.93	0.67
1:A:193:LYS:HD3	1:A:236:MET:SD	2.34	0.67
1:C:31:ARG:N	1:C:31:ARG:NE	2.43	0.67
1:B:508:THR:O	1:B:510:ARG:HD3	1.95	0.67
1:D:240:GLU:O	1:D:244:ILE:HG22	1.95	0.67
1:C:344:ILE:HD12	1:C:379:GLN:NE2	2.06	0.67
1:B:447:ILE:HD11	1:E:141:ILE:HD12	1.77	0.67
1:F:128:ALA:O	1:F:165:ILE:HG21	1.95	0.67
1:E:478:TYR:O	1:E:482:GLU:HG3	1.93	0.67
1:B:9:VAL:O	1:B:13:ILE:HG23	1.95	0.67
1:F:29:ASP:HA	1:F:32:ILE:HG12	1.75	0.67
1:A:243:ALA:O	1:A:247:THR:HG23	1.95	0.67
1:C:7:PRO:HG2	1:C:8:PRO:HD3	1.76	0.67
1:B:468:ALA:O	1:B:472:LYS:HG2	1.95	0.67
1:D:445:VAL:HG21	1:D:467:ILE:HD12	1.76	0.67
1:A:518:HIS:HE1	1:D:358:ASP:OD1	1.78	0.67
1:A:145:ALA:CB	1:D:436:ILE:HD11	2.25	0.66
1:A:410:SER:OG	1:A:415:HIS:HD2	1.78	0.66
1:C:344:ILE:HG23	1:C:379:GLN:OE1	1.94	0.66
1:C:215:VAL:CG2	1:C:220:LEU:HD21	2.22	0.66
1:E:316:ILE:HD12	1:E:346:ALA:HB1	1.77	0.66
1:C:199:MET:O	1:C:226:HIS:HE1	1.79	0.66

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:208:LYS:HD2	1:D:214:GLU:HG2	1.77	0.66
1:D:451:LYS:N	1:D:451:LYS:HE2	2.09	0.66
1:E:273:ARG:CB	1:E:497:ARG:HG3	2.11	0.66
1:F:316:ILE:HG22	2:F:527:HOH:O	1.94	0.66
1:C:215:VAL:HB	1:C:220:LEU:HD11	1.78	0.66
1:C:265:ILE:O	1:C:265:ILE:HG23	1.96	0.66
1:B:269:ASP:N	1:B:270:PRO:CD	2.57	0.66
1:E:276:THR:HG22	1:E:279:GLU:OE2	1.96	0.66
1:B:466:ARG:HH12	1:B:468:ALA:HB2	1.61	0.66
1:F:273:ARG:HE	1:F:275:ALA:HB2	1.61	0.66
1:E:195:ASP:O	1:E:197:TYR:N	2.29	0.66
1:C:273:ARG:NH2	1:C:274:ASP:O	2.29	0.65
1:C:264:TYR:HE2	1:C:507:LYS:HZ1	1.44	0.65
1:F:74:LYS:HD3	1:F:75:GLN:N	2.11	0.65
1:A:490:ILE:CD1	1:A:491:GLU:H	2.09	0.65
1:C:192:ILE:HG21	1:C:195:ASP:CB	2.22	0.65
1:C:31:ARG:O	1:C:34:PHE:HB3	1.97	0.65
1:C:211:LEU:CG	1:C:212:GLY:H	2.08	0.65
1:D:206:ILE:O	1:D:206:ILE:HD13	1.96	0.65
1:D:191:MET:SD	1:D:198:TYR:HB3	2.37	0.65
1:C:6:LYS:NZ	1:C:11:LYS:HG2	2.12	0.65
1:E:182:SER:HB3	1:E:183:PRO:HD3	1.78	0.65
1:A:497:ARG:HA	1:A:500:VAL:HG12	1.79	0.65
1:E:206:ILE:H	1:E:206:ILE:HD12	1.61	0.65
1:F:269:ASP:OD1	1:F:324:ALA:HA	1.96	0.65
1:A:378:ASP:OD1	1:A:382:LYS:HE2	1.97	0.65
1:A:169:THR:HG23	1:A:186:THR:OG1	1.96	0.65
1:B:385:ILE:HD12	1:E:180:VAL:CG1	2.26	0.65
1:F:490:ILE:HD11	1:F:494:ASP:HB2	1.79	0.65
1:D:197:TYR:N	1:D:197:TYR:CD1	2.65	0.65
1:E:450:ARG:C	1:E:452:GLU:H	2.00	0.65
1:E:316:ILE:HG23	1:E:346:ALA:HB1	1.79	0.65
1:D:273:ARG:H	1:D:497:ARG:HG3	1.61	0.65
1:A:240:GLU:O	1:A:244:ILE:HG23	1.97	0.65
1:C:42:THR:OG1	1:C:45:GLU:HG3	1.97	0.65
1:A:141:ILE:CD1	1:A:141:ILE:H	2.10	0.65
1:C:431:TRP:HE1	1:C:495:THR:CG2	2.10	0.65
1:A:462:VAL:HA	1:A:465:GLN:CG	2.27	0.65
1:A:170:ILE:HD11	1:A:247:THR:HG21	1.78	0.65
1:C:145:ALA:HB2	1:F:436:ILE:HD11	1.79	0.65
1:C:129:PRO:HA	1:C:165:ILE:HG23	1.78	0.64
1:C:369:ASP:OD1	1:C:408:ARG:HB3	1.98	0.64

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:493:LYS:HD3	1:D:493:LYS:H	1.58	0.64
1:C:264:TYR:HD2	1:C:326:ASN:HD22	1.44	0.64
1:E:203:GLY:O	1:E:207:THR:HG23	1.97	0.64
1:C:30:GLU:HB3	1:C:31:ARG:HE	1.62	0.64
1:D:464:LYS:HA	1:D:467:ILE:HG12	1.78	0.64
1:A:355:ARG:HH12	1:D:521:ILE:HD13	1.62	0.64
1:A:7:PRO:HG2	1:A:8:PRO:HD3	1.80	0.64
1:E:89:VAL:HG21	1:E:251:LEU:HD13	1.80	0.64
1:C:315:ASN:HD21	1:C:343:ASP:CB	2.10	0.64
1:B:40:LYS:NZ	1:B:197:TYR:HE2	1.95	0.64
1:F:27:GLY:O	1:F:31:ARG:HD3	1.98	0.64
1:A:151:TYR:O	1:A:154:VAL:HG13	1.98	0.64
1:C:481:ALA:HA	1:C:486:VAL:HG22	1.79	0.64
1:D:199:MET:O	1:D:226:HIS:HE1	1.80	0.64
1:C:271:ALA:HB1	1:C:500:VAL:HG21	1.80	0.64
1:D:182:SER:HB3	1:D:183:PRO:HD3	1.79	0.64
1:E:464:LYS:O	1:E:467:ILE:HG12	1.96	0.64
1:A:354:ILE:HD11	1:A:394:ALA:CB	2.27	0.64
1:E:120:TYR:CE2	1:E:130:VAL:HG11	2.33	0.64
1:D:508:THR:O	1:D:510:ARG:HD3	1.98	0.64
1:E:225:VAL:HA	1:E:229:LYS:HD3	1.80	0.64
1:A:284:ASN:HD21	1:B:7:PRO:CB	2.02	0.64
1:D:195:ASP:C	1:D:197:TYR:H	2.00	0.64
1:F:343:ASP:H	1:F:346:ALA:HB3	1.62	0.64
1:C:241:GLN:O	1:C:244:ILE:HG13	1.97	0.64
1:C:197:TYR:CE2	1:C:218:GLN:HB2	2.32	0.64
1:B:447:ILE:HD11	1:E:141:ILE:CD1	2.28	0.63
1:E:228:THR:OG1	1:E:229:LYS:HD2	1.98	0.63
1:C:172:ALA:HA	1:C:196:ALA:HB1	1.80	0.63
1:C:38:LYS:HD2	1:C:40:LYS:H	1.62	0.63
1:A:6:LYS:HZ1	1:A:8:PRO:HG2	1.63	0.63
1:D:7:PRO:HB2	1:E:284:ASN:HB3	1.78	0.63
1:F:205:GLU:H	1:F:205:GLU:CD	2.02	0.63
1:E:6:LYS:HD2	1:E:7:PRO:CD	2.27	0.63
1:D:158:ASN:HA	1:D:167:GLN:HE22	1.63	0.63
1:C:451:LYS:HE2	1:C:452:GLU:H	1.63	0.63
1:F:285:ASP:CG	1:F:288:LYS:HD3	2.18	0.63
1:E:273:ARG:HD3	1:E:497:ARG:CD	2.29	0.63
1:C:25:LYS:HD2	1:C:32:ILE:HD11	1.78	0.63
1:D:6:LYS:HB3	1:D:6:LYS:NZ	2.13	0.63
1:B:450:ARG:HH12	1:B:453:ILE:CD1	2.11	0.63
1:C:32:ILE:O	1:C:35:GLN:CB	2.44	0.63

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:452:GLU:C	1:C:454:GLN:H	2.01	0.63
1:A:449:TYR:H	1:A:450:ARG:HH11	1.46	0.63
1:F:257:ASN:ND2	1:F:259:MET:H	1.95	0.63
1:F:432:PRO:HD3	1:F:490:ILE:O	1.99	0.63
1:D:198:TYR:CE1	1:D:223:ALA:HB2	2.34	0.63
1:A:354:ILE:HD11	1:A:394:ALA:HB3	1.79	0.63
1:F:464:LYS:O	1:F:467:ILE:HG22	1.98	0.63
1:E:315:ASN:HD21	1:E:343:ASP:CB	2.10	0.63
1:C:510:ARG:HH11	1:C:510:ARG:HG2	1.61	0.63
1:E:228:THR:HG22	1:E:311:HIS:HB3	1.80	0.63
1:C:435:GLU:HG3	1:C:475:ALA:HB1	1.80	0.63
1:E:447:ILE:C	1:E:447:ILE:HD12	2.19	0.63
1:D:483:LYS:HB3	1:F:66:ARG:HH22	1.63	0.63
1:D:452:GLU:H	1:D:452:GLU:CD	2.01	0.63
1:C:442:GLU:HB2	1:C:467:ILE:HD11	1.81	0.62
1:A:450:ARG:O	1:A:453:ILE:HG22	1.99	0.62
1:F:269:ASP:N	1:F:270:PRO:HD2	2.12	0.62
1:A:479:TRP:CH2	1:D:146:LEU:HD23	2.34	0.62
1:D:204:PRO:HB3	1:D:215:VAL:HG13	1.81	0.62
1:B:446:ARG:HB3	1:B:446:ARG:CZ	2.29	0.62
1:B:191:MET:CE	1:B:199:MET:HG3	2.29	0.62
1:C:55:LYS:NZ	1:C:55:LYS:HB3	2.14	0.62
1:F:58:GLU:CG	1:F:61:THR:HG22	2.30	0.62
1:A:265:ILE:HG22	1:A:322:ARG:HD3	1.81	0.62
1:C:476:ASN:HD22	1:C:476:ASN:C	2.03	0.62
1:B:110:GLU:OE1	1:B:146:LEU:HG	1.99	0.62
1:D:451:LYS:H	1:D:451:LYS:HE2	1.62	0.62
1:B:194:GLY:C	1:B:196:ALA:H	2.01	0.62
1:A:273:ARG:HD2	1:A:273:ARG:C	2.20	0.62
1:A:205:GLU:HG2	1:A:206:ILE:CD1	2.21	0.62
1:A:450:ARG:NH2	1:A:450:ARG:HA	2.14	0.62
1:F:6:LYS:HZ3	1:F:8:PRO:C	2.03	0.62
1:B:204:PRO:HD2	1:B:205:GLU:OE1	1.99	0.62
1:B:40:LYS:HD2	1:B:197:TYR:CE2	2.35	0.62
1:A:203:GLY:O	1:A:207:THR:HG23	2.00	0.61
1:A:344:ILE:HG13	1:A:379:GLN:OE1	2.00	0.61
1:F:10:GLU:CD	1:F:10:GLU:H	2.03	0.61
1:A:333:ASN:HD22	1:A:369:ASP:H	1.45	0.61
1:A:451:LYS:C	1:A:453:ILE:N	2.50	0.61
1:E:448:LEU:C	1:E:450:ARG:HE	2.01	0.61
1:A:466:ARG:HD2	1:A:469:GLU:OE1	2.00	0.61
1:B:385:ILE:HG12	2:B:549:HOH:O	2.00	0.61

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:267:THR:HG22	1:C:267:THR:O	2.00	0.61
1:C:295:ILE:O	1:C:299:ILE:HG13	1.99	0.61
1:B:7:PRO:HG2	1:B:8:PRO:HD3	1.82	0.61
1:C:445:VAL:CG1	1:C:466:ARG:HB3	2.30	0.61
1:D:194:GLY:N	1:D:198:TYR:OH	2.25	0.61
1:C:197:TYR:HB2	2:C:525:HOH:O	2.01	0.61
1:F:241:GLN:O	1:F:244:ILE:HG13	1.99	0.61
1:C:244:ILE:HD12	1:C:245:ASN:N	2.15	0.61
1:D:277:GLY:HA2	1:D:280:GLN:HG3	1.82	0.61
1:C:57:ASN:HB3	1:C:86:TRP:CH2	2.35	0.61
1:D:460:ASP:O	1:D:463:LEU:HB3	2.01	0.61
1:E:6:LYS:N	1:E:7:PRO:CD	2.64	0.61
1:A:451:LYS:H	1:A:451:LYS:CD	2.11	0.61
1:A:466:ARG:O	1:A:469:GLU:HG2	2.00	0.61
1:A:158:ASN:HA	1:A:167:GLN:HE22	1.65	0.61
1:F:452:GLU:HG2	1:F:452:GLU:O	2.00	0.61
1:C:28:GLY:C	1:C:30:GLU:N	2.51	0.60
1:C:32:ILE:HG12	1:C:33:GLN:N	2.15	0.60
1:E:316:ILE:HG22	2:E:527:HOH:O	2.00	0.60
1:D:316:ILE:CD1	1:D:346:ALA:HB1	2.31	0.60
1:D:296:ILE:HD13	1:D:297:TYR:N	2.16	0.60
1:D:410:SER:OG	1:D:415:HIS:HD2	1.85	0.60
1:B:182:SER:HB3	1:B:183:PRO:HD3	1.82	0.60
1:B:466:ARG:N	1:B:466:ARG:HD3	2.16	0.60
1:B:463:LEU:HB3	1:B:466:ARG:NE	2.16	0.60
1:A:269:ASP:C	1:A:270:PRO:O	2.40	0.60
1:D:450:ARG:HA	1:D:454:GLN:HG3	1.83	0.60
1:B:169:THR:HG22	1:B:186:THR:OG1	2.00	0.60
1:C:495:THR:O	1:C:499:ILE:HG12	2.01	0.60
1:F:129:PRO:HA	1:F:165:ILE:CG2	2.31	0.60
1:A:221:GLY:HA2	1:A:225:VAL:HG21	1.83	0.60
1:E:521:ILE:HG13	1:E:522:PRO:HD2	1.83	0.60
1:E:74:LYS:HE3	1:E:74:LYS:H	1.66	0.60
1:B:6:LYS:HA	1:B:6:LYS:HE2	1.83	0.60
1:C:344:ILE:H	1:C:344:ILE:HD13	1.67	0.60
1:E:198:TYR:CE2	1:E:218:GLN:OE1	2.54	0.60
1:D:197:TYR:HD1	1:D:197:TYR:N	2.00	0.60
1:C:451:LYS:HD2	1:C:452:GLU:N	2.17	0.60
1:B:141:ILE:HG13	1:E:447:ILE:HG12	1.84	0.60
1:B:432:PRO:HG3	1:C:16:LEU:HD22	1.82	0.60
1:A:273:ARG:NH1	1:A:497:ARG:HD3	2.16	0.60
1:E:197:TYR:CD1	1:E:197:TYR:N	2.64	0.60

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:273:ARG:HG3	1:C:273:ARG:NH2	2.16	0.60
1:E:198:TYR:CD2	1:E:222:GLY:CA	2.76	0.60
1:B:205:GLU:O	1:B:209:VAL:HG23	2.02	0.60
1:E:391:MET:HE2	1:E:418:MET:HE2	1.84	0.60
1:B:6:LYS:HG3	1:B:11:LYS:HD3	1.82	0.59
1:C:273:ARG:HG3	1:C:273:ARG:HH21	1.66	0.59
1:B:237:VAL:HG22	1:B:242:GLU:OE2	2.01	0.59
1:D:195:ASP:O	1:D:197:TYR:N	2.26	0.59
1:D:226:HIS:HD2	1:D:230:SER:OG	1.85	0.59
1:B:135:ASP:HA	1:B:173:GLY:HA3	1.84	0.59
1:B:194:GLY:C	1:B:196:ALA:N	2.52	0.59
1:A:6:LYS:NZ	1:A:8:PRO:HG2	2.17	0.59
1:A:318:VAL:HA	1:A:330:ILE:O	2.01	0.59
1:D:198:TYR:CE2	1:D:218:GLN:NE2	2.62	0.59
1:B:40:LYS:HZ2	1:B:197:TYR:HE2	1.42	0.59
1:D:340:GLY:HA3	2:D:700:HOH:O	2.03	0.59
1:C:497:ARG:HG2	1:C:497:ARG:HH11	1.67	0.59
1:A:237:VAL:HG21	1:A:242:GLU:CB	2.32	0.59
1:F:262:PRO:HB2	1:F:327:VAL:HG13	1.83	0.59
1:D:464:LYS:C	1:D:467:ILE:HG12	2.22	0.59
1:D:126:VAL:CG1	1:E:505:MET:HE1	2.33	0.59
1:B:205:GLU:H	1:B:205:GLU:CD	2.06	0.59
1:E:342:ILE:HD12	1:E:343:ASP:N	2.17	0.59
1:C:6:LYS:HZ3	1:C:11:LYS:HG2	1.66	0.59
1:C:461:ASP:CG	1:C:462:VAL:N	2.56	0.59
1:E:316:ILE:HD12	1:E:346:ALA:CB	2.33	0.59
1:C:444:ALA:O	1:C:448:LEU:HB2	2.02	0.59
1:D:455:GLN:HE21	1:D:455:GLN:HA	1.68	0.59
1:B:463:LEU:O	1:B:466:ARG:HD3	2.02	0.59
1:F:445:VAL:HG13	1:F:449:TYR:CD1	2.37	0.59
1:C:31:ARG:HH21	1:C:31:ARG:HG3	1.66	0.59
1:D:460:ASP:O	1:D:463:LEU:HD12	2.03	0.59
1:C:197:TYR:CZ	1:C:218:GLN:CB	2.85	0.59
1:F:452:GLU:OE2	1:F:466:ARG:NH2	2.31	0.59
1:B:432:PRO:HD3	1:B:490:ILE:O	2.01	0.59
1:B:385:ILE:HD13	1:E:201:VAL:HG23	1.85	0.59
1:C:465:GLN:O	1:C:466:ARG:HD2	2.03	0.58
1:D:285:ASP:OD1	1:D:287:ALA:HB3	2.03	0.58
1:E:199:MET:O	1:E:226:HIS:CE1	2.56	0.58
1:B:453:ILE:CG1	1:B:454:GLN:N	2.65	0.58
1:E:206:ILE:HD12	1:E:206:ILE:N	2.18	0.58
1:C:266:ASP:O	1:C:268:GLY:N	2.35	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:342:ILE:HD12	1:A:343:ASP:N	2.18	0.58
1:C:107:SER:OG	1:C:140:ARG:HA	2.03	0.58
1:C:11:LYS:HE3	1:C:11:LYS:HA	1.85	0.58
1:D:265:ILE:CG2	1:D:266:ASP:N	2.54	0.58
1:C:208:LYS:HA	1:C:211:LEU:CD2	2.33	0.58
1:C:215:VAL:HB	1:C:220:LEU:CG	2.34	0.58
1:A:439:THR:HG22	1:A:440:GLY:H	1.69	0.58
1:C:182:SER:HB3	1:C:183:PRO:HD3	1.85	0.58
1:B:291:ASN:HD21	1:B:293:ARG:HB2	1.68	0.58
1:C:450:ARG:HA	1:C:450:ARG:CZ	2.33	0.58
1:E:198:TYR:CD2	1:E:223:ALA:N	2.71	0.58
1:A:120:TYR:CE2	1:A:130:VAL:HG11	2.38	0.58
1:D:316:ILE:HG13	1:D:346:ALA:HB1	1.85	0.58
1:E:193:LYS:HA	1:E:198:TYR:OH	2.03	0.58
1:A:206:ILE:N	1:A:206:ILE:HD12	2.17	0.58
1:C:215:VAL:CG1	1:C:220:LEU:HG	2.33	0.58
1:C:34:PHE:CZ	1:C:38:LYS:HB2	2.39	0.58
1:A:316:ILE:HD12	1:A:346:ALA:CB	2.32	0.58
1:D:444:ALA:O	1:D:448:LEU:HB2	2.04	0.58
1:B:208:LYS:HD2	1:B:213:GLU:N	2.18	0.58
1:A:479:TRP:CZ3	1:D:146:LEU:HD23	2.38	0.58
1:F:169:THR:HG22	1:F:186:THR:OG1	2.03	0.58
1:F:215:VAL:HG23	1:F:219:ASP:HB2	1.86	0.58
1:A:350:ALA:O	1:A:354:ILE:HD13	2.03	0.58
1:B:454:GLN:NE2	1:B:455:GLN:HG3	2.15	0.58
1:B:173:GLY:O	1:B:197:TYR:HB3	2.04	0.58
1:A:458:ASN:ND2	1:A:458:ASN:N	2.50	0.58
1:C:10:GLU:O	1:C:14:GLU:HG3	2.04	0.58
1:A:28:GLY:O	1:A:32:ILE:HG23	2.04	0.58
1:E:273:ARG:HH21	1:E:497:ARG:CG	2.17	0.57
1:D:266:ASP:O	1:D:267:THR:C	2.41	0.57
1:A:207:THR:O	1:A:211:LEU:HB2	2.04	0.57
1:B:458:ASN:HB3	1:B:462:VAL:CG2	2.34	0.57
1:C:34:PHE:O	1:C:38:LYS:HG2	2.04	0.57
1:C:257:ASN:ND2	1:C:259:MET:HB2	2.19	0.57
1:C:71:GLY:O	1:C:74:LYS:HB3	2.04	0.57
1:A:497:ARG:HH11	1:A:497:ARG:CG	2.16	0.57
1:F:471:ARG:O	1:F:475:ALA:HB3	2.04	0.57
1:D:461:ASP:C	1:D:461:ASP:OD2	2.42	0.57
1:A:182:SER:HB3	1:A:183:PRO:HD3	1.86	0.57
1:F:450:ARG:C	1:F:452:GLU:H	2.07	0.57
1:D:293:ARG:HA	1:D:296:ILE:HG23	1.87	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:148:LEU:HD11	1:D:438:VAL:HA	1.86	0.57
1:E:273:ARG:NH2	1:E:497:ARG:HD2	2.17	0.57
1:D:195:ASP:O	1:D:197:TYR:HD1	1.88	0.57
1:E:316:ILE:CG2	1:E:346:ALA:HB1	2.34	0.57
1:A:315:ASN:ND2	1:A:343:ASP:HB2	2.18	0.57
1:A:191:MET:SD	1:A:199:MET:HE2	2.44	0.57
1:C:458:ASN:O	1:C:461:ASP:OD1	2.22	0.57
1:C:344:ILE:HD13	1:C:345:ASP:H	1.69	0.57
1:F:191:MET:CE	1:F:199:MET:SD	2.93	0.57
1:A:399:THR:CG2	1:A:513:ARG:HE	2.18	0.57
1:E:490:ILE:CD1	1:E:491:GLU:H	2.17	0.57
1:B:466:ARG:NE	1:B:467:ILE:HG12	2.20	0.57
1:F:8:PRO:HG2	1:F:11:LYS:HB3	1.85	0.57
1:C:435:GLU:CG	1:C:475:ALA:HB1	2.34	0.57
1:B:138:GLY:HA2	1:B:179:ALA:HB2	1.87	0.57
1:B:344:ILE:H	1:B:379:GLN:HE22	1.53	0.57
1:B:204:PRO:HB3	1:B:215:VAL:HG13	1.86	0.57
1:B:410:SER:OG	1:B:415:HIS:HD2	1.88	0.57
1:A:499:ILE:O	1:A:499:ILE:HD13	2.05	0.57
1:F:441:PRO:HG3	1:F:471:ARG:HH21	1.69	0.57
1:F:357:CYS:CB	1:F:364:LEU:HD11	2.35	0.57
1:D:246:LEU:O	1:D:246:LEU:HD23	2.04	0.57
1:A:145:ALA:HB3	1:D:479:TRP:HZ3	1.69	0.57
1:A:237:VAL:HG22	1:A:238:ASP:N	2.20	0.57
1:A:458:ASN:OD1	1:A:462:VAL:HG13	2.04	0.57
1:D:344:ILE:HG23	1:D:387:HIS:CG	2.39	0.57
1:B:70:PHE:CE2	1:E:448:LEU:HD21	2.40	0.56
1:E:448:LEU:HD12	1:E:449:TYR:H	1.69	0.56
1:A:120:TYR:HE2	1:A:167:GLN:HE21	1.52	0.56
1:C:291:ASN:ND2	1:C:293:ARG:H	2.02	0.56
1:F:269:ASP:O	1:F:270:PRO:O	2.23	0.56
1:D:464:LYS:CA	1:D:467:ILE:HG12	2.33	0.56
1:F:127:GLY:CA	1:F:165:ILE:HD11	2.35	0.56
1:D:316:ILE:HG12	2:D:550:HOH:O	2.06	0.56
1:A:274:ASP:N	1:A:274:ASP:OD2	2.36	0.56
1:D:450:ARG:HB3	1:D:451:LYS:HZ3	1.70	0.56
1:C:211:LEU:HG	1:C:213:GLU:OE2	2.06	0.56
1:F:128:ALA:O	1:F:165:ILE:HD13	2.05	0.56
1:A:72:LEU:HD21	1:A:142:GLN:HB3	1.88	0.56
1:E:436:ILE:H	1:E:436:ILE:HD13	1.70	0.56
1:D:156:LYS:O	1:D:160:MET:HG2	2.05	0.56
1:E:108:LEU:HD22	1:E:151:TYR:CD2	2.40	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:450:ARG:HA	1:B:450:ARG:NE	2.21	0.56
1:D:463:LEU:HD13	1:D:464:LYS:N	2.21	0.56
1:D:6:LYS:HD3	1:D:11:LYS:CD	2.35	0.56
1:E:496:ARG:O	1:E:500:VAL:HG23	2.06	0.56
1:D:276:THR:HG22	1:D:277:GLY:N	2.14	0.56
1:A:447:ILE:C	1:A:450:ARG:HE	2.09	0.56
1:D:32:ILE:HG13	1:D:33:GLN:N	2.19	0.56
1:D:273:ARG:H	1:D:497:ARG:HD3	1.70	0.56
1:D:458:ASN:HB2	1:D:461:ASP:HB3	1.87	0.56
1:B:422:SER:O	1:E:156:LYS:HE2	2.05	0.56
1:E:265:ILE:HG22	1:E:322:ARG:CZ	2.35	0.56
1:C:464:LYS:HA	1:C:467:ILE:HG22	1.87	0.56
1:D:198:TYR:HB2	1:D:221:GLY:O	2.05	0.56
1:D:191:MET:CE	1:D:199:MET:SD	2.94	0.56
1:C:31:ARG:CA	1:C:31:ARG:NE	2.69	0.56
1:C:451:LYS:CE	1:C:452:GLU:HG3	2.32	0.56
1:B:241:GLN:NE2	1:B:241:GLN:H	2.00	0.56
1:F:262:PRO:HB2	1:F:327:VAL:CG1	2.36	0.56
1:D:295:ILE:O	1:D:299:ILE:HG13	2.06	0.56
1:F:35:GLN:NE2	1:F:40:LYS:HE2	2.21	0.56
1:A:316:ILE:HG23	1:A:346:ALA:HB1	1.88	0.56
1:E:283:PRO:C	1:E:285:ASP:H	2.09	0.56
1:C:172:ALA:HA	1:C:196:ALA:CB	2.35	0.56
1:D:274:ASP:OD1	1:D:275:ALA:N	2.39	0.56
1:F:453:ILE:HG22	1:F:454:GLN:OE1	2.04	0.56
1:E:171:MET:HG2	1:E:191:MET:CE	2.29	0.56
1:C:453:ILE:O	1:C:459:PRO:HA	2.06	0.56
1:C:272:ASP:O	1:C:273:ARG:HB2	2.06	0.56
1:C:215:VAL:HB	1:C:220:LEU:CD1	2.34	0.56
1:C:382:LYS:HE3	1:F:382:LYS:HZ2	1.69	0.56
1:C:13:ILE:HD12	1:C:14:GLU:N	2.20	0.56
1:D:344:ILE:HG23	1:D:387:HIS:CD2	2.41	0.56
1:D:28:GLY:O	1:D:32:ILE:HG23	2.06	0.56
1:B:385:ILE:CD1	1:E:180:VAL:HG11	2.36	0.55
1:B:450:ARG:HH22	1:B:453:ILE:HD13	1.71	0.55
1:D:273:ARG:NH1	1:D:276:THR:OG1	2.39	0.55
1:E:206:ILE:O	1:E:210:VAL:HG12	2.06	0.55
1:A:146:LEU:HD23	1:D:479:TRP:CH2	2.40	0.55
1:B:281:ILE:HD13	1:B:294:GLU:HB3	1.87	0.55
1:D:13:ILE:HG13	1:D:14:GLU:N	2.20	0.55
1:F:316:ILE:HD11	1:F:349:LYS:HD3	1.88	0.55
1:F:257:ASN:ND2	1:F:259:MET:HB2	2.21	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:30:GLU:HG2	1:C:31:ARG:NH1	2.18	0.55
1:A:465:GLN:NE2	1:A:466:ARG:HG2	2.22	0.55
1:F:436:ILE:HD12	1:F:437:ALA:N	2.21	0.55
1:C:169:THR:HG23	1:C:189:ILE:HG12	1.88	0.55
1:D:285:ASP:OD1	1:D:288:LYS:HE3	2.06	0.55
1:E:239:SER:OG	1:E:242:GLU:HG3	2.07	0.55
1:F:88:LYS:HA	1:F:92:ARG:O	2.05	0.55
1:A:237:VAL:CG2	1:A:242:GLU:HB3	2.35	0.55
1:C:110:GLU:OE1	1:C:146:LEU:HD22	2.05	0.55
1:D:273:ARG:H	1:D:497:ARG:CD	2.20	0.55
1:A:72:LEU:HD21	1:A:142:GLN:CB	2.37	0.55
1:D:343:ASP:OD1	1:D:344:ILE:N	2.39	0.55
1:F:350:ALA:O	1:F:354:ILE:HG12	2.06	0.55
1:B:177:GLY:O	1:B:180:VAL:HG12	2.06	0.55
1:E:342:ILE:HD12	1:E:346:ALA:HB3	1.89	0.55
1:D:284:ASN:OD1	1:D:285:ASP:N	2.33	0.55
1:A:73:ASP:OD2	1:A:74:LYS:HG2	2.05	0.55
1:E:271:ALA:HB3	2:E:579:HOH:O	2.06	0.55
1:B:273:ARG:CG	1:B:497:ARG:HH12	2.19	0.55
1:D:479:TRP:O	1:D:483:LYS:HG2	2.07	0.55
1:D:169:THR:CG2	1:D:186:THR:OG1	2.54	0.55
1:F:182:SER:HB3	1:F:183:PRO:HD3	1.89	0.55
1:D:99:GLN:HE21	1:D:112:HIS:CE1	2.25	0.55
1:D:342:ILE:HD12	1:D:391:MET:SD	2.46	0.55
1:F:273:ARG:NE	1:F:275:ALA:HB2	2.22	0.55
1:C:316:ILE:HG12	1:C:346:ALA:HB1	1.88	0.55
1:D:483:LYS:HB2	1:D:485:LEU:HG	1.87	0.55
1:F:191:MET:HE2	1:F:199:MET:SD	2.46	0.55
1:A:273:ARG:HH21	1:A:273:ARG:C	2.09	0.55
1:F:455:GLN:HE21	1:F:455:GLN:CA	2.03	0.55
1:E:6:LYS:N	1:E:7:PRO:HD2	2.20	0.55
1:C:454:GLN:OE1	1:C:455:GLN:HG2	2.07	0.55
1:E:467:ILE:HG13	1:E:468:ALA:N	2.22	0.55
1:A:490:ILE:CG1	1:A:491:GLU:N	2.69	0.55
1:C:344:ILE:CD1	1:C:344:ILE:H	2.20	0.55
1:B:450:ARG:O	1:B:450:ARG:HD3	2.07	0.55
1:B:193:LYS:HA	1:B:223:ALA:HB3	1.88	0.55
1:E:270:PRO:HG2	1:E:496:ARG:NH2	2.21	0.55
1:F:495:THR:O	1:F:499:ILE:HG12	2.07	0.55
1:D:449:TYR:HE1	1:D:469:GLU:OE2	1.90	0.54
1:C:266:ASP:C	1:C:268:GLY:H	2.09	0.54
1:A:54:GLY:C	1:A:55:LYS:HG2	2.27	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:463:LEU:C	1:B:465:GLN:H	2.11	0.54
1:F:342:ILE:HG23	1:F:373:TYR:CD2	2.41	0.54
1:C:31:ARG:CA	1:C:31:ARG:CZ	2.83	0.54
1:A:483:LYS:CB	1:D:146:LEU:HD21	2.38	0.54
1:A:6:LYS:HE2	1:A:6:LYS:HA	1.88	0.54
1:D:491:GLU:OE1	1:F:17:ARG:HD3	2.08	0.54
1:A:490:ILE:HG13	1:A:491:GLU:N	2.22	0.54
1:C:120:TYR:CZ	1:C:130:VAL:HG11	2.42	0.54
1:E:17:ARG:HD3	1:F:491:GLU:OE2	2.07	0.54
1:B:343:ASP:HB3	1:B:374:VAL:CG1	2.37	0.54
1:C:205:GLU:HA	1:C:208:LYS:HG2	1.90	0.54
1:F:58:GLU:OE2	1:F:83:VAL:HG13	2.08	0.54
1:E:273:ARG:HD3	1:E:497:ARG:HD2	1.88	0.54
1:A:443:GLY:O	1:A:447:ILE:HG12	2.07	0.54
1:E:450:ARG:HB2	1:E:450:ARG:CZ	2.38	0.54
1:E:240:GLU:O	1:E:244:ILE:HG23	2.07	0.54
1:D:7:PRO:N	1:D:8:PRO:HD2	2.23	0.54
1:A:351:ALA:HA	1:A:354:ILE:HD13	1.88	0.54
1:F:435:GLU:CG	1:F:475:ALA:HB1	2.36	0.54
1:F:269:ASP:HB2	1:F:496:ARG:HH22	1.70	0.54
1:C:288:LYS:N	1:C:288:LYS:HE3	2.22	0.54
1:C:514:TYR:CZ	1:F:124:LEU:HD21	2.43	0.54
1:E:170:ILE:HD11	1:E:247:THR:OG1	2.08	0.54
1:A:418:MET:O	1:A:419:SER:HB3	2.08	0.54
1:B:210:VAL:HG12	1:B:211:LEU:N	2.22	0.54
1:A:42:THR:OG1	1:A:45:GLU:HG3	2.07	0.54
1:C:344:ILE:N	1:C:344:ILE:HD13	2.21	0.54
1:A:447:ILE:HD12	1:D:141:ILE:HG13	1.90	0.54
1:A:462:VAL:HA	1:A:465:GLN:NE2	2.22	0.54
1:F:369:ASP:OD1	1:F:409:LYS:HG2	2.07	0.54
1:D:277:GLY:HA2	1:D:280:GLN:CG	2.38	0.53
1:C:451:LYS:CE	1:C:452:GLU:H	2.20	0.53
1:B:174:PRO:HB3	1:B:197:TYR:CE1	2.42	0.53
1:B:168:ILE:CD1	1:B:250:LEU:HD13	2.38	0.53
1:E:274:ASP:OD2	1:E:275:ALA:N	2.41	0.53
1:C:169:THR:HG22	1:C:186:THR:OG1	2.08	0.53
1:E:191:MET:HE1	1:E:199:MET:HG2	1.89	0.53
1:E:180:VAL:HG22	1:E:199:MET:HB2	1.91	0.53
1:F:490:ILE:HD11	1:F:494:ASP:HB3	1.90	0.53
1:F:6:LYS:HE2	1:F:12:LEU:CD2	2.38	0.53
1:D:269:ASP:O	1:D:271:ALA:N	2.39	0.53
1:B:483:LYS:HB2	1:B:485:LEU:HG	1.90	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:389:ALA:HB1	1:F:185:LEU:HD13	1.89	0.53
1:B:463:LEU:CB	1:B:466:ARG:NE	2.71	0.53
1:F:273:ARG:HD2	1:F:275:ALA:N	2.18	0.53
1:C:215:VAL:HB	1:C:220:LEU:HG	1.90	0.53
1:A:237:VAL:HG23	2:A:733:HOH:O	2.08	0.53
1:E:499:ILE:C	1:E:499:ILE:HD13	2.28	0.53
1:D:108:LEU:HD22	1:D:151:TYR:CD2	2.43	0.53
1:A:235:PHE:CE2	1:A:306:LEU:HD21	2.43	0.53
1:B:463:LEU:HA	1:B:466:ARG:CD	2.39	0.53
1:D:244:ILE:HD12	1:D:244:ILE:O	2.09	0.53
1:C:496:ARG:O	1:C:500:VAL:HG23	2.08	0.53
1:F:31:ARG:HB3	1:F:102:THR:HB	1.90	0.53
1:A:175:ALA:O	1:A:199:MET:HA	2.09	0.53
1:E:265:ILE:HG23	1:E:265:ILE:O	2.08	0.53
1:A:138:GLY:HA2	1:A:179:ALA:HB2	1.91	0.53
1:B:518:HIS:HE1	1:E:358:ASP:OD2	1.91	0.53
1:B:466:ARG:H	1:B:466:ARG:HH21	1.56	0.53
1:D:192:ILE:O	1:D:198:TYR:CE1	2.61	0.53
1:E:448:LEU:HG	1:E:449:TYR:CD1	2.43	0.53
1:C:510:ARG:NH1	1:C:510:ARG:HG2	2.23	0.53
1:A:158:ASN:HD22	1:A:167:GLN:NE2	2.07	0.53
1:D:195:ASP:C	1:D:197:TYR:N	2.61	0.53
1:A:451:LYS:N	1:A:451:LYS:HD2	2.15	0.53
1:A:292:MET:O	1:A:292:MET:HE3	2.08	0.53
1:F:192:ILE:N	1:F:192:ILE:HD12	2.24	0.53
1:C:436:ILE:O	1:C:436:ILE:HD13	2.09	0.53
1:A:497:ARG:HH11	1:A:497:ARG:HG3	1.73	0.53
1:A:451:LYS:O	1:A:453:ILE:N	2.42	0.53
1:C:257:ASN:ND2	1:C:259:MET:H	1.98	0.53
1:A:313:ALA:C	1:A:315:ASN:H	2.11	0.53
1:E:275:ALA:O	1:E:276:THR:O	2.27	0.53
1:A:439:THR:HG22	1:A:440:GLY:N	2.23	0.53
1:F:168:ILE:HD12	1:F:251:LEU:HD13	1.89	0.53
1:B:463:LEU:O	1:B:466:ARG:CZ	2.56	0.53
1:C:445:VAL:HG11	1:C:466:ARG:HB3	1.91	0.53
1:E:7:PRO:N	1:E:8:PRO:HD2	2.23	0.53
1:E:210:VAL:O	1:E:211:LEU:HD13	2.08	0.53
1:A:458:ASN:HD21	1:A:462:VAL:HG11	1.73	0.53
1:F:211:LEU:N	1:F:211:LEU:HD23	2.23	0.53
1:D:378:ASP:HB3	2:D:663:HOH:O	2.08	0.53
1:A:146:LEU:HD21	1:D:483:LYS:HB3	1.91	0.52
1:C:11:LYS:HE3	1:C:14:GLU:OE1	2.09	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:308:VAL:HB	1:C:318:VAL:HG12	1.90	0.52
1:B:108:LEU:HD22	1:B:151:TYR:CD2	2.44	0.52
1:E:494:ASP:CB	1:E:497:ARG:HH11	2.14	0.52
1:E:71:GLY:C	1:E:74:LYS:HE2	2.28	0.52
1:E:169:THR:HG21	1:E:183:PRO:HB3	1.91	0.52
1:B:73:ASP:OD2	1:B:74:LYS:HG3	2.10	0.52
1:C:490:ILE:CD1	1:C:491:GLU:H	2.21	0.52
1:A:453:ILE:HG23	1:A:453:ILE:O	2.09	0.52
1:C:410:SER:OG	1:C:415:HIS:CD2	2.56	0.52
1:E:490:ILE:HG13	1:E:491:GLU:N	2.25	0.52
1:D:471:ARG:HA	1:D:475:ALA:CB	2.40	0.52
1:B:375:PRO:HG3	1:E:210:VAL:CG1	2.39	0.52
1:A:449:TYR:N	1:A:450:ARG:HH11	2.06	0.52
1:C:266:ASP:C	1:C:268:GLY:N	2.62	0.52
1:C:431:TRP:HE1	1:C:495:THR:HG22	1.74	0.52
1:A:369:ASP:HA	1:A:409:LYS:O	2.10	0.52
1:B:276:THR:HG22	1:B:276:THR:O	2.09	0.52
1:E:273:ARG:HG3	1:E:493:LYS:O	2.10	0.52
1:B:445:VAL:CG2	1:B:467:ILE:HG23	2.38	0.52
1:F:14:GLU:O	1:F:18:GLN:HG3	2.10	0.52
1:D:412:GLY:O	1:D:415:HIS:HB3	2.10	0.52
1:C:296:ILE:HD11	1:C:305:PHE:HB2	1.91	0.52
1:E:507:LYS:HG3	1:E:508:THR:N	2.23	0.52
1:F:6:LYS:HE2	1:F:12:LEU:HG	1.91	0.52
1:E:464:LYS:HD2	1:E:464:LYS:O	2.09	0.52
1:A:269:ASP:HB2	1:A:270:PRO:CA	2.39	0.52
1:D:443:GLY:O	1:D:447:ILE:HG23	2.10	0.52
1:F:208:LYS:HA	1:F:213:GLU:O	2.10	0.52
1:B:257:ASN:HD21	1:B:260:GLU:HG3	1.73	0.52
1:B:415:HIS:NE2	1:B:436:ILE:HD12	2.25	0.52
1:B:466:ARG:HH22	1:B:468:ALA:HB3	1.73	0.52
1:B:450:ARG:NH2	1:B:453:ILE:HD13	2.25	0.52
1:A:450:ARG:NE	1:A:450:ARG:HA	2.23	0.52
1:C:205:GLU:HA	1:C:208:LYS:HE2	1.92	0.52
1:F:13:ILE:O	1:F:17:ARG:HG3	2.10	0.52
1:E:108:LEU:HD22	1:E:151:TYR:CE2	2.45	0.52
1:D:456:ALA:O	1:D:457:SER:C	2.47	0.52
1:C:432:PRO:HD3	1:C:490:ILE:O	2.10	0.52
1:C:56:PHE:HB2	1:C:86:TRP:O	2.10	0.52
1:B:458:ASN:HB3	1:B:462:VAL:HG21	1.91	0.52
1:A:200:PHE:CE2	1:A:203:GLY:HA2	2.45	0.52
1:D:466:ARG:NE	1:D:469:GLU:OE2	2.35	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:369:ASP:CG	1:C:408:ARG:HB3	2.30	0.52
1:C:160:MET:HE2	2:F:544:HOH:O	2.09	0.52
1:B:318:VAL:HA	1:B:330:ILE:O	2.09	0.52
1:D:177:GLY:O	1:D:180:VAL:HG22	2.10	0.52
1:D:470:TYR:O	1:D:474:PHE:N	2.43	0.52
1:B:463:LEU:HA	1:B:466:ARG:HD2	1.91	0.51
1:C:445:VAL:HG13	1:C:466:ARG:HB3	1.92	0.51
1:C:452:GLU:O	1:C:454:GLN:N	2.43	0.51
1:E:445:VAL:O	1:E:448:LEU:O	2.28	0.51
1:D:466:ARG:NH1	1:D:469:GLU:HB2	2.25	0.51
1:C:6:LYS:CA	1:C:6:LYS:HE3	2.40	0.51
1:C:226:HIS:HA	1:C:230:SER:HG	1.75	0.51
1:A:208:LYS:O	1:A:212:GLY:HA2	2.10	0.51
1:E:192:ILE:O	1:E:198:TYR:HE1	1.93	0.51
1:D:198:TYR:HE2	1:D:218:GLN:CD	2.12	0.51
1:A:244:ILE:CD1	1:A:248:LYS:HE3	2.40	0.51
1:C:264:TYR:HB3	2:C:560:HOH:O	2.11	0.51
1:C:514:TYR:CE1	1:F:124:LEU:HD21	2.45	0.51
1:E:31:ARG:HG3	1:E:31:ARG:HH11	1.73	0.51
1:E:177:GLY:O	1:E:180:VAL:HB	2.10	0.51
1:C:461:ASP:CG	1:C:462:VAL:H	2.13	0.51
1:D:315:ASN:N	1:D:315:ASN:ND2	2.44	0.51
1:C:342:ILE:HG12	1:C:373:TYR:CE2	2.46	0.51
1:D:493:LYS:N	1:D:493:LYS:CD	2.61	0.51
1:E:210:VAL:HG22	1:E:210:VAL:O	2.10	0.51
1:A:455:GLN:O	1:A:455:GLN:HG3	2.09	0.51
1:C:453:ILE:HG13	1:C:462:VAL:HG21	1.92	0.51
1:F:342:ILE:HD12	1:F:346:ALA:HB3	1.92	0.51
1:C:316:ILE:HD12	1:C:316:ILE:O	2.11	0.51
1:C:512:TYR:O	1:C:513:ARG:HG3	2.10	0.51
1:F:215:VAL:HG23	1:F:219:ASP:CB	2.41	0.51
1:F:418:MET:O	1:F:419:SER:HB3	2.11	0.51
1:B:442:GLU:O	1:B:446:ARG:HB2	2.10	0.51
1:F:435:GLU:HG3	1:F:475:ALA:CB	2.35	0.51
1:C:75:GLN:C	1:C:75:GLN:HE21	2.14	0.51
1:C:75:GLN:C	1:C:75:GLN:NE2	2.64	0.51
1:A:466:ARG:HA	1:A:469:GLU:HG2	1.92	0.51
1:A:469:GLU:HA	1:A:472:LYS:CD	2.40	0.51
1:C:145:ALA:HB3	1:F:479:TRP:HZ3	1.75	0.51
1:C:169:THR:CG2	1:C:189:ILE:HG12	2.41	0.51
1:F:62:PHE:O	1:F:64:THR:HG23	2.11	0.51
1:A:280:GLN:NE2	1:A:280:GLN:HA	2.26	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:450:ARG:CA	1:A:450:ARG:NE	2.74	0.51
1:A:451:LYS:NZ	1:A:451:LYS:HB3	2.25	0.51
1:A:168:ILE:HD13	1:A:250:LEU:HD23	1.92	0.51
1:A:95:PHE:HZ	1:C:505:MET:HE3	1.75	0.51
1:E:460:ASP:OD2	1:E:460:ASP:N	2.43	0.51
1:B:466:ARG:HH22	1:B:468:ALA:CB	2.24	0.51
1:C:462:VAL:O	1:C:466:ARG:HB2	2.11	0.51
1:D:269:ASP:C	1:D:271:ALA:H	2.14	0.51
1:F:273:ARG:HB2	1:F:493:LYS:HB2	1.93	0.51
1:B:206:ILE:O	1:B:210:VAL:HB	2.11	0.51
1:C:135:ASP:HA	1:C:173:GLY:HA3	1.91	0.51
1:C:8:PRO:HG2	1:C:11:LYS:HB3	1.93	0.51
1:D:99:GLN:HE21	1:D:112:HIS:HE1	1.57	0.51
1:E:396:ALA:O	1:E:513:ARG:NH1	2.44	0.51
1:E:168:ILE:HD13	1:E:250:LEU:HD23	1.93	0.51
1:B:7:PRO:HG2	1:B:8:PRO:CD	2.40	0.51
1:F:6:LYS:HE2	1:F:12:LEU:HD21	1.92	0.51
1:B:518:HIS:HD2	1:B:519:GLY:O	1.94	0.51
1:C:418:MET:O	1:C:419:SER:HB3	2.10	0.51
1:C:316:ILE:HD11	1:C:349:LYS:HD3	1.92	0.51
1:C:342:ILE:HD12	1:C:343:ASP:N	2.26	0.51
1:E:499:ILE:O	1:E:499:ILE:HD13	2.11	0.51
1:E:192:ILE:O	1:E:198:TYR:CE1	2.64	0.50
1:C:197:TYR:CE1	1:C:218:GLN:HB3	2.46	0.50
1:C:431:TRP:HE1	1:C:495:THR:HG21	1.76	0.50
1:D:316:ILE:CG1	1:D:346:ALA:HB1	2.42	0.50
1:E:175:ALA:O	1:E:199:MET:HA	2.11	0.50
1:A:6:LYS:HZ3	1:A:8:PRO:CD	2.23	0.50
1:B:169:THR:CG2	1:B:186:THR:OG1	2.59	0.50
1:F:481:ALA:HA	1:F:486:VAL:HG22	1.91	0.50
1:C:202:THR:HG21	1:C:206:ILE:CD1	2.41	0.50
1:A:494:ASP:O	1:A:498:VAL:HG13	2.12	0.50
1:C:313:ALA:HB2	1:C:345:ASP:HB3	1.92	0.50
1:C:127:GLY:CA	1:C:165:ILE:HD11	2.40	0.50
1:F:288:LYS:HD2	1:F:288:LYS:N	2.27	0.50
1:C:287:ALA:C	1:C:288:LYS:HE3	2.31	0.50
1:D:471:ARG:HA	1:D:475:ALA:HB2	1.93	0.50
1:D:191:MET:SD	1:D:198:TYR:CD1	3.05	0.50
1:B:40:LYS:CD	1:B:197:TYR:HE2	2.24	0.50
1:B:342:ILE:HG13	1:B:343:ASP:N	2.26	0.50
1:B:344:ILE:HG23	1:B:387:HIS:CG	2.46	0.50
1:C:512:TYR:CD2	1:C:513:ARG:N	2.80	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:199:MET:O	1:C:226:HIS:CE1	2.64	0.50
1:E:418:MET:O	1:E:419:SER:HB3	2.10	0.50
1:C:15:GLU:O	1:C:19:LEU:HD13	2.11	0.50
1:C:476:ASN:ND2	1:C:476:ASN:C	2.65	0.50
1:B:485:LEU:HD11	1:E:146:LEU:HD12	1.94	0.50
1:B:275:ALA:O	1:B:276:THR:C	2.50	0.50
1:D:434:ALA:HB3	1:D:477:PRO:HG3	1.93	0.50
1:F:344:ILE:HG13	1:F:379:GLN:OE1	2.12	0.50
1:A:467:ILE:HG13	1:A:468:ALA:N	2.25	0.50
1:A:315:ASN:HD21	1:A:343:ASP:HB2	1.74	0.50
1:F:126:VAL:O	1:F:126:VAL:HG13	2.12	0.50
1:E:197:TYR:O	1:E:198:TYR:CD1	2.65	0.50
1:D:191:MET:HE2	1:D:199:MET:SD	2.52	0.50
1:F:309:HIS:HB3	1:F:349:LYS:HE3	1.92	0.50
1:E:208:LYS:O	1:E:208:LYS:HD2	2.12	0.50
1:D:318:VAL:HG13	1:D:353:PHE:CG	2.47	0.50
1:E:55:LYS:HD2	1:E:88:LYS:HB2	1.94	0.50
1:B:332:ALA:CB	1:B:367:LEU:HB2	2.42	0.50
1:B:277:GLY:HA2	1:B:280:GLN:CG	2.42	0.50
1:F:342:ILE:HD12	1:F:343:ASP:H	1.76	0.50
1:B:375:PRO:HG3	1:E:210:VAL:HG11	1.94	0.50
1:E:490:ILE:CG1	1:E:491:GLU:N	2.74	0.50
1:A:226:HIS:HA	1:A:230:SER:OG	2.11	0.50
1:E:89:VAL:CG2	1:E:89:VAL:O	2.60	0.50
1:B:8:PRO:HG2	1:B:11:LYS:HB2	1.93	0.50
1:D:241:GLN:O	1:D:244:ILE:HG23	2.12	0.49
1:C:490:ILE:HG13	1:C:494:ASP:HB2	1.93	0.49
1:C:471:ARG:O	1:C:475:ALA:HB3	2.12	0.49
1:C:269:ASP:C	1:C:271:ALA:N	2.62	0.49
1:B:159:VAL:HG21	1:E:396:ALA:HB3	1.93	0.49
1:D:265:ILE:CG2	1:D:266:ASP:H	2.08	0.49
1:C:471:ARG:HA	1:C:475:ALA:CB	2.42	0.49
1:A:145:ALA:HB3	1:D:479:TRP:CZ3	2.46	0.49
1:C:217:PHE:CG	1:C:218:GLN:N	2.76	0.49
1:E:276:THR:HG22	1:E:279:GLU:CD	2.33	0.49
1:F:443:GLY:O	1:F:447:ILE:HD13	2.11	0.49
1:D:453:ILE:HD13	1:D:462:VAL:HB	1.94	0.49
1:C:14:GLU:O	1:C:18:GLN:HG3	2.12	0.49
1:B:485:LEU:HD11	1:E:146:LEU:CD1	2.43	0.49
1:A:273:ARG:O	1:A:273:ARG:NH2	2.43	0.49
1:B:466:ARG:CZ	1:B:467:ILE:CG1	2.91	0.49
1:E:226:HIS:HA	1:E:230:SER:OG	2.12	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:453:ILE:HG12	1:B:454:GLN:N	2.27	0.49
1:A:447:ILE:HA	1:A:450:ARG:NE	2.26	0.49
1:D:126:VAL:HG11	1:E:505:MET:CE	2.41	0.49
1:D:138:GLY:HA2	1:D:179:ALA:HB2	1.94	0.49
1:A:272:ASP:O	1:A:273:ARG:O	2.30	0.49
1:D:68:THR:O	1:D:73:ASP:HB3	2.13	0.49
1:D:461:ASP:O	1:D:465:GLN:HB2	2.13	0.49
1:B:447:ILE:CD1	1:E:141:ILE:HD12	2.43	0.49
1:E:343:ASP:H	1:E:346:ALA:HB3	1.78	0.49
1:A:469:GLU:HA	1:A:472:LYS:HD3	1.95	0.49
1:A:6:LYS:HE2	1:A:6:LYS:CA	2.43	0.49
1:C:6:LYS:CE	1:C:8:PRO:HD2	2.43	0.49
1:A:190:ILE:HD12	1:A:247:THR:HG22	1.93	0.49
1:B:293:ARG:HA	1:B:296:ILE:HG23	1.95	0.49
1:B:436:ILE:HD11	1:E:145:ALA:HB1	1.93	0.49
1:F:171:MET:HE2	1:F:173:GLY:N	2.23	0.49
1:A:471:ARG:O	1:A:475:ALA:HB3	2.12	0.49
1:E:73:ASP:OD1	1:E:74:LYS:HG3	2.13	0.49
1:A:7:PRO:HG2	1:A:8:PRO:HD2	1.95	0.49
1:F:169:THR:CG2	1:F:186:THR:OG1	2.61	0.49
1:B:315:ASN:HA	1:B:337:GLU:HB2	1.95	0.49
1:E:83:VAL:O	1:E:97:TYR:HA	2.13	0.49
1:A:494:ASP:CB	1:A:497:ARG:NH1	2.73	0.49
1:B:463:LEU:CD1	1:B:466:ARG:NE	2.69	0.49
1:E:226:HIS:HA	1:E:230:SER:HG	1.78	0.49
1:A:473:LEU:HD23	1:A:474:PHE:CE2	2.48	0.49
1:D:197:TYR:HD1	1:D:197:TYR:H	1.59	0.48
1:F:270:PRO:HA	2:F:688:HOH:O	2.12	0.48
1:C:382:LYS:HE3	1:F:382:LYS:HZ1	1.77	0.48
1:C:204:PRO:HD2	1:C:205:GLU:OE1	2.13	0.48
1:A:292:MET:CE	1:A:295:ILE:HB	2.43	0.48
1:D:269:ASP:H	1:D:270:PRO:HD2	1.75	0.48
1:B:237:VAL:HG21	1:B:242:GLU:HB3	1.95	0.48
1:B:483:LYS:HB3	1:E:146:LEU:HD11	1.95	0.48
1:B:66:ARG:NH2	1:D:146:LEU:HG	2.27	0.48
1:E:455:GLN:O	1:E:455:GLN:CG	2.60	0.48
1:C:145:ALA:CB	1:F:436:ILE:HD11	2.41	0.48
1:A:83:VAL:O	1:A:97:TYR:HA	2.13	0.48
1:F:309:HIS:CB	1:F:349:LYS:HE3	2.43	0.48
1:A:354:ILE:HG12	1:A:355:ARG:N	2.28	0.48
1:C:264:TYR:CD1	1:C:264:TYR:N	2.81	0.48
1:E:344:ILE:HG13	1:E:379:GLN:OE1	2.14	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:497:ARG:CB	1:A:497:ARG:NH1	2.72	0.48
1:E:7:PRO:N	1:E:8:PRO:CD	2.76	0.48
1:D:458:ASN:O	1:D:462:VAL:HG22	2.13	0.48
2:D:574:HOH:O	1:F:17:ARG:HG2	2.14	0.48
1:B:169:THR:HG21	1:B:183:PRO:HA	1.96	0.48
1:F:168:ILE:CD1	1:F:251:LEU:HD13	2.44	0.48
1:B:408:ARG:NE	1:B:409:LYS:HZ3	2.11	0.48
1:A:446:ARG:C	1:A:450:ARG:NH1	2.66	0.48
1:C:452:GLU:C	1:C:454:GLN:N	2.67	0.48
1:B:268:GLY:C	1:B:270:PRO:HD2	2.34	0.48
1:D:108:LEU:HD22	1:D:151:TYR:CE2	2.48	0.48
1:F:226:HIS:HA	1:F:230:SER:OG	2.13	0.48
1:A:60:MET:O	1:A:115:LYS:HE3	2.13	0.48
1:D:315:ASN:HA	1:D:337:GLU:HB2	1.96	0.48
1:E:208:LYS:O	1:E:211:LEU:O	2.31	0.48
1:C:451:LYS:HE3	1:C:452:GLU:CG	2.36	0.48
1:D:442:GLU:HA	1:D:445:VAL:HG22	1.96	0.48
1:B:352:ARG:CD	1:E:520:ASN:HD21	2.21	0.48
1:B:40:LYS:HD2	1:B:197:TYR:HE2	1.76	0.48
1:C:270:PRO:HG2	1:C:496:ARG:NH2	2.28	0.48
1:F:10:GLU:O	1:F:13:ILE:HG12	2.14	0.48
1:C:438:VAL:HG13	1:C:439:THR:HG22	1.95	0.48
1:E:496:ARG:O	1:E:499:ILE:HG22	2.14	0.48
1:A:192:ILE:N	1:A:192:ILE:HD12	2.28	0.48
1:E:74:LYS:HE3	1:E:74:LYS:N	2.29	0.48
1:A:244:ILE:O	1:A:244:ILE:HD12	2.13	0.48
1:E:391:MET:CE	1:E:418:MET:HE2	2.44	0.48
1:E:313:ALA:HB2	1:E:345:ASP:HB3	1.95	0.48
1:E:272:ASP:HB3	1:E:273:ARG:NH1	2.28	0.48
1:E:206:ILE:H	1:E:206:ILE:CD1	2.26	0.48
1:D:466:ARG:HA	1:D:469:GLU:HB3	1.96	0.48
1:A:469:GLU:O	1:A:472:LYS:HD3	2.13	0.48
1:E:285:ASP:OD1	1:E:286:ALA:N	2.47	0.48
1:D:439:THR:HG22	1:D:440:GLY:N	2.28	0.48
1:B:446:ARG:HB3	1:B:446:ARG:NH2	2.28	0.48
1:E:17:ARG:HG2	2:F:621:HOH:O	2.13	0.48
1:F:316:ILE:HD11	1:F:349:LYS:CD	2.43	0.48
1:C:412:GLY:O	1:C:415:HIS:HB3	2.14	0.48
1:D:269:ASP:N	1:D:270:PRO:CD	2.77	0.48
1:C:226:HIS:HD2	1:C:230:SER:OG	1.97	0.48
1:A:150:GLY:O	1:A:154:VAL:HG12	2.14	0.48
1:C:124:LEU:HD13	1:F:514:TYR:CE2	2.48	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:131:VAL:HA	1:A:168:ILE:O	2.13	0.48
1:A:244:ILE:HD11	1:A:248:LYS:HE3	1.96	0.48
1:E:450:ARG:C	1:E:452:GLU:N	2.67	0.48
1:F:511:GLU:HG3	1:F:512:TYR:H	1.79	0.48
1:C:344:ILE:CD1	1:C:379:GLN:HE22	2.13	0.47
1:B:180:VAL:HG23	1:B:199:MET:HE2	1.94	0.47
1:A:315:ASN:ND2	1:A:343:ASP:CB	2.76	0.47
1:D:344:ILE:HG13	1:D:379:GLN:NE2	2.29	0.47
1:E:42:THR:OG1	1:E:45:GLU:HG3	2.13	0.47
1:C:210:VAL:HG12	1:C:210:VAL:O	2.13	0.47
1:F:275:ALA:C	1:F:277:GLY:N	2.65	0.47
1:D:175:ALA:O	1:D:199:MET:HA	2.14	0.47
1:B:171:MET:CG	1:B:191:MET:HE3	2.39	0.47
1:D:463:LEU:HD13	1:D:464:LYS:HB3	1.95	0.47
1:D:285:ASP:C	1:D:287:ALA:H	2.18	0.47
1:C:296:ILE:HD12	1:C:296:ILE:O	2.13	0.47
1:B:315:ASN:ND2	1:B:346:ALA:HB2	2.29	0.47
1:A:393:TYR:HA	1:D:159:VAL:HG21	1.96	0.47
1:D:205:GLU:CD	1:D:205:GLU:H	2.17	0.47
1:C:53:ASP:HB3	2:C:545:HOH:O	2.13	0.47
1:F:315:ASN:HD21	1:F:343:ASP:CB	2.14	0.47
1:A:139:ALA:O	1:A:141:ILE:HD12	2.14	0.47
1:F:35:GLN:HG3	1:F:40:LYS:HG3	1.95	0.47
1:F:227:ALA:O	1:F:312:TRP:HB2	2.14	0.47
1:B:295:ILE:O	1:B:299:ILE:HG13	2.13	0.47
1:C:516:LYS:HE2	1:F:164:VAL:HG23	1.97	0.47
1:C:342:ILE:HD12	1:C:343:ASP:H	1.78	0.47
1:B:375:PRO:HB2	1:E:207:THR:CG2	2.35	0.47
1:C:171:MET:HB3	1:C:191:MET:HG3	1.96	0.47
1:A:6:LYS:HE2	1:A:7:PRO:N	2.29	0.47
1:F:344:ILE:HG23	1:F:387:HIS:CG	2.49	0.47
1:E:66:ARG:NH2	1:F:483:LYS:O	2.44	0.47
1:D:432:PRO:HD3	1:D:490:ILE:O	2.15	0.47
1:A:21:GLU:OE2	1:A:21:GLU:N	2.48	0.47
1:F:204:PRO:HG3	1:F:220:LEU:HD22	1.96	0.47
1:F:83:VAL:O	1:F:97:TYR:HA	2.14	0.47
1:C:6:LYS:HZ3	1:C:11:LYS:CG	2.28	0.47
1:A:458:ASN:HD21	1:A:462:VAL:CG1	2.28	0.47
1:D:369:ASP:HB2	1:D:407:VAL:CG1	2.44	0.47
1:E:265:ILE:HG22	1:E:322:ARG:NH2	2.30	0.47
1:A:54:GLY:O	1:A:55:LYS:HG2	2.15	0.47
1:A:497:ARG:HA	1:A:500:VAL:CG1	2.43	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:466:ARG:CG	1:B:467:ILE:N	2.56	0.47
1:E:447:ILE:HD12	1:E:448:LEU:N	2.30	0.47
1:C:211:LEU:CG	1:C:212:GLY:N	2.77	0.47
1:C:193:LYS:HE2	1:C:238:ASP:OD1	2.15	0.47
1:E:316:ILE:HD11	1:E:349:LYS:HD3	1.95	0.47
1:A:237:VAL:CG2	1:A:242:GLU:CB	2.93	0.47
1:A:225:VAL:HG23	1:A:226:HIS:N	2.30	0.47
1:D:6:LYS:C	1:D:8:PRO:HD2	2.35	0.47
1:A:215:VAL:HG22	1:A:216:SER:O	2.15	0.47
1:A:215:VAL:HG23	1:A:219:ASP:HB2	1.97	0.47
1:C:34:PHE:CE1	1:C:38:LYS:HB2	2.50	0.47
1:A:446:ARG:O	1:A:446:ARG:HG2	2.14	0.47
1:A:108:LEU:HD22	1:A:151:TYR:CD2	2.49	0.47
1:C:358:ASP:HA	1:C:400:VAL:CG1	2.45	0.47
1:A:50:LEU:CA	1:A:244:ILE:HD13	2.38	0.47
1:C:264:TYR:HE2	1:C:507:LYS:NZ	2.11	0.47
1:A:265:ILE:HG22	1:A:322:ARG:CD	2.45	0.47
1:C:318:VAL:HG13	1:C:353:PHE:CG	2.50	0.47
1:A:455:GLN:O	1:A:455:GLN:CG	2.61	0.47
1:F:273:ARG:O	1:F:274:ASP:OD2	2.33	0.47
1:D:483:LYS:HB3	1:F:66:ARG:NH2	2.28	0.47
1:D:483:LYS:HD2	1:F:66:ARG:NH2	2.28	0.47
1:A:483:LYS:HB3	1:D:146:LEU:HD21	1.97	0.47
1:F:29:ASP:HA	1:F:32:ILE:CG1	2.43	0.47
1:E:55:LYS:HG3	1:E:55:LYS:O	2.14	0.47
1:A:516:LYS:CE	1:D:162:SER:O	2.62	0.47
1:A:521:ILE:HG13	1:A:522:PRO:HD2	1.97	0.47
1:F:89:VAL:CG2	1:F:89:VAL:O	2.63	0.47
1:A:204:PRO:HD2	1:A:205:GLU:OE1	2.15	0.46
1:A:354:ILE:HG12	1:A:394:ALA:HB1	1.95	0.46
1:D:407:VAL:HG13	1:D:408:ARG:N	2.30	0.46
1:B:494:ASP:O	1:B:498:VAL:HG12	2.14	0.46
1:F:29:ASP:O	1:F:33:GLN:HG3	2.15	0.46
1:E:499:ILE:HD11	1:E:503:LEU:HD11	1.96	0.46
1:E:504:GLU:O	1:E:507:LYS:HE3	2.14	0.46
1:F:205:GLU:HA	1:F:208:LYS:CE	2.29	0.46
1:D:171:MET:HG2	1:D:191:MET:CE	2.37	0.46
1:B:193:LYS:O	1:B:194:GLY:O	2.33	0.46
1:F:58:GLU:CD	1:F:61:THR:HG22	2.36	0.46
1:F:35:GLN:CD	1:F:40:LYS:HG3	2.35	0.46
1:A:464:LYS:NZ	1:A:464:LYS:HB3	2.30	0.46
1:A:494:ASP:CB	1:A:497:ARG:HH12	2.19	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:169:THR:HG22	1:D:186:THR:OG1	2.14	0.46
1:A:518:HIS:HD2	1:A:519:GLY:O	1.98	0.46
1:A:204:PRO:HG2	1:A:217:PHE:CD1	2.50	0.46
1:F:496:ARG:O	1:F:500:VAL:HG23	2.15	0.46
1:C:296:ILE:C	1:C:296:ILE:HD12	2.36	0.46
1:A:135:ASP:HA	1:A:173:GLY:HA3	1.98	0.46
1:C:469:GLU:O	1:C:473:LEU:HD13	2.15	0.46
1:D:266:ASP:CG	1:D:266:ASP:O	2.54	0.46
1:D:208:LYS:HD2	1:D:214:GLU:CG	2.45	0.46
1:C:192:ILE:CG2	1:C:195:ASP:HB2	2.33	0.46
1:C:274:ASP:OD2	1:C:275:ALA:N	2.48	0.46
1:B:32:ILE:HD12	1:B:32:ILE:C	2.35	0.46
1:A:122:LEU:HB3	1:C:505:MET:HE3	1.98	0.46
1:D:260:GLU:HG2	2:D:614:HOH:O	2.16	0.46
1:F:108:LEU:HD22	1:F:151:TYR:CD2	2.50	0.46
1:A:273:ARG:HD2	1:A:274:ASP:N	2.31	0.46
1:C:74:LYS:HD3	1:C:75:GLN:CA	2.46	0.46
1:F:191:MET:HE1	1:F:199:MET:SD	2.56	0.46
1:F:29:ASP:HA	1:F:32:ILE:CD1	2.45	0.46
1:A:269:ASP:OD1	1:A:269:ASP:N	2.46	0.46
1:C:472:LYS:HB3	1:C:473:LEU:HD12	1.98	0.46
1:E:49:LEU:HG	1:E:241:GLN:HE22	1.80	0.46
1:D:120:TYR:O	1:D:124:LEU:HB2	2.15	0.46
1:F:473:LEU:HD23	1:F:474:PHE:CD2	2.51	0.46
1:E:205:GLU:H	1:E:205:GLU:CD	2.18	0.46
1:F:275:ALA:O	1:F:277:GLY:N	2.49	0.46
1:D:208:LYS:CE	1:D:212:GLY:HA2	2.45	0.46
1:A:266:ASP:O	1:A:267:THR:O	2.33	0.46
1:A:342:ILE:HD11	1:A:347:ALA:HB2	1.98	0.46
1:C:175:ALA:O	1:C:199:MET:HA	2.16	0.46
1:B:297:TYR:O	1:B:303:GLY:HA2	2.16	0.46
1:C:418:MET:O	1:C:419:SER:CB	2.64	0.46
1:B:446:ARG:CZ	1:B:446:ARG:CB	2.94	0.46
1:E:225:VAL:CG2	1:E:226:HIS:N	2.78	0.46
1:B:269:ASP:O	1:B:271:ALA:N	2.42	0.46
1:C:193:LYS:O	1:C:219:ASP:OD1	2.34	0.46
1:D:316:ILE:HD12	1:D:346:ALA:HB1	1.96	0.46
1:D:293:ARG:O	1:D:296:ILE:HD13	2.16	0.46
1:B:296:ILE:HG13	1:B:297:TYR:N	2.19	0.46
1:C:217:PHE:HD2	1:C:217:PHE:H	1.63	0.46
1:E:393:TYR:CD2	1:E:521:ILE:HD12	2.50	0.46
1:F:180:VAL:HG21	1:F:201:VAL:HG12	1.98	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:160:MET:HA	1:C:160:MET:CE	2.45	0.46
1:E:281:ILE:HD12	1:E:294:GLU:OE2	2.15	0.46
1:F:72:LEU:HD11	1:F:142:GLN:HB2	1.97	0.46
1:D:334:ASN:ND2	1:D:336:GLU:H	2.13	0.46
1:B:466:ARG:CZ	1:B:467:ILE:HG12	2.46	0.45
1:B:273:ARG:HG2	1:B:497:ARG:HH12	1.82	0.45
1:F:6:LYS:HD2	1:F:8:PRO:CD	2.29	0.45
1:B:450:ARG:CZ	1:B:453:ILE:HD13	2.46	0.45
1:A:447:ILE:CD1	1:D:141:ILE:HG13	2.46	0.45
1:B:343:ASP:HB3	1:B:374:VAL:HG12	1.97	0.45
1:C:107:SER:OG	1:C:140:ARG:CA	2.64	0.45
1:F:450:ARG:C	1:F:452:GLU:N	2.70	0.45
1:D:455:GLN:CA	1:D:455:GLN:HE21	2.27	0.45
1:B:168:ILE:HD13	1:B:250:LEU:HD13	1.97	0.45
1:B:72:LEU:HD11	1:B:142:GLN:HB2	1.98	0.45
1:B:442:GLU:HA	1:B:467:ILE:CG2	2.46	0.45
1:F:204:PRO:O	1:F:208:LYS:HG2	2.16	0.45
1:B:211:LEU:HB3	1:B:212:GLY:H	1.62	0.45
1:D:318:VAL:HG13	1:D:353:PHE:CD2	2.52	0.45
1:B:332:ALA:HB2	1:B:367:LEU:HB2	1.97	0.45
1:B:277:GLY:HA2	1:B:280:GLN:HG3	1.99	0.45
1:F:511:GLU:C	1:F:512:TYR:CD1	2.89	0.45
1:D:257:ASN:HD22	1:D:259:MET:H	1.64	0.45
1:B:442:GLU:HA	1:B:467:ILE:HG21	1.99	0.45
1:D:50:LEU:HB2	1:D:244:ILE:HD13	1.99	0.45
1:C:171:MET:HE2	1:C:173:GLY:N	2.26	0.45
1:A:171:MET:HG2	1:A:199:MET:CE	2.46	0.45
1:A:95:PHE:CZ	1:C:505:MET:HE3	2.51	0.45
1:E:81:GLY:HA3	2:E:558:HOH:O	2.16	0.45
1:D:42:THR:OG1	1:D:45:GLU:HG3	2.16	0.45
1:E:174:PRO:HB2	1:E:197:TYR:CD2	2.51	0.45
1:E:225:VAL:HG23	1:E:226:HIS:N	2.30	0.45
1:E:71:GLY:O	1:E:74:LYS:NZ	2.48	0.45
1:C:13:ILE:C	1:C:13:ILE:HD12	2.37	0.45
1:F:192:ILE:H	1:F:192:ILE:HD12	1.81	0.45
1:E:504:GLU:O	1:E:507:LYS:HG2	2.17	0.45
1:C:332:ALA:HB2	1:C:367:LEU:HB2	1.99	0.45
1:B:196:ALA:O	1:B:197:TYR:CD1	2.69	0.45
1:B:40:LYS:NZ	1:B:197:TYR:CE2	2.72	0.45
1:E:410:SER:OG	1:E:415:HIS:CD2	2.63	0.45
1:F:418:MET:O	1:F:419:SER:CB	2.64	0.45
1:C:83:VAL:O	1:C:97:TYR:HA	2.17	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:6:LYS:HE2	1:F:12:LEU:CG	2.46	0.45
1:D:273:ARG:N	1:D:497:ARG:HG3	2.28	0.45
1:C:490:ILE:CG1	1:C:491:GLU:N	2.80	0.45
1:C:34:PHE:CD2	1:C:38:LYS:NZ	2.84	0.45
1:B:510:ARG:HB2	1:B:510:ARG:HE	1.57	0.45
1:B:393:TYR:HA	1:E:159:VAL:HG21	1.99	0.45
1:E:60:MET:HA	2:F:603:HOH:O	2.17	0.45
1:E:135:ASP:HA	1:E:173:GLY:HA3	1.97	0.45
1:E:6:LYS:HG2	2:E:705:HOH:O	2.16	0.45
1:C:490:ILE:HG13	1:C:491:GLU:N	2.32	0.45
1:C:217:PHE:CD2	1:C:217:PHE:N	2.85	0.45
1:C:226:HIS:HA	1:C:230:SER:OG	2.17	0.45
1:E:89:VAL:HG13	1:E:94:VAL:HG13	1.99	0.45
1:C:438:VAL:HB	1:F:144:GLY:HA2	1.99	0.45
1:A:171:MET:HG2	1:A:199:MET:HE2	1.98	0.45
1:D:342:ILE:HD11	1:D:347:ALA:HB2	1.98	0.45
1:A:496:ARG:HA	1:A:499:ILE:HG22	1.99	0.45
1:F:490:ILE:CG1	1:F:491:GLU:N	2.79	0.45
1:A:449:TYR:C	1:A:450:ARG:NH1	2.70	0.45
1:A:483:LYS:HG3	1:D:146:LEU:HD21	1.97	0.45
1:B:343:ASP:HB3	1:B:374:VAL:HG11	1.99	0.45
1:A:51:PHE:O	1:A:52:ASP:C	2.55	0.45
1:D:463:LEU:C	1:D:463:LEU:HD13	2.37	0.45
1:B:383:GLY:O	1:B:387:HIS:HD2	2.00	0.45
1:C:271:ALA:HB1	1:C:500:VAL:HG11	1.98	0.45
1:B:412:GLY:O	1:B:415:HIS:HB3	2.15	0.45
1:E:31:ARG:NH1	1:E:31:ARG:HG3	2.31	0.45
1:E:28:GLY:O	1:E:32:ILE:HG23	2.17	0.45
1:A:25:LYS:HE3	1:A:29:ASP:OD2	2.17	0.45
1:E:369:ASP:HA	1:E:409:LYS:O	2.17	0.45
1:A:497:ARG:CA	1:A:500:VAL:HG12	2.46	0.45
1:F:273:ARG:HD2	1:F:275:ALA:HB2	1.98	0.45
1:B:461:ASP:O	1:B:462:VAL:C	2.54	0.45
1:F:316:ILE:O	1:F:316:ILE:HD12	2.17	0.45
1:D:273:ARG:N	1:D:497:ARG:HD3	2.32	0.45
1:C:34:PHE:CE2	1:C:38:LYS:NZ	2.82	0.45
1:D:6:LYS:HB3	1:D:6:LYS:HZ3	1.81	0.45
1:C:56:PHE:CG	1:C:57:ASN:N	2.83	0.45
1:D:447:ILE:C	1:D:447:ILE:HD12	2.36	0.45
1:E:110:GLU:HG3	2:E:697:HOH:O	2.17	0.45
1:D:290:TYR:CZ	1:D:335:PRO:HG2	2.52	0.45
1:A:490:ILE:HD11	1:A:494:ASP:OD2	2.16	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:342:ILE:HD12	1:C:346:ALA:HB3	1.99	0.44
1:C:316:ILE:HD11	1:C:349:LYS:CD	2.47	0.44
1:E:449:TYR:N	1:E:450:ARG:NH1	2.57	0.44
1:C:217:PHE:HD2	1:C:217:PHE:N	2.16	0.44
1:A:72:LEU:O	1:A:76:ARG:NE	2.50	0.44
1:B:257:ASN:HD21	1:B:260:GLU:CG	2.29	0.44
1:C:10:GLU:O	1:C:13:ILE:HG13	2.16	0.44
1:E:436:ILE:HD11	2:E:556:HOH:O	2.17	0.44
1:E:156:LYS:O	1:E:160:MET:HG2	2.17	0.44
1:F:265:ILE:O	1:F:267:THR:HG23	2.16	0.44
1:B:521:ILE:HG13	1:B:522:PRO:HD2	1.99	0.44
1:C:214:GLU:N	1:C:214:GLU:CD	2.70	0.44
1:A:461:ASP:O	1:A:465:GLN:HG2	2.17	0.44
1:F:180:VAL:C	1:F:183:PRO:HD2	2.37	0.44
1:D:411:TYR:CD1	1:D:437:ALA:HB3	2.52	0.44
1:C:209:VAL:O	1:C:209:VAL:HG12	2.18	0.44
1:A:272:ASP:HB3	1:A:273:ARG:HH22	1.83	0.44
1:B:466:ARG:CZ	1:B:467:ILE:HG13	2.47	0.44
1:A:202:THR:HG21	1:D:375:PRO:HB3	1.99	0.44
1:F:441:PRO:CG	1:F:471:ARG:HH21	2.30	0.44
1:C:220:LEU:HB3	1:C:221:GLY:H	1.68	0.44
1:D:450:ARG:HB3	1:D:451:LYS:NZ	2.31	0.44
1:B:173:GLY:HA2	1:B:197:TYR:CD2	2.53	0.44
1:C:431:TRP:NE1	1:C:495:THR:CG2	2.78	0.44
1:F:106:GLY:O	1:F:136:SER:CB	2.64	0.44
1:A:190:ILE:HD13	1:A:246:LEU:HD13	1.99	0.44
1:F:512:TYR:O	1:F:513:ARG:HD3	2.17	0.44
1:B:266:ASP:O	1:B:267:THR:C	2.56	0.44
1:B:57:ASN:O	1:B:85:GLY:HA3	2.17	0.44
1:D:208:LYS:HE3	1:D:208:LYS:CA	2.34	0.44
1:A:450:ARG:CA	1:A:450:ARG:CZ	2.92	0.44
1:C:75:GLN:HE21	1:C:76:ARG:N	2.15	0.44
1:B:240:GLU:O	1:B:244:ILE:HG23	2.18	0.44
1:A:158:ASN:HD22	1:A:167:GLN:HE22	1.64	0.44
1:E:285:ASP:OD1	1:E:287:ALA:N	2.41	0.44
1:D:342:ILE:HD13	1:D:373:TYR:CE2	2.52	0.44
1:C:473:LEU:HD12	1:C:473:LEU:N	2.33	0.44
1:A:81:GLY:HA3	2:A:533:HOH:O	2.18	0.44
1:B:462:VAL:O	1:B:462:VAL:HG12	2.18	0.44
1:B:342:ILE:HG12	1:B:373:TYR:CE2	2.53	0.44
1:C:497:ARG:HH11	1:C:497:ARG:CG	2.29	0.44
1:D:455:GLN:CA	1:D:455:GLN:NE2	2.80	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:281:ILE:HD13	1:B:294:GLU:CB	2.48	0.44
1:F:369:ASP:CG	1:F:408:ARG:HB3	2.38	0.44
1:B:393:TYR:OH	1:B:519:GLY:HA3	2.17	0.44
1:B:481:ALA:HA	1:B:486:VAL:HG22	1.98	0.44
1:A:34:PHE:CZ	1:A:38:LYS:HE3	2.52	0.44
1:F:313:ALA:HB2	1:F:345:ASP:HB3	2.00	0.44
1:E:198:TYR:CE2	1:E:223:ALA:N	2.76	0.44
1:C:343:ASP:CG	1:C:344:ILE:HD13	2.37	0.44
1:D:208:LYS:CE	1:D:208:LYS:HA	2.33	0.44
1:D:472:LYS:HD3	1:D:472:LYS:C	2.38	0.44
1:F:369:ASP:HA	1:F:409:LYS:O	2.17	0.44
1:B:58:GLU:OE2	1:B:61:THR:HB	2.18	0.44
1:A:490:ILE:HG13	1:A:491:GLU:O	2.18	0.44
1:E:16:LEU:HD22	1:F:432:PRO:HG3	1.98	0.44
1:D:225:VAL:HG13	2:D:738:HOH:O	2.17	0.44
1:D:493:LYS:HA	2:D:588:HOH:O	2.16	0.44
1:C:28:GLY:O	1:C:31:ARG:N	2.51	0.44
1:D:466:ARG:O	1:D:469:GLU:HB3	2.18	0.44
1:B:405:VAL:HG21	1:B:499:ILE:HD11	2.00	0.44
1:D:126:VAL:HG21	1:E:505:MET:HE2	2.00	0.44
1:C:485:LEU:HD11	1:F:146:LEU:HD12	2.00	0.44
1:B:273:ARG:HG3	1:B:497:ARG:CZ	2.47	0.44
1:C:34:PHE:CE1	1:C:38:LYS:CB	3.01	0.44
1:E:89:VAL:O	1:E:89:VAL:HG23	2.16	0.44
1:A:54:GLY:O	1:A:55:LYS:CG	2.66	0.44
1:F:474:PHE:O	1:F:476:ASN:N	2.45	0.44
1:C:479:TRP:HZ3	1:F:145:ALA:HB3	1.82	0.44
1:B:466:ARG:NH1	1:B:467:ILE:CG1	2.79	0.44
1:E:171:MET:CG	1:E:191:MET:HE3	2.34	0.44
1:F:467:ILE:O	1:F:471:ARG:HG3	2.18	0.44
1:D:407:VAL:HG23	1:D:431:TRP:CE3	2.53	0.44
1:E:418:MET:O	1:E:419:SER:CB	2.66	0.44
1:B:281:ILE:CD1	1:B:294:GLU:HB3	2.48	0.44
1:C:160:MET:HG3	1:F:514:TYR:HD2	1.83	0.44
1:F:456:ALA:C	1:F:458:ASN:H	2.21	0.44
1:D:67:ALA:HB3	1:D:72:LEU:HD23	1.99	0.44
1:A:432:PRO:HD3	1:A:490:ILE:O	2.18	0.43
1:B:466:ARG:N	1:B:466:ARG:HH21	2.15	0.43
1:B:7:PRO:N	1:B:8:PRO:HD2	2.32	0.43
1:C:197:TYR:CE2	1:C:219:ASP:OD1	2.70	0.43
1:A:76:ARG:HH21	1:A:76:ARG:HG2	1.83	0.43
1:B:6:LYS:HG3	1:B:11:LYS:CD	2.47	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:434:ALA:HB3	1:F:477:PRO:CG	2.35	0.43
1:F:257:ASN:HD21	1:F:259:MET:HB2	1.81	0.43
1:B:244:ILE:O	1:B:248:LYS:HG3	2.19	0.43
1:C:431:TRP:NE1	1:C:495:THR:HG21	2.34	0.43
1:A:399:THR:CG2	1:A:513:ARG:NE	2.81	0.43
1:C:182:SER:N	1:C:183:PRO:CD	2.81	0.43
1:E:151:TYR:O	1:E:154:VAL:CG1	2.66	0.43
1:B:265:ILE:O	1:B:266:ASP:HB2	2.18	0.43
1:D:31:ARG:HB3	1:D:102:THR:HB	2.00	0.43
1:E:430:ALA:O	1:E:489:VAL:HA	2.17	0.43
1:B:19:LEU:O	1:B:22:LYS:HB3	2.17	0.43
1:B:460:ASP:O	1:B:460:ASP:OD1	2.36	0.43
1:D:241:GLN:N	1:D:241:GLN:NE2	2.57	0.43
1:D:191:MET:HE1	1:D:199:MET:SD	2.58	0.43
1:F:257:ASN:HD21	1:F:260:GLU:HG3	1.84	0.43
1:C:451:LYS:O	1:C:454:GLN:HG3	2.17	0.43
1:E:342:ILE:HG23	1:E:373:TYR:CD2	2.53	0.43
1:C:513:ARG:HG2	2:C:698:HOH:O	2.18	0.43
1:D:369:ASP:HB2	1:D:407:VAL:HG13	2.00	0.43
1:E:504:GLU:HG2	1:E:507:LYS:HE3	2.00	0.43
1:B:14:GLU:HG3	2:B:722:HOH:O	2.17	0.43
1:F:445:VAL:HG13	1:F:449:TYR:HD1	1.83	0.43
1:C:205:GLU:OE1	1:C:205:GLU:N	2.47	0.43
1:A:466:ARG:HH21	1:A:469:GLU:CD	2.21	0.43
1:A:169:THR:CG2	1:A:186:THR:OG1	2.66	0.43
1:F:29:ASP:CA	1:F:32:ILE:HG12	2.46	0.43
1:A:126:VAL:HG21	1:C:505:MET:HE2	2.00	0.43
1:C:316:ILE:CG1	1:C:346:ALA:HB1	2.49	0.43
1:A:464:LYS:CB	1:A:464:LYS:NZ	2.80	0.43
1:B:20:LYS:HD2	1:B:62:PHE:HZ	1.84	0.43
1:E:16:LEU:HD11	1:E:20:LYS:HE3	1.99	0.43
1:F:490:ILE:CD1	1:F:498:VAL:CG2	2.93	0.43
1:F:11:LYS:NZ	1:F:15:GLU:HG3	2.33	0.43
1:D:493:LYS:N	1:D:493:LYS:HD2	2.28	0.43
1:B:241:GLN:HE21	1:B:241:GLN:N	2.09	0.43
1:A:313:ALA:C	1:A:315:ASN:N	2.69	0.43
1:E:412:GLY:O	1:E:415:HIS:HB3	2.19	0.43
1:A:378:ASP:CG	1:A:382:LYS:HE2	2.39	0.43
1:D:16:LEU:HD11	1:D:20:LYS:HE3	1.99	0.43
1:B:16:LEU:C	1:B:16:LEU:HD13	2.39	0.43
1:E:74:LYS:CE	1:E:74:LYS:H	2.30	0.43
1:F:6:LYS:HZ2	1:F:7:PRO:C	2.20	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:7:PRO:HG2	1:F:8:PRO:HD3	2.01	0.43
1:F:316:ILE:HD11	1:F:349:LYS:CG	2.49	0.43
1:B:180:VAL:HG22	1:E:385:ILE:HG23	2.00	0.43
1:C:208:LYS:HA	1:C:211:LEU:HD21	2.01	0.43
1:A:7:PRO:CG	1:A:8:PRO:CD	2.95	0.43
1:F:182:SER:N	1:F:183:PRO:CD	2.82	0.43
1:C:462:VAL:O	1:C:464:LYS:N	2.49	0.43
1:C:265:ILE:O	1:C:266:ASP:HB2	2.19	0.43
1:D:466:ARG:HH11	1:D:469:GLU:CB	2.32	0.43
1:F:214:GLU:O	1:F:215:VAL:O	2.37	0.43
1:B:434:ALA:HB3	1:B:477:PRO:HB3	2.01	0.43
1:E:273:ARG:CG	1:E:493:LYS:O	2.66	0.43
1:F:206:ILE:HG13	1:F:207:THR:N	2.32	0.43
1:E:269:ASP:C	1:E:271:ALA:H	2.22	0.43
1:A:306:LEU:HD23	1:A:306:LEU:C	2.39	0.43
1:B:318:VAL:HB	1:B:353:PHE:CD2	2.53	0.43
1:F:473:LEU:CD2	1:F:474:PHE:CD2	3.02	0.43
1:D:75:GLN:HB3	2:D:745:HOH:O	2.19	0.43
1:B:445:VAL:C	1:B:447:ILE:H	2.23	0.43
1:B:458:ASN:ND2	1:B:462:VAL:HG11	2.34	0.43
1:D:199:MET:O	1:D:221:GLY:HA3	2.18	0.43
1:C:257:ASN:HD22	1:C:259:MET:N	2.00	0.43
1:B:291:ASN:ND2	1:B:293:ARG:HB2	2.34	0.43
1:D:344:ILE:HG13	1:D:379:GLN:HE22	1.84	0.43
1:E:282:VAL:HA	1:E:283:PRO:HD3	1.87	0.43
1:E:175:ALA:N	1:E:198:TYR:O	2.50	0.42
1:D:174:PRO:HB3	1:D:197:TYR:CE2	2.54	0.42
1:D:276:THR:HA	2:D:588:HOH:O	2.18	0.42
1:B:180:VAL:HG21	1:E:385:ILE:HD13	2.01	0.42
1:A:141:ILE:HD11	2:A:610:HOH:O	2.18	0.42
1:E:432:PRO:HD3	1:E:490:ILE:O	2.19	0.42
1:E:393:TYR:OH	1:E:519:GLY:HA3	2.19	0.42
1:C:214:GLU:N	1:C:214:GLU:OE1	2.51	0.42
1:F:276:THR:HA	1:F:279:GLU:OE2	2.19	0.42
1:F:316:ILE:C	1:F:316:ILE:HD12	2.39	0.42
1:D:275:ALA:O	1:D:276:THR:O	2.37	0.42
1:C:215:VAL:CB	1:C:220:LEU:HG	2.48	0.42
1:C:30:GLU:CB	1:C:31:ARG:HE	2.30	0.42
1:B:193:LYS:O	1:B:194:GLY:C	2.56	0.42
1:A:296:ILE:HG13	1:A:297:TYR:N	2.33	0.42
1:A:73:ASP:CG	1:A:74:LYS:HE3	2.38	0.42
1:C:516:LYS:HE2	1:F:164:VAL:CG2	2.48	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:274:ASP:O	1:F:277:GLY:HA3	2.19	0.42
1:E:74:LYS:CE	1:E:75:GLN:N	2.67	0.42
1:F:15:GLU:O	1:F:19:LEU:HD13	2.19	0.42
1:D:197:TYR:C	1:D:198:TYR:CG	2.93	0.42
1:E:449:TYR:N	1:E:450:ARG:HE	2.17	0.42
1:C:191:MET:CE	1:C:198:TYR:HA	2.49	0.42
1:F:357:CYS:HB2	1:F:364:LEU:HD11	2.01	0.42
1:C:247:THR:HG22	1:C:251:LEU:HD23	2.01	0.42
1:B:452:GLU:O	1:B:452:GLU:HG2	2.19	0.42
1:D:277:GLY:O	1:D:280:GLN:HB2	2.19	0.42
1:C:471:ARG:HA	1:C:475:ALA:HB2	2.00	0.42
1:E:244:ILE:O	1:E:244:ILE:HD12	2.20	0.42
1:A:412:GLY:O	1:A:415:HIS:HB3	2.18	0.42
1:E:32:ILE:HD12	1:E:36:HIS:CE1	2.54	0.42
1:E:476:ASN:HB2	1:E:477:PRO:HD2	2.01	0.42
1:D:502:GLY:O	1:D:506:LEU:HD22	2.19	0.42
1:A:109:GLY:N	1:A:112:HIS:HB3	2.34	0.42
1:A:504:GLU:O	1:A:507:LYS:HG2	2.20	0.42
1:E:228:THR:OG1	1:E:229:LYS:CD	2.67	0.42
1:C:215:VAL:HG11	1:C:220:LEU:HG	2.01	0.42
1:C:29:ASP:HA	1:C:32:ILE:HD13	2.00	0.42
1:C:511:GLU:C	1:C:513:ARG:HH22	2.23	0.42
1:E:490:ILE:HG13	1:E:491:GLU:O	2.20	0.42
1:C:36:HIS:CE1	1:C:45:GLU:OE2	2.73	0.42
1:F:287:ALA:C	1:F:288:LYS:HD2	2.40	0.42
1:E:151:TYR:O	1:E:154:VAL:HG12	2.19	0.42
1:F:35:GLN:O	1:F:40:LYS:HG2	2.19	0.42
1:A:54:GLY:O	1:A:55:LYS:CD	2.67	0.42
1:D:439:THR:HG22	1:D:440:GLY:H	1.84	0.42
1:A:516:LYS:HA	1:D:258:ASN:HD21	1.84	0.42
1:D:418:MET:O	1:D:419:SER:CB	2.67	0.42
1:D:418:MET:O	1:D:419:SER:HB3	2.19	0.42
1:B:180:VAL:HG21	1:E:385:ILE:CD1	2.50	0.42
1:B:257:ASN:HD22	1:B:259:MET:N	2.12	0.42
1:C:6:LYS:NZ	1:C:8:PRO:HG2	2.34	0.42
1:F:241:GLN:NE2	1:F:241:GLN:H	2.17	0.42
1:B:334:ASN:ND2	2:B:618:HOH:O	2.51	0.42
1:C:502:GLY:O	1:C:506:LEU:HG	2.20	0.42
1:C:344:ILE:HG12	1:C:345:ASP:N	2.34	0.42
1:C:316:ILE:HD11	1:C:349:LYS:CG	2.50	0.42
1:F:269:ASP:OD1	1:F:270:PRO:N	2.53	0.42
1:C:46:ARG:HH12	1:C:135:ASP:HB2	1.85	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:146:LEU:HD21	1:D:483:LYS:CB	2.50	0.42
1:A:193:LYS:HB3	1:A:223:ALA:HB3	2.01	0.42
1:F:29:ASP:O	1:F:32:ILE:HG12	2.18	0.42
1:B:369:ASP:HA	1:B:409:LYS:O	2.20	0.42
1:C:141:ILE:HG12	2:C:588:HOH:O	2.18	0.42
1:C:156:LYS:HE2	2:F:733:HOH:O	2.19	0.42
1:D:282:VAL:HA	1:D:283:PRO:HD3	1.82	0.42
1:A:497:ARG:NH1	1:A:497:ARG:CG	2.80	0.42
1:B:385:ILE:HG22	1:E:184:ALA:HB2	2.01	0.42
1:F:11:LYS:HZ3	1:F:15:GLU:HG3	1.84	0.42
1:D:198:TYR:CE2	1:D:218:GLN:OE1	2.72	0.42
1:B:197:TYR:HB3	1:B:198:TYR:H	1.67	0.42
1:E:72:LEU:HD21	1:E:142:GLN:HB3	2.01	0.42
1:B:204:PRO:HB3	1:B:215:VAL:CG1	2.48	0.42
1:E:495:THR:O	1:E:499:ILE:HG22	2.19	0.42
1:F:332:ALA:HB2	1:F:367:LEU:HB2	2.01	0.42
1:F:6:LYS:NZ	1:F:8:PRO:N	2.68	0.42
1:C:267:THR:HA	2:C:560:HOH:O	2.19	0.42
1:F:191:MET:HE3	1:F:191:MET:HB2	1.69	0.42
1:A:95:PHE:CZ	1:C:505:MET:CE	3.03	0.42
1:C:84:THR:HG22	1:C:97:TYR:CB	2.49	0.42
1:D:25:LYS:HA	1:D:25:LYS:HD3	1.92	0.42
1:E:155:PHE:CZ	1:E:181:TYR:HB2	2.55	0.42
1:A:499:ILE:HD13	1:A:499:ILE:C	2.41	0.42
1:D:50:LEU:HD13	1:D:244:ILE:CD1	2.49	0.42
1:B:180:VAL:HG22	1:E:385:ILE:CG2	2.50	0.42
1:B:237:VAL:HG21	1:B:242:GLU:CB	2.49	0.42
1:B:227:ALA:O	1:B:312:TRP:HB2	2.20	0.42
1:D:227:ALA:O	1:D:312:TRP:HB2	2.20	0.42
1:A:494:ASP:O	1:A:497:ARG:NH1	2.52	0.41
1:B:443:GLY:O	1:B:447:ILE:HG23	2.20	0.41
1:E:228:THR:HG22	1:E:311:HIS:CB	2.47	0.41
1:F:203:GLY:O	1:F:207:THR:HG23	2.20	0.41
1:F:316:ILE:HG12	1:F:346:ALA:HB1	2.02	0.41
1:B:208:LYS:HD3	1:B:214:GLU:N	2.35	0.41
1:A:446:ARG:C	1:A:450:ARG:CZ	2.89	0.41
1:B:291:ASN:HD22	1:B:294:GLU:HG3	1.85	0.41
1:E:323:ILE:HG21	1:E:499:ILE:HD12	2.01	0.41
1:A:418:MET:O	1:A:419:SER:CB	2.68	0.41
1:D:351:ALA:O	1:D:355:ARG:HG3	2.19	0.41
1:B:451:LYS:HZ2	1:B:451:LYS:HA	1.77	0.41
1:E:244:ILE:C	1:E:244:ILE:HD12	2.41	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:447:ILE:N	1:F:447:ILE:HD12	2.36	0.41
1:B:226:HIS:HA	1:B:230:SER:OG	2.20	0.41
1:B:464:LYS:O	1:B:464:LYS:CG	2.67	0.41
1:C:464:LYS:C	1:C:466:ARG:H	2.24	0.41
1:F:257:ASN:ND2	1:F:260:GLU:HG3	2.35	0.41
1:C:257:ASN:HD21	1:C:259:MET:HB2	1.86	0.41
1:C:55:LYS:HZ2	1:C:55:LYS:HB3	1.85	0.41
1:F:128:ALA:N	1:F:165:ILE:HD13	2.35	0.41
1:A:54:GLY:O	1:A:55:LYS:HD3	2.19	0.41
1:A:278:VAL:HG13	1:A:279:GLU:N	2.35	0.41
1:A:452:GLU:O	1:A:452:GLU:CD	2.59	0.41
1:F:296:ILE:O	1:F:296:ILE:HD12	2.20	0.41
1:A:365:ILE:HD11	1:A:499:ILE:HD11	2.02	0.41
1:B:193:LYS:O	1:B:193:LYS:HG2	2.19	0.41
1:A:342:ILE:HG23	1:A:373:TYR:CD2	2.56	0.41
1:C:6:LYS:HE3	1:C:8:PRO:HD2	2.03	0.41
1:E:168:ILE:CD1	1:E:250:LEU:HD23	2.50	0.41
1:F:507:LYS:HD2	2:F:743:HOH:O	2.19	0.41
1:D:323:ILE:O	1:D:324:ALA:HB3	2.21	0.41
1:F:490:ILE:HG12	1:F:491:GLU:H	1.85	0.41
1:B:208:LYS:HD2	1:B:212:GLY:HA2	2.03	0.41
1:C:451:LYS:CD	1:C:452:GLU:N	2.83	0.41
1:D:461:ASP:C	1:D:463:LEU:H	2.22	0.41
1:C:46:ARG:HD3	1:C:133:ILE:HG21	2.01	0.41
1:F:177:GLY:O	1:F:180:VAL:HG22	2.21	0.41
1:A:179:ALA:HB1	2:A:667:HOH:O	2.21	0.41
1:C:247:THR:O	1:C:251:LEU:HD23	2.20	0.41
1:A:256:SER:HB2	1:A:260:GLU:OE1	2.20	0.41
1:E:9:VAL:HG13	1:E:10:GLU:N	2.36	0.41
1:C:376:GLY:HA3	2:C:655:HOH:O	2.19	0.41
1:F:273:ARG:CB	1:F:497:ARG:HH12	2.09	0.41
1:B:495:THR:HA	1:B:498:VAL:CG1	2.50	0.41
1:F:512:TYR:N	1:F:512:TYR:CD1	2.88	0.41
1:F:89:VAL:HG22	1:F:89:VAL:O	2.20	0.41
1:D:255:PRO:HB2	1:D:260:GLU:HB3	2.03	0.41
1:F:273:ARG:CD	1:F:275:ALA:HB2	2.50	0.41
1:F:15:GLU:HA	1:F:18:GLN:HE21	1.86	0.41
1:D:198:TYR:HB2	1:D:199:MET:H	1.72	0.41
1:A:450:ARG:CZ	1:A:450:ARG:N	2.84	0.41
1:D:453:ILE:O	1:D:454:GLN:HG3	2.21	0.41
1:D:464:LYS:O	1:D:467:ILE:HG12	2.21	0.41
1:E:344:ILE:CD1	1:E:382:LYS:HB2	2.50	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:129:PRO:HA	1:F:165:ILE:HG23	2.01	0.41
1:A:190:ILE:CD1	1:A:246:LEU:HD13	2.50	0.41
1:C:358:ASP:HA	1:C:400:VAL:HG11	2.03	0.41
1:F:318:VAL:HG13	1:F:353:PHE:CD1	2.56	0.41
1:D:399:THR:HG22	1:D:513:ARG:NH1	2.36	0.41
1:D:17:ARG:HG2	2:E:614:HOH:O	2.21	0.41
1:A:392:LEU:HD23	1:A:417:ALA:HA	2.01	0.41
1:B:458:ASN:HA	1:B:459:PRO:HD3	1.84	0.41
1:E:200:PHE:CE1	1:E:203:GLY:HA2	2.55	0.41
1:A:146:LEU:HD23	1:D:479:TRP:CZ3	2.56	0.41
1:A:467:ILE:O	1:A:471:ARG:HG3	2.21	0.41
1:F:71:GLY:O	1:F:74:LYS:HB3	2.21	0.41
1:A:109:GLY:O	1:A:112:HIS:HB3	2.21	0.41
1:B:225:VAL:CG2	1:B:226:HIS:N	2.84	0.41
1:B:392:LEU:HD23	1:B:417:ALA:HA	2.02	0.41
1:A:274:ASP:HB2	1:A:275:ALA:H	1.46	0.41
1:A:490:ILE:CG1	1:A:494:ASP:HB2	2.51	0.41
1:F:490:ILE:CD1	1:F:494:ASP:HB2	2.48	0.41
1:F:212:GLY:O	1:F:213:GLU:HG3	2.21	0.41
1:C:344:ILE:HG12	1:C:345:ASP:OD1	2.21	0.41
1:B:449:TYR:O	1:B:453:ILE:HG22	2.21	0.41
1:C:276:THR:HG23	1:C:276:THR:O	2.20	0.41
1:C:494:ASP:O	1:C:498:VAL:HG23	2.21	0.41
1:B:208:LYS:HD2	1:B:212:GLY:C	2.42	0.41
1:A:177:GLY:O	1:A:180:VAL:HB	2.21	0.41
1:D:466:ARG:HB3	1:D:469:GLU:OE2	2.20	0.41
1:C:191:MET:HE1	1:C:198:TYR:HA	2.03	0.41
1:E:51:PHE:O	1:E:52:ASP:C	2.57	0.41
1:B:495:THR:O	1:B:498:VAL:HG13	2.21	0.41
1:D:6:LYS:HB3	1:D:6:LYS:HZ2	1.86	0.41
1:B:146:LEU:HD22	1:E:479:TRP:CH2	2.56	0.41
1:B:429:TYR:OH	1:C:57:ASN:ND2	2.54	0.41
1:D:344:ILE:H	1:D:379:GLN:HE22	1.68	0.41
1:F:369:ASP:OD1	1:F:408:ARG:HB3	2.21	0.41
1:E:49:LEU:HD13	2:E:612:HOH:O	2.21	0.41
1:E:190:ILE:HD13	1:E:246:LEU:HD13	2.02	0.41
1:D:372:GLY:HA2	1:D:414:ALA:HB2	2.03	0.41
1:E:22:LYS:HG3	2:E:715:HOH:O	2.19	0.41
1:D:68:THR:HA	1:D:73:ASP:HB3	2.03	0.41
1:C:7:PRO:HG2	1:C:8:PRO:CD	2.46	0.41
1:A:108:LEU:HD22	1:A:151:TYR:CG	2.56	0.41
1:F:450:ARG:C	1:F:451:LYS:HG2	2.41	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:214:GLU:H	1:F:214:GLU:CD	2.24	0.41
1:A:95:PHE:HZ	1:C:505:MET:CE	2.34	0.41
1:E:198:TYR:CE2	1:E:218:GLN:NE2	2.89	0.40
1:B:451:LYS:HZ1	1:B:454:GLN:HE22	1.69	0.40
1:F:441:PRO:O	1:F:445:VAL:HG23	2.21	0.40
1:F:442:GLU:HB2	1:F:467:ILE:HD11	2.03	0.40
1:D:461:ASP:OD2	1:D:465:GLN:NE2	2.53	0.40
1:B:321:ALA:O	1:B:327:VAL:HA	2.21	0.40
1:C:481:ALA:CA	1:C:486:VAL:HG22	2.47	0.40
1:E:270:PRO:C	1:E:496:ARG:HH21	2.24	0.40
1:B:20:LYS:HD2	1:B:62:PHE:CZ	2.56	0.40
1:D:281:ILE:CD1	1:D:294:GLU:HG2	2.51	0.40
1:B:300:VAL:HA	1:B:323:ILE:HD13	2.03	0.40
1:C:262:PRO:HB2	1:C:327:VAL:CG2	2.51	0.40
1:A:57:ASN:O	1:A:85:GLY:HA3	2.21	0.40
1:D:266:ASP:OD1	1:D:266:ASP:O	2.39	0.40
1:A:446:ARG:O	1:A:450:ARG:CZ	2.69	0.40
1:D:452:GLU:CD	1:D:452:GLU:N	2.69	0.40
1:C:439:THR:CG2	1:C:444:ALA:HB2	2.51	0.40
1:D:432:PRO:HG3	1:F:16:LEU:HD22	2.02	0.40
1:B:310:LYS:HG2	1:B:311:HIS:CE1	2.56	0.40
1:E:204:PRO:HG2	1:E:217:PHE:CD2	2.56	0.40
1:A:273:ARG:NH1	1:A:497:ARG:CD	2.84	0.40
1:F:464:LYS:NZ	1:F:464:LYS:HB3	2.36	0.40
1:A:449:TYR:C	1:A:450:ARG:CZ	2.89	0.40
1:E:448:LEU:HD12	1:E:449:TYR:N	2.36	0.40
1:D:445:VAL:HG21	1:D:467:ILE:CD1	2.46	0.40
1:E:471:ARG:O	1:E:475:ALA:HB3	2.21	0.40
1:D:125:LYS:NZ	1:E:511:GLU:OE1	2.34	0.40
1:F:342:ILE:HG13	1:F:343:ASP:N	2.35	0.40
1:B:374:VAL:O	1:B:374:VAL:HG13	2.21	0.40
1:C:270:PRO:HG2	1:C:496:ARG:HH21	1.86	0.40
1:E:244:ILE:CD1	1:E:248:LYS:HE3	2.52	0.40
1:D:358:ASP:CG	1:D:398:ALA:HA	2.42	0.40
1:B:274:ASP:O	1:B:275:ALA:C	2.60	0.40
1:B:280:GLN:NE2	2:B:671:HOH:O	2.54	0.40
1:B:464:LYS:HD2	1:B:464:LYS:O	2.21	0.40
1:C:385:ILE:HG22	1:F:184:ALA:HB2	2.03	0.40
1:A:449:TYR:H	1:A:450:ARG:NH1	2.14	0.40
1:A:451:LYS:N	1:A:451:LYS:CD	2.82	0.40
1:F:382:LYS:HE2	1:F:382:LYS:HB3	1.87	0.40
1:A:237:VAL:HG22	1:A:238:ASP:H	1.85	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:70:PHE:CZ	1:F:448:LEU:HD13	2.56	0.40
1:A:33:GLN:HB2	2:A:690:HOH:O	2.21	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

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	516/522 (99%)	471 (91%)	31 (6%)	14 (3%)	8	3
1	B	516/522 (99%)	471 (91%)	30 (6%)	15 (3%)	7	3
1	C	516/522 (99%)	461 (89%)	37 (7%)	18 (4%)	6	2
1	D	516/522 (99%)	474 (92%)	25 (5%)	17 (3%)	6	2
1	E	516/522 (99%)	468 (91%)	37 (7%)	11 (2%)	11	5
1	F	516/522 (99%)	479 (93%)	25 (5%)	12 (2%)	10	5
All	All	3096/3132 (99%)	2824 (91%)	185 (6%)	87 (3%)	8	3

All (87) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	7	PRO
1	A	52	ASP
1	A	267	THR
1	A	270	PRO
1	A	273	ARG
1	A	459	PRO
1	B	194	GLY
1	B	265	ILE
1	B	464	LYS
1	C	195	ASP
1	C	216	SER
1	C	266	ASP
1	C	267	THR

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Mol	Chain	Res	Type
1	C	453	ILE
1	D	197	TYR
1	D	266	ASP
1	D	267	THR
1	D	273	ARG
1	D	276	THR
1	E	52	ASP
1	E	196	ALA
1	E	197	TYR
1	E	273	ARG
1	E	274	ASP
1	E	276	THR
1	F	215	VAL
1	F	270	PRO
1	F	275	ALA
1	F	459	PRO
1	A	53	ASP
1	B	196	ALA
1	B	276	THR
1	C	27	GLY
1	C	277	GLY
1	C	464	LYS
1	D	265	ILE
1	D	268	GLY
1	D	442	GLU
1	D	454	GLN
1	D	457	SER
1	E	53	ASP
1	E	265	ILE
1	F	212	GLY
1	F	276	THR
1	A	419	SER
1	B	267	THR
1	B	275	ALA
1	B	419	SER
1	C	37	SER
1	C	211	LEU
1	C	212	GLY
1	C	419	SER
1	C	452	GLU
1	D	419	SER
1	E	419	SER

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Mol	Chain	Res	Type
1	F	269	ASP
1	F	419	SER
1	A	275	ALA
1	A	369	ASP
1	B	207	THR
1	B	459	PRO
1	C	7	PRO
1	C	56	PHE
1	C	219	ASP
1	D	286	ALA
1	D	450	ARG
1	A	174	PRO
1	A	210	VAL
1	A	266	ASP
1	B	266	ASP
1	B	457	SER
1	C	77	PHE
1	C	302	ASN
1	D	196	ALA
1	D	198	TYR
1	D	270	PRO
1	E	518	HIS
1	F	278	VAL
1	F	302	ASN
1	F	475	ALA
1	A	458	ASN
1	B	277	GLY
1	B	462	VAL
1	D	462	VAL
1	F	268	GLY
1	B	7	PRO
1	E	174	PRO

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	413/416 (99%)	376 (91%)	37 (9%)	14 13

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	413/416 (99%)	372 (90%)	41 (10%)	11	10
1	C	413/416 (99%)	372 (90%)	41 (10%)	11	10
1	D	413/416 (99%)	376 (91%)	37 (9%)	14	13
1	E	413/416 (99%)	377 (91%)	36 (9%)	15	14
1	F	413/416 (99%)	380 (92%)	33 (8%)	17	16
All	All	2478/2496 (99%)	2253 (91%)	225 (9%)	14	13

All (225) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	LYS
1	A	11	LYS
1	A	21	GLU
1	A	32	ILE
1	A	49	LEU
1	A	61	THR
1	A	68	THR
1	A	76	ARG
1	A	154	VAL
1	A	208	LYS
1	A	244	ILE
1	A	246	LEU
1	A	266	ASP
1	A	269	ASP
1	A	273	ARG
1	A	274	ASP
1	A	276	THR
1	A	298	LYS
1	A	316	ILE
1	A	334	ASN
1	A	342	ILE
1	A	352	ARG
1	A	354	ILE
1	A	435	GLU
1	A	450	ARG
1	A	451	LYS
1	A	452	GLU
1	A	455	GLN
1	A	458	ASN
1	A	459	PRO

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Mol	Chain	Res	Type
1	A	463	LEU
1	A	467	ILE
1	A	472	LYS
1	A	486	VAL
1	A	497	ARG
1	A	499	ILE
1	A	513	ARG
1	B	13	ILE
1	B	14	GLU
1	B	20	LYS
1	B	32	ILE
1	B	61	THR
1	B	112	HIS
1	B	118	ARG
1	B	124	LEU
1	B	146	LEU
1	B	169	THR
1	B	211	LEU
1	B	214	GLU
1	B	225	VAL
1	B	241	GLN
1	B	244	ILE
1	B	250	LEU
1	B	257	ASN
1	B	264	TYR
1	B	296	ILE
1	B	304	GLU
1	B	310	LYS
1	B	315	ASN
1	B	317	ILE
1	B	327	VAL
1	B	334	ASN
1	B	342	ILE
1	B	352	ARG
1	B	365	ILE
1	B	436	ILE
1	B	446	ARG
1	B	447	ILE
1	B	448	LEU
1	B	450	ARG
1	B	451	LYS
1	B	453	ILE

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Mol	Chain	Res	Type
1	B	461	ASP
1	B	465	GLN
1	B	466	ARG
1	B	473	LEU
1	B	505	MET
1	B	510	ARG
1	C	6	LYS
1	C	11	LYS
1	C	31	ARG
1	C	32	ILE
1	C	33	GLN
1	C	38	LYS
1	C	75	GLN
1	C	76	ARG
1	C	108	LEU
1	C	160	MET
1	C	169	THR
1	C	197	TYR
1	C	205	GLU
1	C	206	ILE
1	C	207	THR
1	C	211	LEU
1	C	214	GLU
1	C	217	PHE
1	C	218	GLN
1	C	220	LEU
1	C	264	TYR
1	C	288	LYS
1	C	296	ILE
1	C	298	LYS
1	C	304	GLU
1	C	315	ASN
1	C	318	VAL
1	C	342	ILE
1	C	344	ILE
1	C	377	THR
1	C	407	VAL
1	C	427	LEU
1	C	436	ILE
1	C	448	LEU
1	C	450	ARG
1	C	451	LYS

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Mol	Chain	Res	Type
1	C	461	ASP
1	C	462	VAL
1	C	472	LYS
1	C	476	ASN
1	C	497	ARG
1	D	13	ILE
1	D	19	LEU
1	D	32	ILE
1	D	61	THR
1	D	68	THR
1	D	142	GLN
1	D	169	THR
1	D	197	TYR
1	D	206	ILE
1	D	208	LYS
1	D	241	GLN
1	D	244	ILE
1	D	251	LEU
1	D	257	ASN
1	D	260	GLU
1	D	288	LYS
1	D	294	GLU
1	D	296	ILE
1	D	315	ASN
1	D	318	VAL
1	D	334	ASN
1	D	342	ILE
1	D	352	ARG
1	D	427	LEU
1	D	436	ILE
1	D	442	GLU
1	D	448	LEU
1	D	451	LYS
1	D	452	GLU
1	D	455	GLN
1	D	461	ASP
1	D	463	LEU
1	D	467	ILE
1	D	473	LEU
1	D	493	LYS
1	D	506	LEU
1	D	510	ARG

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Mol	Chain	Res	Type
1	E	6	LYS
1	E	11	LYS
1	E	32	ILE
1	E	49	LEU
1	E	53	ASP
1	E	61	THR
1	E	68	THR
1	E	74	LYS
1	E	146	LEU
1	E	180	VAL
1	E	197	TYR
1	E	208	LYS
1	E	211	LEU
1	E	244	ILE
1	E	246	LEU
1	E	259	MET
1	E	273	ARG
1	E	276	THR
1	E	278	VAL
1	E	299	ILE
1	E	316	ILE
1	E	318	VAL
1	E	327	VAL
1	E	342	ILE
1	E	436	ILE
1	E	450	ARG
1	E	452	GLU
1	E	455	GLN
1	E	458	ASN
1	E	460	ASP
1	E	462	VAL
1	E	464	LYS
1	E	469	GLU
1	E	486	VAL
1	E	499	ILE
1	E	505	MET
1	F	6	LYS
1	F	10	GLU
1	F	66	ARG
1	F	89	VAL
1	F	108	LEU
1	F	124	LEU

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Mol	Chain	Res	Type
1	F	126	VAL
1	F	146	LEU
1	F	169	THR
1	F	185	LEU
1	F	206	ILE
1	F	211	LEU
1	F	214	GLU
1	F	241	GLN
1	F	244	ILE
1	F	250	LEU
1	F	251	LEU
1	F	270	PRO
1	F	273	ARG
1	F	291	ASN
1	F	296	ILE
1	F	315	ASN
1	F	327	VAL
1	F	342	ILE
1	F	364	LEU
1	F	407	VAL
1	F	427	LEU
1	F	436	ILE
1	F	446	ARG
1	F	455	GLN
1	F	473	LEU
1	F	510	ARG
1	F	512	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (75) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	GLN
1	A	167	GLN
1	A	241	GLN
1	A	280	GLN
1	A	284	ASN
1	A	326	ASN
1	A	333	ASN
1	A	334	ASN
1	A	415	HIS
1	A	455	GLN
1	A	458	ASN

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Mol	Chain	Res	Type
1	A	465	GLN
1	A	518	HIS
1	B	18	GLN
1	B	241	GLN
1	B	245	ASN
1	B	257	ASN
1	B	291	ASN
1	B	302	ASN
1	B	326	ASN
1	B	334	ASN
1	B	361	ASN
1	B	379	GLN
1	B	387	HIS
1	B	415	HIS
1	B	454	GLN
1	B	455	GLN
1	B	458	ASN
1	B	465	GLN
1	B	518	HIS
1	C	36	HIS
1	C	57	ASN
1	C	75	GLN
1	C	218	GLN
1	C	226	HIS
1	C	245	ASN
1	C	257	ASN
1	C	291	ASN
1	C	326	ASN
1	C	379	GLN
1	C	415	HIS
1	C	476	ASN
1	D	18	GLN
1	D	57	ASN
1	D	75	GLN
1	D	112	HIS
1	D	142	GLN
1	D	167	GLN
1	D	226	HIS
1	D	241	GLN
1	D	245	ASN
1	D	257	ASN
1	D	315	ASN

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Mol	Chain	Res	Type
1	D	334	ASN
1	D	361	ASN
1	D	379	GLN
1	D	415	HIS
1	D	454	GLN
1	D	455	GLN
1	E	18	GLN
1	E	226	HIS
1	E	241	GLN
1	E	280	GLN
1	E	302	ASN
1	E	311	HIS
1	E	415	HIS
1	E	520	ASN
1	F	18	GLN
1	F	241	GLN
1	F	245	ASN
1	F	257	ASN
1	F	291	ASN
1	F	302	ASN
1	F	326	ASN
1	F	455	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

There are no ligands in this entry.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å <sup>2</sup> )	Q<0.9
1	A	518/522 (99%)	-0.05	26 (5%)	28 27	8, 17, 57, 83	0
1	B	518/522 (99%)	-0.06	29 (5%)	24 23	7, 19, 61, 82	0
1	C	518/522 (99%)	0.15	49 (9%)	8 8	9, 19, 68, 81	0
1	D	518/522 (99%)	-0.05	30 (5%)	22 22	10, 19, 60, 83	0
1	E	518/522 (99%)	-0.01	32 (6%)	20 19	9, 17, 57, 81	0
1	F	518/522 (99%)	-0.00	26 (5%)	28 27	9, 19, 61, 82	0
All	All	3108/3132 (99%)	-0.00	192 (6%)	20 19	7, 19, 61, 83	0

All (192) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	276	THR	12.1
1	C	54	GLY	10.2
1	C	215	VAL	9.2
1	E	456	ALA	9.0
1	D	461	ASP	8.3
1	D	268	GLY	7.8
1	D	456	ALA	7.7
1	B	269	ASP	7.5
1	D	462	VAL	7.4
1	D	269	ASP	7.2
1	F	7	PRO	7.1
1	C	7	PRO	7.1
1	B	462	VAL	7.1
1	A	275	ALA	6.9
1	A	7	PRO	6.6
1	F	210	VAL	6.5
1	B	266	ASP	6.4
1	E	275	ALA	6.4
1	A	456	ALA	6.3

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Mol	Chain	Res	Type	RSRZ
1	C	37	SER	6.2
1	A	457	SER	6.2
1	C	33	GLN	6.0
1	F	275	ALA	6.0
1	C	36	HIS	5.9
1	B	457	SER	5.7
1	C	275	ALA	5.6
1	E	455	GLN	5.6
1	C	461	ASP	5.6
1	A	458	ASN	5.5
1	A	462	VAL	5.5
1	E	197	TYR	5.4
1	F	211	LEU	5.2
1	E	512	TYR	5.2
1	C	34	PHE	5.2
1	D	198	TYR	5.1
1	E	198	TYR	5.1
1	A	276	THR	5.0
1	E	211	LEU	5.0
1	A	54	GLY	5.0
1	D	459	PRO	4.9
1	D	197	TYR	4.9
1	B	455	GLN	4.9
1	A	461	ASP	4.9
1	D	458	ASN	4.8
1	C	462	VAL	4.8
1	B	275	ALA	4.8
1	B	6	LYS	4.8
1	E	457	SER	4.8
1	A	514	TYR	4.7
1	E	212	GLY	4.7
1	D	455	GLN	4.7
1	E	206	ILE	4.7
1	F	209	VAL	4.6
1	E	6	LYS	4.6
1	C	217	PHE	4.6
1	E	54	GLY	4.6
1	E	276	THR	4.6
1	F	213	GLU	4.6
1	F	453	ILE	4.5
1	F	457	SER	4.5
1	C	212	GLY	4.5

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Mol	Chain	Res	Type	RSRZ
1	F	458	ASN	4.3
1	D	449	TYR	4.2
1	E	210	VAL	4.2
1	C	32	ILE	4.2
1	D	452	GLU	4.2
1	A	266	ASP	4.1
1	C	216	SER	4.1
1	E	458	ASN	4.1
1	B	265	ILE	4.1
1	C	457	SER	4.1
1	C	56	PHE	4.0
1	C	218	GLN	4.0
1	E	207	THR	3.9
1	A	459	PRO	3.9
1	C	210	VAL	3.9
1	B	451	LYS	3.8
1	D	267	THR	3.8
1	C	206	ILE	3.8
1	F	475	ALA	3.7
1	F	208	LYS	3.7
1	A	211	LEU	3.7
1	F	270	PRO	3.7
1	B	206	ILE	3.6
1	A	452	GLU	3.6
1	E	213	GLU	3.6
1	B	197	TYR	3.6
1	D	451	LYS	3.6
1	D	275	ALA	3.5
1	B	196	ALA	3.5
1	A	207	THR	3.5
1	B	268	GLY	3.5
1	C	456	ALA	3.4
1	C	459	PRO	3.4
1	F	206	ILE	3.4
1	C	465	GLN	3.4
1	B	456	ALA	3.4
1	F	269	ASP	3.4
1	D	6	LYS	3.4
1	B	276	THR	3.4
1	F	474	PHE	3.3
1	C	57	ASN	3.3
1	F	514	TYR	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	264	TYR	3.3
1	D	514	TYR	3.3
1	C	55	LYS	3.2
1	E	447	ILE	3.2
1	C	207	THR	3.2
1	E	273	ARG	3.1
1	C	268	GLY	3.1
1	A	455	GLN	3.1
1	C	475	ALA	3.1
1	C	6	LYS	3.1
1	E	265	ILE	3.1
1	B	7	PRO	3.1
1	D	213	GLU	3.0
1	A	213	GLU	3.0
1	C	195	ASP	3.0
1	C	451	LYS	3.0
1	C	35	GLN	3.0
1	B	213	GLU	2.9
1	C	194	GLY	2.9
1	B	449	TYR	2.9
1	E	448	LEU	2.8
1	D	515	PRO	2.8
1	C	270	PRO	2.8
1	B	212	GLY	2.7
1	E	452	GLU	2.7
1	C	211	LEU	2.7
1	A	447	ILE	2.7
1	E	269	ASP	2.7
1	A	273	ARG	2.7
1	A	268	GLY	2.7
1	B	465	GLN	2.7
1	B	270	PRO	2.7
1	D	453	ILE	2.7
1	F	212	GLY	2.7
1	E	270	PRO	2.7
1	B	208	LYS	2.6
1	F	459	PRO	2.6
1	B	447	ILE	2.6
1	F	512	TYR	2.5
1	C	209	VAL	2.5
1	B	514	TYR	2.5
1	F	451	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
1	E	53	ASP	2.5
1	C	196	ALA	2.5
1	B	515	PRO	2.5
1	C	271	ALA	2.5
1	F	515	PRO	2.5
1	C	450	ARG	2.4
1	E	459	PRO	2.4
1	F	6	LYS	2.4
1	A	450	ARG	2.4
1	C	214	GLU	2.4
1	C	272	ASP	2.4
1	D	467	ILE	2.3
1	C	276	THR	2.3
1	A	212	GLY	2.3
1	E	208	LYS	2.3
1	B	277	GLY	2.3
1	C	269	ASP	2.3
1	E	7	PRO	2.3
1	C	513	ARG	2.2
1	C	454	GLN	2.2
1	E	450	ARG	2.2
1	A	206	ILE	2.2
1	D	266	ASP	2.2
1	F	207	THR	2.2
1	D	270	PRO	2.2
1	E	454	GLN	2.2
1	C	267	THR	2.2
1	D	463	LEU	2.2
1	D	7	PRO	2.1
1	D	447	ILE	2.1
1	F	271	ALA	2.1
1	D	457	SER	2.1
1	F	456	ALA	2.1
1	C	197	TYR	2.1
1	A	284	ASN	2.1
1	C	514	TYR	2.1
1	A	267	THR	2.1
1	C	220	LEU	2.1
1	C	213	GLU	2.1
1	E	267	THR	2.1
1	E	71	GLY	2.0
1	D	209	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	446	ARG	2.0
1	A	463	LEU	2.0
1	D	460	ASP	2.0
1	D	284	ASN	2.0
1	B	273	ARG	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

There are no ligands in this entry.

## 6.5 Other polymers ⓘ

There are no such residues in this entry.