



# Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 03:58 AM GMT

PDB ID : 1PWQ  
Title : Crystal structure of Anthrax Lethal Factor complexed with Thioacetyl-Tyr-Pro-Met-Amide, a metal-chelating peptidyl small molecule inhibitor  
Authors : Wong, T.Y.; Schwarzenbacher, R.; Liddington, R.C.  
Deposited on : 2003-07-02  
Resolution : 3.52 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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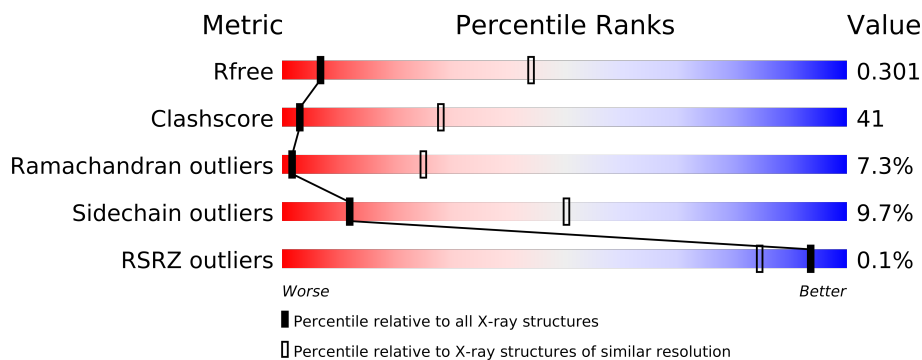
The following versions of software and data (see [references](#)) were used in the production of this report:

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 3.52 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	1256 (3.74-3.30)
Clashscore	79885	1020 (3.68-3.36)
Ramachandran outliers	78287	1082 (3.70-3.34)
Sidechain outliers	78261	1082 (3.70-3.34)
RSRZ outliers	66119	1256 (3.74-3.30)

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	776	
1	B	776	

## 2 Entry composition i

There are 3 unique types of molecules in this entry. The entry contains 12120 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.

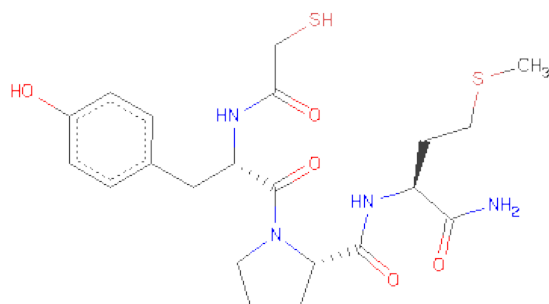
- Molecule 1 is a protein called Lethal factor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	732	Total	C	N	O	S	0	0	0
			6020	3827	1015	1171	7			
1	B	734	Total	C	N	O	S	0	0	0
			6034	3834	1017	1176	7			

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Zn	0	0
			1	1		
2	A	1	Total	Zn	0	0
			1	1		

- Molecule 3 is N-(SULFANYLACETYL)TYROSYLPROLYLMETHIONINAMIDE (three-letter code: SD2) (formula: C<sub>21</sub>H<sub>30</sub>N<sub>4</sub>O<sub>5</sub>S<sub>2</sub>).

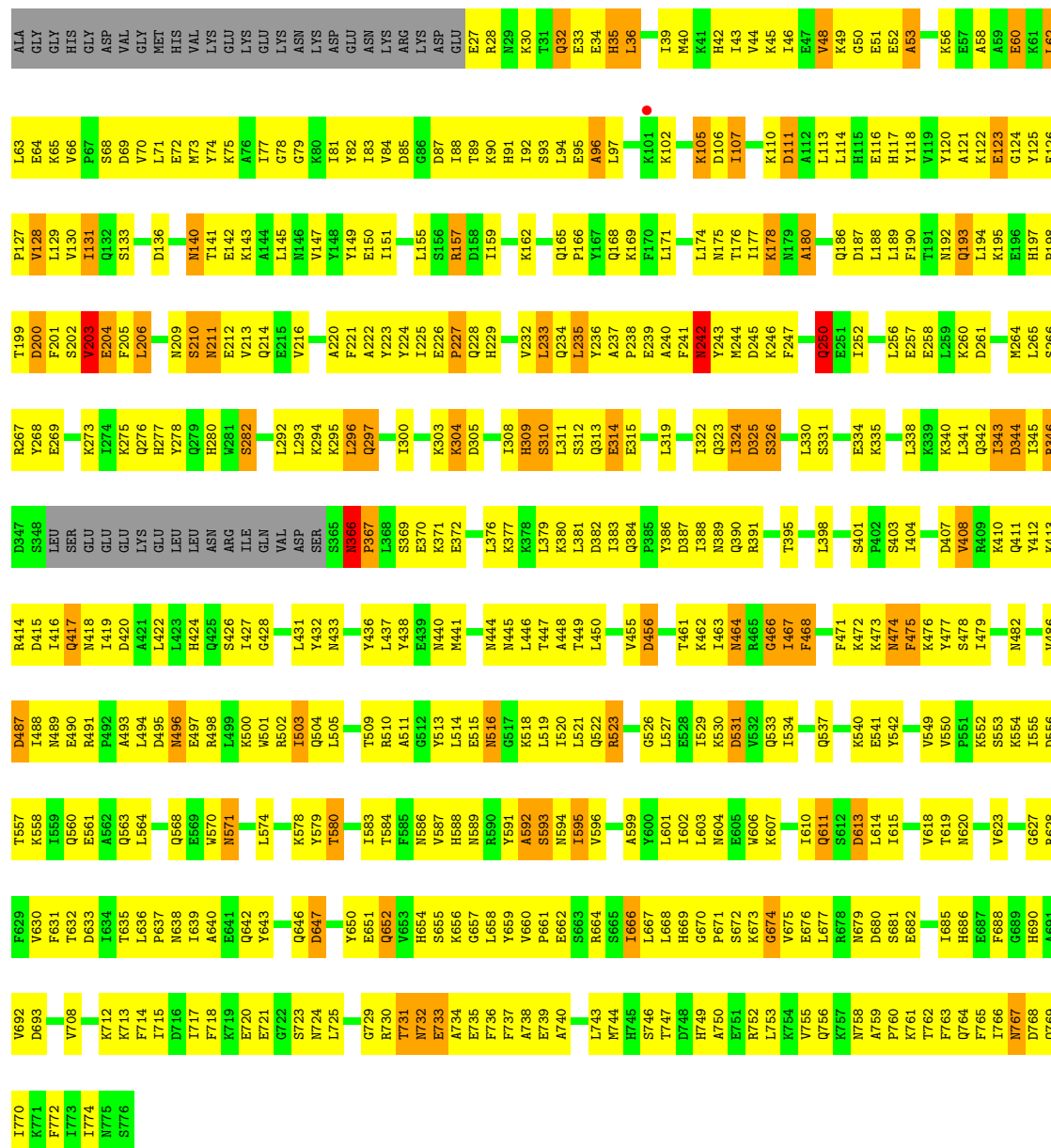


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			32	21	4	5	2		
3	B	1	Total	C	N	O	S	0	0
			32	21	4	5	2		



● Molecule 1: Lethal factor

Chain B:



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	96.70Å 137.40Å 98.30Å 90.00° 98.00° 90.00°	Depositor
Resolution (Å)	24.86 – 3.52 24.86 – 3.51	Depositor EDS
% Data completeness (in resolution range)	86.7 (24.86-3.52) 82.4 (24.86-3.51)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.16	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.81 (at 3.54Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.228 , 0.311 0.226 , 0.301	Depositor DCC
$R_{free}$ test set	1330 reflections (4.90%)	DCC
Wilson B-factor (Å <sup>2</sup> )	49.5	Xtriage
Anisotropy	0.099	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , -5.9	EDS
Estimated twinning fraction	0.066 for l,-k,h	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	0 of 31681 reflections	Xtriage
$F_o, F_c$ correlation	0.88	EDS
Total number of atoms	12120	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.35% 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

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, SD2

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	0.48	0/6128	0.70	0/8253
1	B	0.50	0/6142	0.72	0/8272
All	All	0.49	0/12270	0.71	0/16525

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 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	6020	0	6008	498	0
1	B	6034	0	6017	501	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	32	0	28	9	0
3	B	32	0	29	9	0
All	All	12120	0	12082	1000	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 41.



All (1000) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:91:HIS:CD2	1:B:93:SER:HB3	1.69	1.27
1:A:635:THR:HG22	1:A:637:PRO:HD2	1.21	1.16
1:B:366:ASN:HB2	1:B:367:PRO:HD3	1.16	1.12
1:A:308:ILE:HD12	1:A:345:ILE:HD11	1.32	1.10
1:B:91:HIS:HD2	1:B:93:SER:HB3	0.92	1.09
1:B:91:HIS:CD2	1:B:93:SER:CB	2.38	1.07
1:A:49:LYS:HG3	1:A:50:GLY:H	1.24	1.02
1:B:340:LYS:O	1:B:344:ASP:OD1	1.81	0.99
1:B:366:ASN:CB	1:B:367:PRO:HD3	1.92	0.98
1:A:440:ASN:HD21	1:A:500:LYS:HE2	1.29	0.98
1:B:175:ASN:ND2	1:B:200:ASP:HB3	1.81	0.96
1:B:366:ASN:HB2	1:B:367:PRO:CD	1.89	0.96
1:B:175:ASN:HD21	1:B:200:ASP:HB3	1.28	0.95
1:B:165:GLN:HG3	1:B:166:PRO:HA	1.48	0.95
1:A:304:LYS:HD2	1:A:304:LYS:H	1.31	0.95
1:A:477:TYR:H	1:A:593:SER:HB2	1.30	0.94
1:B:296:LEU:HD22	1:B:419:ILE:HD13	1.48	0.94
1:A:426:SER:HA	1:A:510:ARG:HA	1.50	0.93
1:B:273:LYS:HD2	1:B:431:LEU:HD22	1.53	0.91
1:A:31:THR:O	1:A:35:HIS:HB3	1.70	0.91
1:A:643:TYR:HB3	1:A:652:GLN:OE1	1.72	0.90
3:B:9003:SD2:OAT	3:B:9003:SD2:HAL	1.74	0.88
1:A:500:LYS:HZ2	1:A:500:LYS:HB3	1.36	0.88
1:A:301:GLU:HG3	1:A:385:PRO:HG3	1.56	0.88
1:A:373:LYS:HG2	1:A:377:LYS:HE3	1.54	0.87
1:A:655:SER:HB2	3:A:9002:SD2:OAH	1.75	0.86
1:A:173:VAL:O	1:A:177:ILE:HG12	1.75	0.86
1:B:221:PHE:HA	1:B:244:MET:HE2	1.57	0.86
1:A:40:MET:O	1:A:44:VAL:HB	1.76	0.85
1:B:686:HIS:ND1	3:B:9003:SD2:HAK	1.92	0.85
1:A:412:TYR:O	1:A:416:ILE:HG13	1.77	0.85
1:B:516:ASN:H	1:B:516:ASN:HD22	1.23	0.84
1:B:366:ASN:HD22	1:B:367:PRO:CD	1.90	0.84
1:B:516:ASN:N	1:B:516:ASN:HD22	1.75	0.84
1:A:308:ILE:HD12	1:A:345:ILE:CD1	2.06	0.84
1:A:469:ASN:N	1:A:469:ASN:HD22	1.74	0.84
1:B:140:ASN:HD22	1:B:140:ASN:C	1.79	0.83
1:A:442:ASN:HB2	1:A:496:ASN:HD22	1.44	0.82
1:A:59:ALA:HB1	1:A:83:ILE:HD13	1.62	0.82
1:B:516:ASN:ND2	1:B:516:ASN:H	1.75	0.82
1:B:91:HIS:CD2	1:B:93:SER:H	1.98	0.81
1:B:468:PHE:CZ	1:B:534:ILE:HG13	2.16	0.81

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:36:LEU:HD13	1:B:64:GLU:OE1	1.80	0.81
1:A:440:ASN:ND2	1:A:500:LYS:HE2	1.96	0.81
1:A:167:TYR:CZ	1:A:536:LYS:HB2	2.16	0.80
1:A:308:ILE:CD1	1:A:345:ILE:HD11	2.11	0.80
1:A:102:LYS:HA	1:A:114:LEU:HD11	1.61	0.80
1:A:490:GLU:OE2	1:A:544:ARG:NH2	2.12	0.80
1:A:608:ASN:C	1:A:609:ASN:HD22	1.85	0.79
1:B:113:LEU:O	1:B:116:GLU:HG2	1.83	0.79
1:B:81:ILE:HG23	1:B:129:LEU:HD22	1.65	0.79
1:B:570:TRP:CE3	1:B:574:LEU:HD21	2.17	0.78
1:B:557:THR:O	1:B:561:GLU:HG3	1.82	0.78
1:B:401:SER:CB	1:B:638:ASN:HD22	1.96	0.77
1:B:221:PHE:HD1	1:B:244:MET:HE1	1.50	0.77
1:B:186:GLN:HE21	1:B:195:LYS:HB2	1.50	0.77
1:B:75:LYS:O	1:B:78:GLY:N	2.16	0.76
1:B:611:GLN:HE21	1:B:774:ILE:CD1	1.99	0.76
1:B:304:LYS:H	1:B:304:LYS:HD3	1.47	0.76
1:B:224:TYR:HD2	1:B:225:ILE:HD13	1.51	0.76
1:A:167:TYR:CE1	1:A:536:LYS:HB2	2.21	0.76
1:B:324:ILE:O	1:B:326:SER:N	2.18	0.76
1:A:233:LEU:O	1:A:237:ALA:HB3	1.85	0.76
1:A:676:GLU:O	1:A:677:LEU:HD23	1.85	0.75
1:A:518:LYS:O	1:A:519:LEU:HD23	1.86	0.75
1:B:463:ILE:HD12	1:B:534:ILE:HG23	1.68	0.75
1:A:61:LYS:HA	1:A:61:LYS:HE2	1.69	0.75
1:A:764:GLN:O	1:A:768:ASP:HB2	1.87	0.75
1:A:73:MET:HG2	1:A:256:LEU:HD23	1.69	0.75
1:B:343:ILE:N	1:B:343:ILE:HD13	2.02	0.74
1:A:87:ASP:HB3	1:A:90:LYS:HE3	1.69	0.74
1:A:87:ASP:O	1:A:90:LYS:HG2	1.87	0.74
1:A:49:LYS:HG3	1:A:50:GLY:N	1.97	0.74
1:B:635:THR:HB	1:B:637:PRO:HD2	1.69	0.74
1:B:366:ASN:HD22	1:B:367:PRO:HD3	1.50	0.74
1:A:709:THR:HG21	1:A:734:ALA:HA	1.67	0.74
1:A:500:LYS:NZ	1:A:500:LYS:HB3	2.02	0.74
1:A:389:ASN:OD1	1:A:482:ASN:HB2	1.88	0.74
1:B:401:SER:HB2	1:B:638:ASN:HD22	1.51	0.73
1:A:658:LEU:HD23	3:A:9002:SD2:SAE	2.28	0.73
1:B:708:VAL:HG21	1:B:769:GLN:NE2	2.03	0.73
1:B:610:ILE:HD12	1:B:610:ILE:H	1.53	0.72
1:A:611:GLN:HE21	1:A:774:ILE:HD11	1.54	0.72
1:A:258:GLU:HG3	1:A:502:ARG:HH12	1.54	0.72

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:211:ASN:HA	1:B:214:GLN:NE2	2.04	0.72
1:A:613:ASP:HB3	1:A:774:ILE:HG23	1.72	0.71
1:B:145:LEU:HD23	1:B:226:GLU:HG3	1.72	0.71
1:A:677:LEU:HD11	3:A:9002:SD2:CAO	2.20	0.71
1:B:343:ILE:O	1:B:346:ARG:HB2	1.90	0.71
1:B:688:PHE:O	1:B:692:VAL:HG23	1.90	0.70
1:B:583:ILE:HG23	1:B:631:PHE:HE1	1.56	0.70
1:A:298:ILE:O	1:A:298:ILE:HD12	1.91	0.70
1:B:88:ILE:HB	1:B:130:VAL:HG11	1.73	0.70
1:B:123:GLU:HG3	1:B:157:ARG:NH1	2.06	0.70
1:A:202:SER:O	1:A:205:PHE:N	2.25	0.70
1:A:107:ILE:HG23	1:A:108:TYR:H	1.57	0.70
1:B:570:TRP:HE3	1:B:574:LEU:HD21	1.55	0.70
1:B:646:GLN:NE2	1:B:652:GLN:HB3	2.07	0.70
1:A:107:ILE:HG23	1:A:108:TYR:N	2.06	0.70
1:B:630:VAL:HB	1:B:667:LEU:HD23	1.74	0.70
1:A:95:GLU:O	1:A:95:GLU:HG3	1.91	0.70
1:B:366:ASN:CB	1:B:367:PRO:CD	2.58	0.69
1:A:567:ASN:C	1:A:569:GLU:H	1.96	0.69
1:A:113:LEU:O	1:A:117:HIS:HB2	1.91	0.69
1:B:27:GLU:O	1:B:27:GLU:HG3	1.92	0.69
1:A:693:ASP:OD2	1:A:707:LEU:HB2	1.93	0.69
1:A:500:LYS:HZ2	1:A:544:ARG:HH21	1.40	0.69
1:B:111:ASP:N	1:B:111:ASP:OD2	2.26	0.69
1:B:461:THR:HG22	1:B:540:LYS:HA	1.74	0.69
1:B:611:GLN:HE22	1:B:613:ASP:HB2	1.57	0.69
1:A:513:TYR:HA	1:A:519:LEU:CD2	2.23	0.69
1:B:70:VAL:HG13	1:B:155:LEU:HD13	1.74	0.68
1:B:278:TYR:HE2	1:B:511:ALA:O	1.76	0.68
1:B:675:VAL:HG23	3:B:9003:SD2:CAZ	2.24	0.68
1:A:513:TYR:HA	1:A:519:LEU:HD22	1.74	0.68
1:B:300:ILE:O	1:B:300:ILE:HG22	1.93	0.68
1:B:114:LEU:HA	1:B:117:HIS:HB3	1.75	0.68
1:B:233:LEU:HD23	1:B:237:ALA:HB3	1.75	0.68
1:A:395:THR:HB	1:A:398:LEU:O	1.93	0.68
1:A:442:ASN:ND2	1:A:496:ASN:HB2	2.09	0.68
1:B:107:ILE:HG21	1:B:145:LEU:HD12	1.75	0.68
1:B:246:LYS:O	1:B:250:GLN:HB2	1.94	0.68
1:B:610:ILE:CG2	1:B:614:LEU:HD23	2.24	0.68
1:A:284:SER:O	1:A:285:LEU:HD23	1.95	0.67
1:B:129:LEU:HD21	1:B:131:ILE:HG12	1.75	0.67
1:B:603:LEU:O	1:B:606:TRP:HB3	1.93	0.67

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:585:PHE:CE1	1:A:596:VAL:HG13	2.30	0.67
1:A:498:ARG:HD3	1:A:542:TYR:CD2	2.30	0.67
1:A:103:LYS:HG3	1:A:113:LEU:HD21	1.77	0.67
1:A:577:PRO:O	1:A:580:THR:HG22	1.95	0.67
1:A:191:THR:HG23	1:A:193:GLN:H	1.60	0.67
1:A:369:SER:OG	1:A:372:GLU:HB2	1.93	0.67
1:B:366:ASN:ND2	1:B:367:PRO:HD3	2.09	0.67
1:B:746:SER:O	1:B:752:ARG:HD2	1.94	0.67
1:B:140:ASN:HD22	1:B:141:THR:N	1.93	0.66
1:B:126:GLU:N	1:B:127:PRO:HD3	2.10	0.66
1:A:102:LYS:HA	1:A:114:LEU:CD1	2.25	0.66
1:B:516:ASN:ND2	1:B:516:ASN:N	2.40	0.66
1:A:277:HIS:CD2	1:A:429:SER:HB2	2.30	0.66
1:B:475:PHE:CD1	1:B:529:ILE:HG12	2.30	0.66
1:B:107:ILE:O	1:B:107:ILE:HD13	1.96	0.66
1:B:643:TYR:HA	1:B:646:GLN:HB2	1.77	0.66
1:B:386:TYR:OH	1:B:411:GLN:HG3	1.95	0.66
1:B:755:VAL:HG12	1:B:763:PHE:HB2	1.78	0.66
1:A:296:LEU:HD12	1:A:419:ILE:HD13	1.78	0.65
1:B:477:TYR:H	1:B:593:SER:HB2	1.62	0.65
1:B:395:THR:HG22	1:B:638:ASN:ND2	2.11	0.65
1:A:427:ILE:HG23	1:A:428:GLY:N	2.09	0.65
1:B:438:TYR:CE2	1:B:502:ARG:HD3	2.32	0.65
1:B:212:GLU:O	1:B:216:VAL:HG23	1.96	0.65
1:A:500:LYS:HZ2	1:A:544:ARG:NH2	1.94	0.65
1:B:655:SER:HB2	3:B:9003:SD2:OAH	1.96	0.65
1:B:627:GLY:O	1:B:628:ARG:HG2	1.96	0.65
1:A:314:GLU:HA	1:A:317:GLU:CD	2.17	0.65
1:A:334:GLU:O	1:A:337:PHE:HB3	1.96	0.65
1:B:377:LYS:O	1:B:380:LYS:HB3	1.97	0.64
1:B:366:ASN:HD22	1:B:367:PRO:HD2	1.62	0.64
1:B:74:TYR:HA	1:B:159:ILE:HD11	1.79	0.64
1:A:59:ALA:CB	1:A:83:ILE:HD13	2.27	0.64
1:B:49:LYS:HG3	1:B:85:ASP:HB3	1.80	0.64
1:B:670:GLY:H	1:B:671:PRO:HD3	1.63	0.64
1:B:36:LEU:O	1:B:40:MET:HG3	1.98	0.64
1:A:304:LYS:H	1:A:304:LYS:CD	2.08	0.64
1:A:485:ILE:HG12	1:A:520:ILE:HG12	1.78	0.64
1:A:394:ASP:O	1:A:634:ILE:HB	1.98	0.63
1:A:427:ILE:CG2	1:A:428:GLY:N	2.61	0.63
1:A:151:ILE:O	1:A:154:ILE:HB	1.99	0.63
1:A:252:ILE:HG23	1:A:253:ASN:N	2.13	0.63

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:611:GLN:HE21	1:B:774:ILE:HD13	1.61	0.63
1:A:329:PHE:N	1:A:329:PHE:HD2	1.97	0.63
1:A:498:ARG:HD3	1:A:542:TYR:CE2	2.34	0.63
1:B:387:ASP:HB3	1:B:390:GLN:HB3	1.81	0.63
1:B:686:HIS:CE1	3:B:9003:SD2:HAK	2.34	0.63
1:A:673:LYS:O	3:A:9002:SD2:HAY	1.99	0.63
1:A:36:LEU:O	1:A:40:MET:HG2	1.99	0.63
1:B:45:LYS:HD2	1:B:82:TYR:CE2	2.33	0.63
1:B:650:TYR:CE1	1:B:651:GLU:HG3	2.33	0.63
1:A:73:MET:HB3	1:A:159:ILE:HD13	1.81	0.62
1:B:257:GLU:O	1:B:260:LYS:HB2	1.99	0.62
1:A:550:VAL:HG12	1:A:551:PRO:HD2	1.81	0.62
1:A:119:VAL:HG13	1:A:131:ILE:HG12	1.81	0.62
1:B:552:LYS:O	1:B:554:LYS:N	2.33	0.62
1:B:456:ASP:HB3	1:B:462:LYS:O	1.98	0.62
1:B:723:SER:HA	1:B:730:ARG:HD3	1.81	0.62
1:B:493:ALA:HB1	1:B:497:GLU:HB2	1.81	0.62
1:B:494:LEU:O	1:B:496:ASN:N	2.31	0.62
1:B:188:LEU:HD11	1:B:223:TYR:CE2	2.34	0.62
1:A:477:TYR:N	1:A:593:SER:HB2	2.10	0.62
1:A:107:ILE:C	1:A:107:ILE:HD13	2.19	0.62
1:B:232:VAL:O	1:B:235:LEU:HD12	2.00	0.62
1:A:126:GLU:O	1:A:128:VAL:HG23	1.99	0.62
1:B:366:ASN:ND2	1:B:367:PRO:CD	2.61	0.62
1:B:43:ILE:HG13	1:B:44:VAL:HG23	1.81	0.62
1:B:570:TRP:HH2	1:B:607:LYS:HB2	1.65	0.62
1:A:635:THR:HG22	1:A:637:PRO:CD	2.14	0.62
1:B:574:LEU:N	1:B:574:LEU:HD23	2.15	0.62
1:A:329:PHE:HD2	1:A:329:PHE:H	1.46	0.61
1:A:256:LEU:HD11	1:A:260:LYS:HE3	1.81	0.61
1:A:707:LEU:HD12	1:A:709:THR:CG2	2.30	0.61
1:B:105:LYS:N	1:B:105:LYS:HD2	2.15	0.61
1:B:240:ALA:O	1:B:244:MET:HB2	2.00	0.61
1:A:221:PHE:O	1:A:225:ILE:HG12	2.00	0.61
1:B:632:THR:HG21	1:B:639:ILE:HD11	1.82	0.61
1:B:650:TYR:CD1	1:B:651:GLU:HG3	2.36	0.61
1:B:503:ILE:HD13	1:B:503:ILE:N	2.15	0.61
1:A:335:LYS:C	1:A:337:PHE:H	2.02	0.61
1:B:686:HIS:HD2	1:B:738:ALA:HB1	1.66	0.61
1:A:296:LEU:HD23	1:A:296:LEU:C	2.20	0.61
1:B:725:LEU:HD12	1:B:736:PHE:CE1	2.36	0.61
1:A:67:PRO:O	1:A:70:VAL:HG22	2.01	0.61

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:73:MET:HG2	1:B:256:LEU:HD12	1.83	0.61
1:B:733:GLU:CD	1:B:733:GLU:H	2.03	0.61
1:B:540:LYS:HD3	1:B:542:TYR:OH	2.00	0.61
1:A:30:LYS:HG3	1:A:30:LYS:O	1.99	0.61
1:B:242:ASN:O	1:B:243:TYR:C	2.39	0.60
1:A:102:LYS:O	1:A:114:LEU:HG	2.01	0.60
1:B:131:ILE:HD11	1:B:147:VAL:CG1	2.30	0.60
1:B:125:TYR:C	1:B:127:PRO:HD3	2.21	0.60
1:A:319:LEU:HA	1:A:322:ILE:HD12	1.81	0.60
1:B:292:LEU:HD11	1:B:418:ASN:HB3	1.82	0.60
1:B:708:VAL:HG21	1:B:769:GLN:HE22	1.67	0.60
1:B:673:LYS:HG3	1:B:673:LYS:O	2.01	0.60
1:A:635:THR:CG2	1:A:637:PRO:HD2	2.14	0.60
1:A:175:ASN:OD1	1:A:200:ASP:HB3	2.01	0.60
1:A:469:ASN:N	1:A:469:ASN:ND2	2.45	0.60
1:A:543:ILE:O	1:A:543:ILE:HG22	2.01	0.60
1:A:76:ALA:C	1:A:78:GLY:H	2.04	0.60
1:A:258:GLU:HG3	1:A:502:ARG:NH1	2.15	0.60
1:A:637:PRO:HG3	1:A:653:VAL:O	2.02	0.60
1:A:329:PHE:N	1:A:329:PHE:CD2	2.69	0.60
1:B:513:TYR:O	1:B:514:LEU:HD23	2.01	0.60
1:B:210:SER:O	1:B:212:GLU:N	2.35	0.60
1:A:191:THR:HG22	1:A:194:LEU:HG	1.83	0.60
1:B:447:THR:HG21	1:B:450:LEU:HD12	1.84	0.60
1:A:766:ILE:O	1:A:770:ILE:HG12	2.02	0.59
1:B:440:ASN:ND2	1:B:500:LYS:HD3	2.17	0.59
1:A:476:LYS:H	1:A:593:SER:CB	2.13	0.59
1:A:301:GLU:HG3	1:A:385:PRO:CG	2.30	0.59
1:B:424:HIS:HA	1:B:510:ARG:HD2	1.82	0.59
1:A:119:VAL:HG21	1:A:147:VAL:HG22	1.85	0.59
1:B:83:ILE:HG23	1:B:131:ILE:HG22	1.83	0.59
1:B:245:ASP:C	1:B:245:ASP:OD2	2.41	0.59
1:A:338:LEU:HD21	1:A:383:ILE:HG21	1.84	0.59
1:A:608:ASN:HD22	1:A:608:ASN:N	1.99	0.59
1:B:557:THR:O	1:B:560:GLN:HG2	2.02	0.59
1:B:202:SER:O	1:B:204:GLU:N	2.35	0.59
1:B:666:ILE:HG22	1:B:667:LEU:N	2.18	0.59
1:A:454:LEU:HA	1:A:467:ILE:HG21	1.85	0.59
1:A:330:LEU:HD21	1:A:380:LYS:HB2	1.83	0.59
1:A:739:GLU:O	1:A:743:LEU:HD12	2.03	0.59
1:B:413:LYS:O	1:B:417:GLN:HG3	2.03	0.59
1:B:636:LEU:HD12	1:B:636:LEU:N	2.16	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:464:ASN:OD1	1:A:467:ILE:HD13	2.03	0.58
1:B:619:THR:O	1:B:623:VAL:HG23	2.03	0.58
1:A:307:ILE:O	1:A:311:LEU:HD13	2.02	0.58
1:A:241:PHE:C	1:A:241:PHE:CD1	2.76	0.58
1:B:656:LYS:HD3	1:B:672:SER:HB3	1.83	0.58
1:A:601:LEU:HD23	1:A:601:LEU:H	1.68	0.58
1:B:221:PHE:O	1:B:225:ILE:HG12	2.04	0.58
1:B:401:SER:HB2	1:B:638:ASN:ND2	2.18	0.58
1:A:267:ARG:O	1:A:489:ASN:ND2	2.36	0.58
1:A:73:MET:CG	1:A:256:LEU:HD23	2.34	0.58
1:B:477:TYR:HB2	1:B:555:ILE:HD13	1.86	0.58
1:B:686:HIS:CD2	1:B:738:ALA:HB1	2.39	0.58
1:B:221:PHE:CD1	1:B:244:MET:HE1	2.35	0.58
1:B:202:SER:OG	1:B:204:GLU:HG3	2.03	0.58
1:A:677:LEU:HD21	3:A:9002:SD2:OAP	2.02	0.58
1:A:461:THR:O	1:A:541:GLU:HB2	2.04	0.58
1:B:155:LEU:O	1:B:159:ILE:HB	2.03	0.57
1:B:338:LEU:O	1:B:341:LEU:HB3	2.03	0.57
1:B:69:ASP:O	1:B:73:MET:HG3	2.04	0.57
1:B:496:ASN:HD22	1:B:497:GLU:N	2.02	0.57
1:A:368:LEU:O	1:A:369:SER:HB3	2.04	0.57
1:B:444:ASN:OD1	1:B:448:ALA:HA	2.04	0.57
3:A:9002:SD2:HAL	3:A:9002:SD2:OAT	2.04	0.57
1:B:224:TYR:CD2	1:B:225:ILE:HD13	2.37	0.57
1:A:338:LEU:HD22	1:A:379:LEU:HD13	1.85	0.57
1:B:571:ASN:HD21	1:B:580:THR:HG22	1.68	0.57
1:B:236:TYR:C	1:B:238:PRO:HD3	2.24	0.57
1:B:510:ARG:O	1:B:522:GLN:HB3	2.04	0.57
1:B:140:ASN:ND2	1:B:140:ASN:C	2.50	0.57
1:A:202:SER:O	1:A:205:PHE:HB3	2.04	0.57
1:B:84:VAL:O	1:B:133:SER:N	2.31	0.57
1:B:330:LEU:O	1:B:335:LYS:HE3	2.03	0.57
1:B:91:HIS:CD2	1:B:93:SER:N	2.71	0.57
1:B:555:ILE:O	1:B:558:LYS:HB2	2.05	0.57
1:B:468:PHE:CE1	1:B:534:ILE:CG1	2.87	0.57
1:A:762:THR:HG22	1:A:766:ILE:HD13	1.87	0.57
1:A:122:LYS:N	1:A:128:VAL:O	2.38	0.57
1:A:601:LEU:N	1:A:601:LEU:HD23	2.20	0.57
1:A:602:ILE:HG23	1:A:681:SER:HA	1.87	0.57
1:B:221:PHE:HD1	1:B:244:MET:CE	2.16	0.57
1:B:438:TYR:HE2	1:B:502:ARG:HD3	1.70	0.56
1:B:257:GLU:O	1:B:260:LYS:N	2.38	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:674:GLY:O	1:A:676:GLU:N	2.38	0.56
1:B:714:PHE:HE2	1:B:733:GLU:HB2	1.70	0.56
1:B:611:GLN:HE21	1:B:774:ILE:HD11	1.70	0.56
1:A:643:TYR:CB	1:A:652:GLN:OE1	2.48	0.56
1:B:94:LEU:O	1:B:96:ALA:N	2.38	0.56
1:B:105:LYS:HE2	1:B:111:ASP:HB3	1.87	0.56
1:B:404:ILE:HD12	1:B:408:VAL:HB	1.87	0.56
1:A:391:ARG:NH2	1:A:399:ILE:O	2.38	0.56
1:B:221:PHE:CE1	1:B:225:ILE:HD11	2.41	0.56
1:A:167:TYR:CE1	1:A:536:LYS:CB	2.88	0.56
1:B:403:SER:OG	1:B:638:ASN:ND2	2.39	0.56
1:B:583:ILE:HG23	1:B:631:PHE:CE1	2.39	0.56
1:B:438:TYR:O	1:B:486:VAL:HB	2.06	0.56
1:B:656:LYS:CD	1:B:672:SER:HB3	2.36	0.56
1:A:598:SER:O	1:A:602:ILE:HG13	2.05	0.56
1:B:131:ILE:HD11	1:B:147:VAL:HG13	1.86	0.56
1:A:737:PHE:HD2	1:A:737:PHE:C	2.09	0.56
1:B:91:HIS:CD2	1:B:93:SER:HB2	2.37	0.56
1:B:68:SER:O	1:B:71:LEU:N	2.39	0.56
1:A:737:PHE:CD2	1:A:737:PHE:C	2.80	0.55
1:A:506:SER:OG	1:A:508:ASP:HB2	2.06	0.55
1:A:658:LEU:HD22	1:A:659:TYR:N	2.21	0.55
1:A:253:ASN:O	1:A:255:SER:N	2.40	0.55
1:B:427:ILE:HG23	1:B:428:GLY:N	2.21	0.55
1:B:127:PRO:O	1:B:128:VAL:HG13	2.07	0.55
1:B:117:HIS:CG	1:B:118:TYR:H	2.24	0.55
1:A:123:GLU:HG3	1:A:123:GLU:O	2.05	0.55
1:A:639:ILE:HG21	1:A:667:LEU:CD2	2.36	0.55
1:A:681:SER:O	1:A:682:GLU:C	2.44	0.55
1:B:602:ILE:HD13	1:B:668:LEU:HD21	1.87	0.55
1:B:280:HIS:C	1:B:282:SER:H	2.10	0.55
1:B:766:ILE:C	1:B:768:ASP:H	2.10	0.55
1:A:107:ILE:CG2	1:A:108:TYR:H	2.18	0.55
1:B:713:LYS:HD2	1:B:765:PHE:HE1	1.72	0.55
1:A:525:ILE:HG22	1:A:526:GLY:N	2.21	0.55
1:B:35:HIS:O	1:B:39:ILE:HG12	2.06	0.55
1:B:319:LEU:HD23	1:B:345:ILE:HD11	1.89	0.55
1:A:642:GLN:OE1	1:A:653:VAL:HG22	2.07	0.55
1:A:304:LYS:HD2	1:A:304:LYS:N	2.12	0.55
1:A:477:TYR:CE1	1:A:593:SER:HA	2.40	0.55
1:B:431:LEU:O	1:B:432:TYR:HB3	2.08	0.54
1:B:714:PHE:HA	1:B:717:ILE:HG12	1.89	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:769:GLN:O	1:A:772:PHE:HB3	2.07	0.54
1:B:32:GLN:O	1:B:34:GLU:N	2.39	0.54
1:A:206:LEU:O	1:A:210:SER:HB3	2.07	0.54
1:B:303:LYS:HD2	1:B:305:ASP:OD1	2.06	0.54
1:A:762:THR:CG2	1:A:766:ILE:HD13	2.37	0.54
1:B:210:SER:O	1:B:211:ASN:C	2.44	0.54
1:A:122:LYS:HB3	1:A:128:VAL:HB	1.89	0.54
1:B:369:SER:OG	1:B:372:GLU:HG3	2.07	0.54
1:A:49:LYS:CG	1:A:50:GLY:N	2.69	0.54
1:A:250:GLN:HG3	1:A:251:GLU:HG2	1.90	0.54
1:A:387:ASP:HB3	1:A:390:GLN:HB3	1.90	0.54
1:B:83:ILE:HD12	1:B:131:ILE:HG21	1.88	0.54
1:A:247:PHE:CZ	1:A:252:ILE:HD12	2.42	0.54
1:B:94:LEU:HD11	1:B:130:VAL:HG21	1.90	0.54
1:B:729:GLY:O	1:B:736:PHE:HB2	2.07	0.54
1:B:275:LYS:HG3	1:B:513:TYR:CE2	2.42	0.54
1:A:749:HIS:O	1:A:752:ARG:N	2.41	0.54
1:B:635:THR:CB	1:B:637:PRO:HD2	2.37	0.54
1:A:563:GLN:HE21	1:A:584:THR:HA	1.72	0.54
1:A:156:SER:HA	1:A:160:LEU:HD12	1.89	0.54
1:A:674:GLY:HA2	3:A:9002:SD2:OAT	2.07	0.54
1:A:146:ASN:O	1:A:149:TYR:HB3	2.08	0.54
1:A:72:GLU:O	1:A:75:LYS:HB3	2.07	0.54
1:A:51:GLU:OE1	1:A:51:GLU:HA	2.08	0.54
1:A:443:ILE:CD1	1:A:454:LEU:HD22	2.36	0.54
1:A:440:ASN:ND2	1:A:493:ALA:HB2	2.23	0.54
1:B:221:PHE:CE2	1:B:225:ILE:HG13	2.42	0.54
1:A:563:GLN:O	1:A:566:ILE:HG22	2.08	0.54
1:B:280:HIS:C	1:B:282:SER:N	2.60	0.54
1:A:614:LEU:O	1:A:618:VAL:HG23	2.08	0.53
1:A:150:GLU:OE2	1:A:153:LYS:HE2	2.07	0.53
1:A:612:SER:O	1:A:616:LYS:HG3	2.08	0.53
1:B:410:LYS:O	1:B:414:ARG:HB2	2.09	0.53
1:B:77:ILE:HG22	1:B:127:PRO:HG2	1.90	0.53
1:A:472:LYS:HE3	1:A:532:VAL:O	2.07	0.53
1:B:467:ILE:O	1:B:468:PHE:C	2.45	0.53
1:A:608:ASN:N	1:A:608:ASN:ND2	2.56	0.53
1:A:585:PHE:CZ	1:A:596:VAL:HG13	2.44	0.53
1:A:314:GLU:HA	1:A:317:GLU:CG	2.38	0.53
1:A:670:GLY:H	1:A:671:PRO:CD	2.20	0.53
1:A:636:LEU:C	1:A:638:ASN:H	2.11	0.53
1:A:265:LEU:O	1:A:269:GLU:HB2	2.08	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:468:PHE:CE1	1:B:534:ILE:HG13	2.44	0.53
1:A:314:GLU:HA	1:A:317:GLU:HG2	1.89	0.53
1:B:478:SER:O	1:B:527:LEU:HB2	2.08	0.53
1:B:636:LEU:O	1:B:637:PRO:C	2.46	0.53
1:B:468:PHE:CE1	1:B:534:ILE:HG12	2.44	0.53
1:A:167:TYR:HD2	1:A:168:GLN:H	1.57	0.53
1:A:204:GLU:O	1:A:207:GLU:HB3	2.09	0.53
1:B:737:PHE:CE1	1:B:766:ILE:HG13	2.43	0.53
1:A:677:LEU:HD11	3:A:9002:SD2:CAN	2.39	0.53
1:B:243:TYR:CD1	1:B:244:MET:N	2.77	0.53
1:B:610:ILE:N	1:B:610:ILE:HD12	2.22	0.53
1:A:190:PHE:CD1	1:A:194:LEU:HB3	2.44	0.53
1:A:210:SER:O	1:A:214:GLN:HG3	2.08	0.53
1:B:40:MET:HA	1:B:44:VAL:HG23	1.90	0.53
1:A:223:TYR:HB3	1:A:233:LEU:HD12	1.91	0.53
1:A:567:ASN:C	1:A:569:GLU:N	2.62	0.53
1:A:293:LEU:O	1:A:296:LEU:HB3	2.09	0.53
1:B:720:GLU:OE2	1:B:761:LYS:HE2	2.08	0.53
1:B:675:VAL:HG23	3:B:9003:SD2:NBF	2.23	0.53
1:B:640:ALA:HA	1:B:643:TYR:CZ	2.44	0.53
1:A:443:ILE:HD11	1:A:471:PHE:CD1	2.44	0.53
1:B:91:HIS:NE2	1:B:93:SER:HB2	2.24	0.53
1:B:243:TYR:HD1	1:B:244:MET:N	2.07	0.53
1:A:146:ASN:O	1:A:147:VAL:C	2.46	0.53
1:A:237:ALA:HB1	1:A:240:ALA:HB3	1.91	0.53
1:A:693:ASP:OD1	1:A:709:THR:HG22	2.09	0.53
1:B:77:ILE:CG2	1:B:127:PRO:HG2	2.39	0.53
1:B:448:ALA:HB3	1:B:672:SER:O	2.09	0.53
1:A:233:LEU:HD23	1:A:237:ALA:CB	2.40	0.52
1:A:253:ASN:C	1:A:255:SER:H	2.12	0.52
1:B:636:LEU:N	1:B:636:LEU:CD1	2.72	0.52
1:A:681:SER:O	1:A:684:PHE:N	2.42	0.52
1:B:441:MET:SD	1:B:446:LEU:HD13	2.48	0.52
1:A:82:TYR:HB2	1:A:130:VAL:HG22	1.90	0.52
1:B:463:ILE:HG13	1:B:541:GLU:HB3	1.92	0.52
1:A:460:ASN:O	1:A:498:ARG:NH2	2.40	0.52
1:A:429:SER:HB3	1:A:432:TYR:CZ	2.44	0.52
1:A:437:LEU:HD12	1:A:505:LEU:HD21	1.92	0.52
1:A:67:PRO:HG2	1:A:248:ASN:OD1	2.09	0.52
1:B:614:LEU:HD13	1:B:770:ILE:HG23	1.90	0.52
1:A:278:TYR:C	1:A:280:HIS:H	2.13	0.52
1:A:286:SER:C	1:A:288:GLU:H	2.11	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:461:THR:O	1:B:541:GLU:HB2	2.10	0.52
1:A:155:LEU:O	1:A:160:LEU:HG	2.09	0.52
1:B:673:LYS:O	1:B:674:GLY:C	2.46	0.52
1:A:103:LYS:HG3	1:A:113:LEU:CD2	2.40	0.52
1:A:584:THR:HG21	1:A:630:VAL:HG22	1.92	0.52
1:B:46:ILE:HG22	1:B:48:VAL:HG13	1.91	0.52
1:B:570:TRP:CZ3	1:B:574:LEU:HD21	2.44	0.52
1:A:314:GLU:O	1:A:318:LEU:HG	2.09	0.52
1:A:701:ASP:O	1:A:703:ASN:N	2.42	0.52
1:A:505:LEU:HD22	1:A:505:LEU:N	2.25	0.52
1:A:253:ASN:C	1:A:255:SER:N	2.62	0.52
1:A:212:GLU:O	1:A:215:GLU:HB3	2.10	0.52
1:A:335:LYS:C	1:A:337:PHE:N	2.63	0.52
1:A:335:LYS:O	1:A:337:PHE:N	2.43	0.52
1:A:196:GLU:O	1:A:197:HIS:C	2.48	0.52
1:B:324:ILE:HG22	1:B:325:ASP:N	2.24	0.52
1:B:640:ALA:HB2	1:B:643:TYR:CZ	2.45	0.52
1:B:632:THR:OG1	1:B:633:ASP:N	2.43	0.52
1:B:319:LEU:CD2	1:B:345:ILE:HD11	2.39	0.52
1:B:732:ASN:OD1	1:B:734:ALA:N	2.43	0.52
1:B:416:ILE:O	1:B:418:ASN:N	2.42	0.52
1:B:178:LYS:HD2	1:B:201:PHE:CE1	2.44	0.52
1:B:276:GLN:NE2	1:B:431:LEU:HD11	2.25	0.51
1:A:468:PHE:HD1	1:A:543:ILE:HD11	1.75	0.51
1:A:456:ASP:OD1	1:A:464:ASN:HB2	2.10	0.51
1:A:55:LYS:HD2	1:A:133:SER:OG	2.10	0.51
1:B:174:LEU:HD22	1:B:216:VAL:HG11	1.92	0.51
1:B:640:ALA:HA	1:B:643:TYR:CE1	2.45	0.51
1:B:493:ALA:O	1:B:494:LEU:HD23	2.10	0.51
1:B:178:LYS:O	1:B:178:LYS:HG3	2.09	0.51
1:A:264:MET:O	1:A:267:ARG:N	2.44	0.51
1:A:437:LEU:HD12	1:A:505:LEU:CD2	2.40	0.51
1:A:73:MET:CB	1:A:159:ILE:HD13	2.41	0.51
1:B:278:TYR:CE2	1:B:511:ALA:O	2.61	0.51
1:B:601:LEU:O	1:B:604:ASN:N	2.39	0.51
1:B:121:ALA:HB2	1:B:150:GLU:HG3	1.92	0.51
1:B:66:VAL:HG21	1:B:151:ILE:HD13	1.91	0.51
1:A:509:THR:OG1	1:A:549:VAL:HG11	2.11	0.51
1:B:552:LYS:C	1:B:554:LYS:H	2.14	0.51
1:A:32:GLN:O	1:A:36:LEU:HB2	2.10	0.51
1:B:592:ALA:O	1:B:593:SER:C	2.49	0.51
1:A:443:ILE:HD13	1:A:454:LEU:HD22	1.91	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:762:THR:HG22	1:B:766:ILE:HD13	1.91	0.51
1:B:293:LEU:O	1:B:297:GLN:HG3	2.11	0.51
1:A:374:GLU:O	1:A:377:LYS:HB2	2.11	0.51
1:A:442:ASN:HB2	1:A:496:ASN:ND2	2.22	0.51
1:B:426:SER:HA	1:B:509:THR:O	2.10	0.51
1:A:634:ILE:O	1:A:635:THR:C	2.48	0.51
1:A:500:LYS:NZ	1:A:544:ARG:NH2	2.58	0.51
1:B:463:ILE:HD11	1:B:541:GLU:C	2.32	0.51
1:A:584:THR:HG22	1:A:629:PHE:O	2.11	0.51
1:B:729:GLY:HA2	1:B:739:GLU:HG3	1.93	0.51
1:B:420:ASP:OD2	1:B:523:ARG:NH1	2.43	0.51
1:B:62:LEU:HD13	1:B:63:LEU:HD23	1.93	0.51
1:B:304:LYS:O	1:B:308:ILE:HG13	2.11	0.51
1:A:156:SER:HB3	1:A:217:PHE:HD2	1.75	0.51
1:B:520:ILE:O	1:B:520:ILE:HG23	2.11	0.51
1:A:505:LEU:CD2	1:A:505:LEU:N	2.74	0.51
1:A:83:ILE:HA	1:A:131:ILE:O	2.11	0.51
1:A:296:LEU:HD23	1:A:296:LEU:O	2.11	0.51
1:B:304:LYS:N	1:B:304:LYS:HD3	2.23	0.50
1:A:516:ASN:ND2	1:A:518:LYS:HD2	2.26	0.50
1:B:721:GLU:OE1	1:B:761:LYS:HB2	2.10	0.50
1:A:294:LYS:O	1:A:297:GLN:N	2.44	0.50
1:B:311:LEU:HD22	1:B:315:GLU:HB3	1.94	0.50
1:B:226:GLU:CD	1:B:229:HIS:HD1	2.14	0.50
1:B:660:VAL:O	1:B:664:ARG:N	2.44	0.50
1:B:269:GLU:O	1:B:273:LYS:HG2	2.12	0.50
1:A:522:GLN:HG3	1:A:523:ARG:O	2.10	0.50
1:B:300:ILE:HB	1:B:386:TYR:HB3	1.92	0.50
1:A:755:VAL:O	1:A:759:ALA:HB3	2.11	0.50
1:B:192:ASN:C	1:B:194:LEU:H	2.14	0.50
1:A:437:LEU:HD12	1:A:505:LEU:HG	1.93	0.50
1:B:379:LEU:O	1:B:380:LYS:C	2.49	0.50
1:A:718:PHE:CD1	1:A:733:GLU:HB3	2.47	0.50
1:B:606:TRP:CE2	1:B:615:ILE:HD12	2.46	0.50
1:A:404:ILE:O	1:A:405:ASN:O	2.30	0.50
1:A:737:PHE:O	1:A:737:PHE:HD2	1.95	0.50
1:B:87:ASP:O	1:B:90:LYS:HG2	2.12	0.50
1:B:319:LEU:HD21	1:B:341:LEU:HD22	1.94	0.50
1:B:390:GLN:HA	1:B:390:GLN:NE2	2.27	0.50
1:B:713:LYS:O	1:B:717:ILE:HD11	2.12	0.50
1:A:279:GLN:O	1:A:279:GLN:HG3	2.11	0.50
1:A:87:ASP:CG	1:A:89:THR:HG1	2.14	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:729:GLY:CA	1:B:739:GLU:HG3	2.42	0.49
1:A:637:PRO:HB3	1:A:652:GLN:NE2	2.27	0.49
1:A:59:ALA:HB1	1:A:83:ILE:CD1	2.38	0.49
1:B:303:LYS:HD3	1:B:304:LYS:HZ1	1.76	0.49
1:B:610:ILE:HB	1:B:615:ILE:HD11	1.93	0.49
1:A:440:ASN:HD21	1:A:500:LYS:CE	2.12	0.49
1:B:125:TYR:HE2	1:B:162:LYS:HE3	1.77	0.49
1:A:30:LYS:CG	1:A:30:LYS:O	2.61	0.49
1:A:505:LEU:HD12	1:A:509:THR:HG21	1.93	0.49
1:A:658:LEU:CD2	1:A:659:TYR:N	2.76	0.49
1:A:185:GLY:HA3	1:A:236:TYR:O	2.13	0.49
3:B:9003:SD2:OAT	3:B:9003:SD2:CAL	2.54	0.49
1:A:78:GLY:O	1:A:127:PRO:HD2	2.12	0.49
1:A:298:ILE:HD12	1:A:299:PRO:O	2.12	0.49
1:B:123:GLU:HG3	1:B:157:ARG:HH11	1.76	0.49
1:B:714:PHE:CE2	1:B:733:GLU:HB2	2.47	0.49
1:A:86:GLY:O	1:A:132:GLN:NE2	2.45	0.49
1:B:83:ILE:HD12	1:B:131:ILE:CG2	2.42	0.49
1:A:202:SER:HB2	1:A:204:GLU:OE2	2.13	0.49
1:B:681:SER:O	1:B:685:ILE:HG13	2.12	0.49
1:B:40:MET:O	1:B:44:VAL:HB	2.13	0.49
1:A:252:ILE:CG2	1:A:253:ASN:N	2.76	0.49
1:A:733:GLU:HG2	1:A:734:ALA:H	1.78	0.49
1:A:152:GLY:O	1:A:153:LYS:C	2.50	0.49
1:A:153:LYS:O	1:A:157:ARG:HB3	2.13	0.49
1:A:528:GLU:OE1	1:A:550:VAL:HG21	2.13	0.49
1:B:759:ALA:N	1:B:760:PRO:HD3	2.27	0.49
1:A:177:ILE:HD12	1:A:238:PRO:HD2	1.95	0.49
1:A:314:GLU:C	1:A:317:GLU:HG2	2.33	0.49
1:A:221:PHE:N	1:A:244:MET:HE2	2.28	0.49
1:A:169:LYS:HE3	1:A:533:GLN:CB	2.43	0.49
1:A:572:LYS:C	1:A:574:LEU:H	2.16	0.49
1:B:91:HIS:CG	1:B:93:SER:H	2.31	0.49
1:A:508:ASP:O	1:A:509:THR:C	2.51	0.49
1:A:278:TYR:O	1:A:280:HIS:N	2.46	0.49
1:A:163:ILE:O	1:A:164:ASN:HB2	2.13	0.49
1:A:65:LYS:HE2	1:A:227:PRO:HG3	1.95	0.49
1:B:730:ARG:O	1:B:731:THR:O	2.31	0.48
1:A:443:ILE:HG13	1:A:499:LEU:HD21	1.95	0.48
1:B:194:LEU:HG	1:B:194:LEU:O	2.12	0.48
1:B:487:ASP:OD1	1:B:518:LYS:HE2	2.13	0.48
1:A:477:TYR:H	1:A:593:SER:CB	2.12	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:40:MET:HA	1:B:43:ILE:HG12	1.95	0.48
1:A:696:ALA:O	1:A:699:LEU:N	2.46	0.48
1:A:442:ASN:CG	1:A:496:ASN:HB2	2.34	0.48
1:B:226:GLU:OE1	1:B:229:HIS:ND1	2.36	0.48
1:A:209:ASN:O	1:A:212:GLU:HB2	2.14	0.48
1:B:718:PHE:CG	1:B:733:GLU:HB3	2.49	0.48
1:A:124:GLY:C	1:A:126:GLU:H	2.15	0.48
1:A:713:LYS:O	1:A:717:ILE:HG13	2.13	0.48
1:A:589:ASN:HB2	1:A:633:ASP:OD2	2.13	0.48
1:B:596:VAL:O	1:B:599:ALA:HB3	2.13	0.48
1:B:366:ASN:ND2	1:B:367:PRO:HD2	2.26	0.48
1:B:40:MET:C	1:B:42:HIS:H	2.17	0.48
1:B:721:GLU:HA	1:B:724:ASN:OD1	2.12	0.48
1:A:465:ARG:O	1:A:469:ASN:ND2	2.46	0.48
1:A:107:ILE:CG2	1:A:108:TYR:N	2.72	0.48
1:B:102:LYS:O	1:B:113:LEU:HD22	2.13	0.48
1:B:312:SER:O	1:B:313:GLN:C	2.51	0.48
1:B:682:GLU:HA	1:B:685:ILE:HD12	1.95	0.48
1:B:675:VAL:HG12	1:B:676:GLU:HG2	1.95	0.48
1:A:442:ASN:CB	1:A:496:ASN:HD22	2.21	0.48
1:A:76:ALA:C	1:A:78:GLY:N	2.66	0.48
1:B:229:HIS:O	1:B:232:VAL:HG23	2.13	0.48
1:B:447:THR:HG23	1:B:447:THR:O	2.13	0.48
1:A:489:ASN:O	1:A:490:GLU:C	2.51	0.48
1:A:267:ARG:HE	1:A:491:ARG:HH21	1.60	0.48
1:B:498:ARG:NH1	1:B:540:LYS:HE3	2.28	0.48
1:B:314:GLU:HG3	1:B:314:GLU:O	2.13	0.48
1:B:635:THR:HG22	1:B:654:HIS:CE1	2.48	0.48
1:A:314:GLU:O	1:A:317:GLU:HG2	2.14	0.48
1:B:322:ILE:HG13	1:B:372:GLU:OE2	2.14	0.48
1:B:369:SER:C	1:B:371:LYS:H	2.17	0.48
1:A:636:LEU:O	1:A:638:ASN:N	2.47	0.48
1:A:187:ASP:HA	1:A:195:LYS:HE2	1.95	0.48
1:A:733:GLU:CD	1:A:733:GLU:H	2.17	0.48
1:B:476:LYS:O	1:B:529:ILE:HB	2.14	0.48
1:B:715:ILE:O	1:B:718:PHE:HB3	2.13	0.48
1:B:65:LYS:HB3	1:B:225:ILE:HG22	1.95	0.48
1:A:741:PHE:O	1:A:744:MET:N	2.47	0.48
1:B:529:ILE:N	1:B:529:ILE:HD12	2.29	0.48
1:B:669:HIS:CE1	1:B:671:PRO:HD2	2.49	0.48
1:B:501:TRP:HB3	1:B:503:ILE:CD1	2.44	0.48
1:A:553:SER:O	1:A:554:LYS:C	2.51	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:72:GLU:HA	1:B:72:GLU:OE2	2.13	0.48
1:B:243:TYR:C	1:B:243:TYR:CD1	2.86	0.47
1:A:107:ILE:HG22	1:A:146:ASN:OD1	2.14	0.47
1:B:749:HIS:O	1:B:752:ARG:N	2.44	0.47
1:A:199:THR:OG1	1:A:200:ASP:N	2.47	0.47
1:A:688:PHE:O	1:A:691:ALA:HB3	2.13	0.47
1:B:636:LEU:H	1:B:636:LEU:CD1	2.27	0.47
1:B:43:ILE:HG13	1:B:44:VAL:N	2.28	0.47
1:A:256:LEU:HD13	1:A:256:LEU:C	2.34	0.47
1:A:87:ASP:OD2	1:A:89:THR:N	2.47	0.47
1:A:770:ILE:O	1:A:774:ILE:HG13	2.14	0.47
1:A:51:GLU:O	1:A:53:ALA:N	2.47	0.47
1:A:294:LYS:O	1:A:295:LYS:C	2.52	0.47
1:B:679:ASN:O	1:B:682:GLU:N	2.46	0.47
1:A:732:ASN:OD1	1:A:732:ASN:C	2.52	0.47
1:B:498:ARG:HH12	1:B:540:LYS:HG2	1.79	0.47
1:B:275:LYS:HG3	1:B:513:TYR:HE2	1.79	0.47
1:B:389:ASN:OD1	1:B:482:ASN:HB2	2.14	0.47
1:A:657:GLY:HA2	1:A:667:LEU:O	2.14	0.47
1:A:584:THR:CG2	1:A:630:VAL:HG22	2.44	0.47
1:B:749:HIS:O	1:B:750:ALA:C	2.52	0.47
1:B:202:SER:C	1:B:204:GLU:N	2.66	0.47
1:A:286:SER:C	1:A:288:GLU:N	2.68	0.47
1:B:606:TRP:CH2	1:B:615:ILE:HG23	2.49	0.47
1:B:587:VAL:O	1:B:588:HIS:CG	2.67	0.47
1:B:530:LYS:O	1:B:531:ASP:HB2	2.14	0.47
1:A:118:TYR:OH	1:A:143:LYS:HA	2.14	0.47
1:B:91:HIS:NE2	1:B:93:SER:CB	2.76	0.47
1:A:391:ARG:NH1	1:A:404:ILE:CD1	2.78	0.47
1:B:674:GLY:O	1:B:677:LEU:HB2	2.14	0.47
1:B:654:HIS:O	3:B:9003:SD2:HBE3	2.15	0.47
1:A:718:PHE:O	1:A:722:GLY:HA3	2.15	0.47
1:A:258:GLU:CG	1:A:502:ARG:HH12	2.25	0.47
1:B:107:ILE:HG12	1:B:149:TYR:CD1	2.49	0.47
1:B:338:LEU:HD21	1:B:379:LEU:HB3	1.96	0.47
1:A:327:SER:HB2	1:A:329:PHE:CE2	2.49	0.47
1:A:401:SER:O	1:A:403:SER:N	2.37	0.47
1:A:104:ILE:HG13	1:A:120:TYR:CE1	2.50	0.47
1:A:656:LYS:O	1:A:668:LEU:HD12	2.14	0.47
1:B:123:GLU:CG	1:B:124:GLY:H	2.28	0.47
1:A:191:THR:HG23	1:A:194:LEU:H	1.80	0.47
1:A:550:VAL:HG12	1:A:551:PRO:CD	2.43	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:476:LYS:N	1:A:593:SER:OG	2.34	0.47
1:B:129:LEU:HD23	1:B:129:LEU:C	2.35	0.47
1:A:693:ASP:OD2	1:A:693:ASP:O	2.33	0.47
1:A:693:ASP:CG	1:A:708:VAL:HG12	2.36	0.47
1:A:718:PHE:HA	1:A:722:GLY:HA3	1.97	0.47
1:B:511:ALA:CB	1:B:521:LEU:HA	2.45	0.47
1:B:84:VAL:HG22	1:B:85:ASP:N	2.30	0.47
1:A:725:LEU:HD12	1:A:736:PHE:CE1	2.50	0.47
1:B:564:LEU:O	1:B:568:GLN:HB2	2.15	0.47
1:A:338:LEU:CD2	1:A:383:ILE:HG21	2.45	0.47
1:A:479:ILE:HG22	1:A:480:SER:N	2.30	0.47
1:B:660:VAL:HG13	1:B:662:GLU:OE2	2.14	0.47
1:A:118:TYR:N	1:A:118:TYR:CD1	2.83	0.47
1:A:495:ASP:C	1:A:497:GLU:N	2.68	0.47
1:A:87:ASP:OD2	1:A:87:ASP:C	2.52	0.46
1:B:614:LEU:O	1:B:618:VAL:HG23	2.14	0.46
1:A:191:THR:HG21	1:A:212:GLU:OE2	2.15	0.46
1:B:280:HIS:O	1:B:282:SER:N	2.48	0.46
1:A:81:ILE:HG12	1:A:129:LEU:HD23	1.98	0.46
1:A:639:ILE:HG23	1:A:641:GLU:OE1	2.15	0.46
1:B:276:GLN:O	1:B:277:HIS:C	2.54	0.46
1:A:696:ALA:O	1:A:697:GLY:C	2.53	0.46
1:B:189:LEU:HD22	1:B:220:ALA:HB2	1.97	0.46
1:A:639:ILE:HG21	1:A:667:LEU:HD21	1.96	0.46
1:A:498:ARG:CD	1:A:542:TYR:CD2	2.97	0.46
1:B:32:GLN:C	1:B:34:GLU:H	2.18	0.46
1:B:526:GLY:HA3	1:B:550:VAL:O	2.16	0.46
1:A:683:GLY:O	1:A:687:GLU:HG2	2.15	0.46
1:B:472:LYS:HG3	1:B:473:LYS:N	2.29	0.46
1:A:437:LEU:HD12	1:A:505:LEU:CG	2.46	0.46
1:B:455:VAL:HG22	1:B:498:ARG:HE	1.79	0.46
1:A:718:PHE:CE1	1:A:733:GLU:N	2.84	0.46
1:A:191:THR:C	1:A:193:GLN:H	2.19	0.46
1:A:636:LEU:C	1:A:638:ASN:N	2.67	0.46
1:A:586:ASN:HB3	1:A:632:THR:OG1	2.14	0.46
1:B:261:ASP:OD1	1:B:490:GLU:HB3	2.15	0.46
1:B:366:ASN:CG	1:B:367:PRO:HD3	2.34	0.46
1:A:264:MET:O	1:A:265:LEU:C	2.54	0.46
1:B:640:ALA:C	1:B:642:GLN:N	2.69	0.46
1:A:272:GLU:HG3	1:B:125:TYR:CE1	2.51	0.46
1:B:77:ILE:HG22	1:B:77:ILE:O	2.16	0.46
1:B:331:SER:HB3	1:B:334:GLU:HB2	1.97	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:488:ILE:HG22	1:B:489:ASN:CG	2.36	0.46
1:A:446:LEU:HG	1:A:591:TYR:HB2	1.98	0.46
1:A:674:GLY:O	1:A:675:VAL:C	2.53	0.46
1:B:769:GLN:O	1:B:772:PHE:HB3	2.16	0.46
1:A:498:ARG:HG2	1:A:498:ARG:HH11	1.81	0.46
1:A:316:LYS:O	1:A:319:LEU:HB3	2.15	0.46
1:B:331:SER:HB3	1:B:334:GLU:CD	2.36	0.46
1:A:439:GLU:OE1	1:A:590:ARG:NH2	2.49	0.46
1:A:410:LYS:NZ	1:A:414:ARG:HH21	2.14	0.46
1:B:171:LEU:O	1:B:175:ASN:HB2	2.15	0.46
1:B:468:PHE:CG	1:B:534:ILE:HD11	2.51	0.46
1:A:54:VAL:O	1:A:57:GLU:HB3	2.16	0.46
1:A:57:GLU:O	1:A:61:LYS:N	2.36	0.46
1:B:238:PRO:O	1:B:241:PHE:HB3	2.15	0.46
1:B:247:PHE:CE2	1:B:252:ILE:HD13	2.51	0.46
1:A:311:LEU:O	1:A:312:SER:HB3	2.15	0.46
1:B:294:LYS:HG3	1:B:295:LYS:N	2.31	0.46
1:B:735:GLU:O	1:B:736:PHE:C	2.52	0.46
1:A:529:ILE:N	1:A:529:ILE:HD13	2.31	0.46
1:A:62:LEU:HD21	1:A:147:VAL:HG11	1.97	0.46
1:A:592:ALA:HA	1:A:595:ILE:HG12	1.97	0.46
1:B:636:LEU:N	1:B:637:PRO:CD	2.79	0.46
1:A:167:TYR:OH	1:A:536:LYS:HB2	2.15	0.46
1:B:376:LEU:HD23	1:B:379:LEU:HD12	1.98	0.46
1:B:557:THR:HA	1:B:560:GLN:HG2	1.97	0.45
1:A:76:ALA:O	1:A:78:GLY:N	2.49	0.45
1:A:205:PHE:CE2	1:A:209:ASN:ND2	2.82	0.45
1:A:46:ILE:O	1:A:47:GLU:HG3	2.16	0.45
1:A:753:LEU:O	1:A:756:GLN:N	2.48	0.45
1:B:643:TYR:HB3	1:B:646:GLN:OE1	2.16	0.45
1:B:670:GLY:H	1:B:671:PRO:CD	2.28	0.45
1:A:481:SER:HA	1:A:524:ASN:HD22	1.80	0.45
1:A:615:ILE:HG22	1:A:616:LYS:N	2.31	0.45
1:A:427:ILE:CG2	1:A:428:GLY:H	2.30	0.45
1:A:314:GLU:CA	1:A:317:GLU:HG2	2.46	0.45
1:A:126:GLU:HG3	1:A:126:GLU:O	2.16	0.45
1:A:615:ILE:O	1:A:619:THR:HG23	2.15	0.45
1:A:695:TYR:O	1:A:698:TYR:HB3	2.17	0.45
1:B:239:GLU:O	1:B:242:ASN:N	2.49	0.45
1:A:299:PRO:O	1:A:300:ILE:HG23	2.16	0.45
1:A:191:THR:OG1	1:A:192:ASN:N	2.50	0.45
1:B:49:LYS:HB2	1:B:50:GLY:H	1.58	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:369:SER:O	1:B:371:LYS:N	2.49	0.45
1:A:264:MET:O	1:A:266:SER:N	2.49	0.45
1:B:467:ILE:N	1:B:467:ILE:HD12	2.32	0.45
1:A:584:THR:HG23	1:A:630:VAL:HA	1.98	0.45
1:B:731:THR:HG22	1:B:732:ASN:H	1.81	0.45
1:A:122:LYS:CB	1:A:128:VAL:HB	2.47	0.45
1:A:220:ALA:C	1:A:244:MET:HE2	2.37	0.45
1:A:682:GLU:O	1:A:685:ILE:N	2.44	0.45
1:B:487:ASP:OD2	1:B:487:ASP:N	2.49	0.45
1:A:88:ILE:HD13	1:A:118:TYR:C	2.36	0.45
1:B:74:TYR:CZ	1:B:79:GLY:HA3	2.52	0.45
1:A:429:SER:HB3	1:A:432:TYR:CE1	2.52	0.45
1:B:717:ILE:HD13	1:B:717:ILE:N	2.31	0.45
1:B:51:GLU:O	1:B:53:ALA:N	2.50	0.45
1:B:563:GLN:NE2	1:B:584:THR:HA	2.32	0.45
1:A:264:MET:HG2	1:A:265:LEU:N	2.31	0.45
1:A:191:THR:HG22	1:A:194:LEU:CG	2.47	0.45
1:B:89:THR:HG21	1:B:97:LEU:HD12	1.98	0.45
1:B:427:ILE:HG23	1:B:428:GLY:H	1.80	0.45
1:B:211:ASN:O	1:B:214:GLN:N	2.49	0.45
1:B:505:LEU:HD11	1:B:521:LEU:HD21	1.98	0.45
1:B:477:TYR:N	1:B:593:SER:HB2	2.30	0.45
1:B:264:MET:O	1:B:267:ARG:N	2.48	0.45
1:B:467:ILE:H	1:B:467:ILE:HD12	1.82	0.45
1:B:303:LYS:HD3	1:B:304:LYS:NZ	2.32	0.45
1:A:73:MET:O	1:A:76:ALA:HB3	2.17	0.45
1:A:566:ILE:HG13	1:A:600:TYR:CE2	2.52	0.45
1:A:739:GLU:O	1:A:743:LEU:CD1	2.65	0.45
1:A:426:SER:HB3	1:A:508:ASP:O	2.17	0.45
1:A:61:LYS:CE	1:A:61:LYS:HA	2.45	0.45
1:A:707:LEU:HD23	1:A:707:LEU:H	1.81	0.45
1:A:611:GLN:NE2	1:A:774:ILE:HD11	2.29	0.45
1:B:587:VAL:HG11	1:B:592:ALA:HA	1.99	0.45
1:A:744:MET:SD	1:A:766:ILE:HG21	2.57	0.44
1:A:766:ILE:N	1:A:766:ILE:HD12	2.32	0.44
1:B:762:THR:C	1:B:764:GLN:N	2.70	0.44
1:A:197:HIS:HA	1:A:198:PRO:HD3	1.85	0.44
1:A:366:ASN:HB2	1:A:367:PRO:HD3	1.99	0.44
1:B:48:VAL:HB	1:B:49:LYS:H	1.51	0.44
1:A:462:LYS:HA	1:A:541:GLU:OE2	2.17	0.44
1:A:169:LYS:HE3	1:A:533:GLN:HB2	2.00	0.44
1:A:187:ASP:HA	1:A:195:LYS:CE	2.47	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:188:LEU:O	1:A:188:LEU:HD12	2.18	0.44
1:B:131:ILE:HD11	1:B:147:VAL:HG11	1.99	0.44
1:B:766:ILE:HG22	1:B:767:ASN:N	2.31	0.44
1:A:311:LEU:O	1:A:315:GLU:HB2	2.17	0.44
1:B:679:ASN:O	1:B:680:ASP:C	2.56	0.44
1:B:594:ASN:O	1:B:595:ILE:C	2.55	0.44
1:A:255:SER:O	1:A:256:LEU:C	2.55	0.44
1:B:155:LEU:HD12	1:B:159:ILE:CG2	2.47	0.44
1:A:427:ILE:O	1:A:428:GLY:C	2.54	0.44
1:B:721:GLU:OE2	1:B:760:PRO:N	2.51	0.44
1:A:185:GLY:CA	1:A:236:TYR:O	2.66	0.44
1:A:588:HIS:C	1:A:589:ASN:HD22	2.20	0.44
1:B:591:TYR:O	1:B:595:ILE:HG12	2.17	0.44
1:B:176:THR:O	1:B:180:ALA:N	2.46	0.44
1:B:479:ILE:O	1:B:589:ASN:C	2.56	0.44
1:B:658:LEU:HD23	1:B:659:TYR:N	2.32	0.44
1:A:639:ILE:HG21	1:A:667:LEU:HD22	2.00	0.44
1:B:640:ALA:CA	1:B:643:TYR:CZ	3.01	0.44
1:B:501:TRP:HB3	1:B:503:ILE:HD11	1.99	0.44
1:A:711:SER:OG	1:A:714:PHE:HB2	2.17	0.44
1:A:661:PRO:O	1:A:664:ARG:HG3	2.17	0.44
1:B:640:ALA:HB2	1:B:643:TYR:OH	2.17	0.44
1:B:122:LYS:HB3	1:B:128:VAL:HG23	1.99	0.44
1:A:391:ARG:NH1	1:A:404:ILE:HD13	2.33	0.44
1:A:566:ILE:O	1:A:566:ILE:HG12	2.18	0.44
1:B:693:ASP:HB2	1:B:737:PHE:CE2	2.52	0.44
1:A:371:LYS:HA	1:A:371:LYS:HD2	1.81	0.44
1:A:31:THR:HG22	1:A:32:GLN:N	2.32	0.44
1:B:466:GLY:O	1:B:467:ILE:C	2.56	0.44
1:A:765:PHE:O	1:A:768:ASP:HB3	2.17	0.44
1:A:523:ARG:O	1:A:524:ASN:HB2	2.17	0.44
1:B:758:ASN:C	1:B:760:PRO:HD3	2.37	0.44
1:B:113:LEU:HB2	1:B:116:GLU:OE1	2.18	0.44
1:B:511:ALA:HB2	1:B:521:LEU:HA	2.00	0.44
1:A:506:SER:O	1:A:507:PRO:C	2.56	0.44
1:B:505:LEU:HD23	1:B:549:VAL:HG21	1.99	0.44
1:A:600:TYR:O	1:A:604:ASN:HB2	2.17	0.44
1:B:670:GLY:N	1:B:671:PRO:CD	2.81	0.44
1:B:765:PHE:O	1:B:768:ASP:HB3	2.18	0.44
1:B:222:ALA:O	1:B:223:TYR:C	2.56	0.44
1:B:416:ILE:C	1:B:418:ASN:N	2.71	0.44
1:A:378:LYS:HG2	1:A:650:TYR:CD2	2.53	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:488:ILE:HG13	1:A:517:GLY:O	2.18	0.44
1:A:440:ASN:CG	1:A:493:ALA:HB2	2.38	0.43
1:A:660:VAL:HA	1:A:661:PRO:HD3	1.91	0.43
1:B:503:ILE:CD1	1:B:503:ILE:N	2.78	0.43
1:A:241:PHE:HD1	1:A:241:PHE:C	2.20	0.43
1:A:522:GLN:HG2	1:A:525:ILE:HD11	1.99	0.43
1:A:335:LYS:CG	1:A:336:GLU:N	2.81	0.43
1:B:766:ILE:C	1:B:768:ASP:N	2.71	0.43
1:B:490:GLU:HG3	1:B:491:ARG:N	2.33	0.43
1:B:89:THR:O	1:B:89:THR:HG22	2.18	0.43
1:B:193:GLN:HB3	1:B:193:GLN:HE21	1.61	0.43
1:A:500:LYS:HB3	1:A:544:ARG:HH21	1.83	0.43
1:A:614:LEU:HD22	1:A:770:ILE:HD12	2.00	0.43
1:B:640:ALA:C	1:B:642:GLN:H	2.20	0.43
1:B:412:TYR:O	1:B:416:ILE:HG12	2.18	0.43
1:A:84:VAL:O	1:A:133:SER:N	2.51	0.43
1:A:345:ILE:HG22	1:A:345:ILE:O	2.18	0.43
1:B:468:PHE:O	1:B:471:PHE:HB3	2.18	0.43
1:B:84:VAL:C	1:B:133:SER:HB3	2.37	0.43
1:A:154:ILE:HA	1:A:158:ASP:OD1	2.19	0.43
1:A:145:LEU:HD22	1:A:229:HIS:NE2	2.33	0.43
1:B:415:ASP:O	1:B:419:ILE:HG13	2.19	0.43
1:A:741:PHE:O	1:A:742:ARG:C	2.57	0.43
1:A:634:ILE:HG13	1:A:635:THR:O	2.18	0.43
1:A:640:ALA:HA	1:A:643:TYR:CZ	2.53	0.43
1:A:435:ILE:HG22	1:A:437:LEU:HG	2.01	0.43
1:B:83:ILE:HG23	1:B:131:ILE:CG2	2.47	0.43
1:B:155:LEU:HD12	1:B:159:ILE:HB	2.01	0.43
1:B:297:GLN:OE1	1:B:514:LEU:HD13	2.19	0.43
1:A:479:ILE:CG2	1:A:480:SER:N	2.82	0.43
1:A:714:PHE:O	1:A:717:ILE:N	2.39	0.43
1:B:309:HIS:O	1:B:310:SER:HB3	2.18	0.43
1:B:239:GLU:O	1:B:240:ALA:C	2.56	0.43
1:A:79:GLY:HA3	1:A:127:PRO:HB2	1.99	0.43
1:B:610:ILE:HG21	1:B:614:LEU:HD23	1.98	0.43
1:B:79:GLY:HA2	1:B:127:PRO:HB2	2.00	0.43
1:B:476:LYS:N	1:B:593:SER:OG	2.42	0.43
1:B:379:LEU:O	1:B:382:ASP:N	2.51	0.43
1:B:690:HIS:CE1	1:B:735:GLU:OE1	2.72	0.43
1:B:388:ILE:HG23	1:B:416:ILE:HD11	2.00	0.43
1:B:679:ASN:C	1:B:681:SER:N	2.72	0.43
1:A:534:ILE:HG22	1:A:535:ILE:N	2.33	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:56:LYS:HG3	1:A:56:LYS:O	2.18	0.43
1:B:125:TYR:CE2	1:B:162:LYS:HE3	2.53	0.43
1:A:429:SER:OG	1:A:430:THR:N	2.52	0.43
1:A:155:LEU:HG	1:A:160:LEU:HD11	2.00	0.43
1:B:257:GLU:O	1:B:258:GLU:C	2.54	0.43
1:A:234:GLN:HG3	1:A:241:PHE:CD2	2.53	0.43
1:A:525:ILE:CG2	1:A:526:GLY:N	2.82	0.43
1:A:140:ASN:HD21	1:A:143:LYS:NZ	2.16	0.43
1:A:640:ALA:HA	1:A:643:TYR:CE2	2.54	0.43
1:A:107:ILE:C	1:A:107:ILE:CD1	2.87	0.43
1:B:639:ILE:O	1:B:642:GLN:N	2.44	0.43
1:B:766:ILE:O	1:B:768:ASP:N	2.52	0.43
1:A:621:TYR:CE1	1:A:664:ARG:CZ	3.02	0.42
1:B:202:SER:O	1:B:205:PHE:N	2.51	0.42
1:B:65:LYS:HA	1:B:65:LYS:HD2	1.81	0.42
1:B:117:HIS:CG	1:B:118:TYR:N	2.87	0.42
1:A:480:SER:HB3	1:A:525:ILE:HB	2.00	0.42
1:A:29:ASN:C	1:A:31:THR:H	2.21	0.42
1:A:32:GLN:O	1:A:36:LEU:CB	2.68	0.42
1:A:611:GLN:HE22	1:A:770:ILE:CG2	2.32	0.42
1:B:718:PHE:HZ	1:B:731:THR:O	2.02	0.42
1:B:496:ASN:C	1:B:496:ASN:HD22	2.21	0.42
1:B:610:ILE:CD1	1:B:610:ILE:H	2.27	0.42
1:A:415:ASP:O	1:A:419:ILE:HG13	2.19	0.42
1:B:713:LYS:HD2	1:B:765:PHE:CE1	2.53	0.42
1:B:737:PHE:O	1:B:740:ALA:HB3	2.19	0.42
1:A:221:PHE:CE1	1:A:225:ILE:HD11	2.54	0.42
1:A:206:LEU:CD1	1:A:213:VAL:HG11	2.49	0.42
1:A:555:ILE:HD12	1:A:555:ILE:N	2.34	0.42
1:B:388:ILE:O	1:B:391:ARG:N	2.47	0.42
1:A:467:ILE:H	1:A:467:ILE:CD1	2.33	0.42
1:B:264:MET:C	1:B:266:SER:N	2.73	0.42
1:B:436:TYR:CE2	1:B:504:GLN:HB2	2.54	0.42
1:A:707:LEU:N	1:A:707:LEU:HD23	2.34	0.42
1:B:237:ALA:N	1:B:238:PRO:HD3	2.35	0.42
1:A:190:PHE:HD1	1:A:194:LEU:HB3	1.84	0.42
1:B:319:LEU:HD23	1:B:345:ILE:CD1	2.49	0.42
1:A:311:LEU:O	1:A:312:SER:CB	2.67	0.42
1:B:60:GLU:O	1:B:62:LEU:N	2.52	0.42
1:A:570:TRP:HH2	1:A:607:LYS:HB2	1.85	0.42
1:A:77:ILE:CG2	1:A:162:LYS:HD2	2.50	0.42
1:B:654:HIS:O	3:B:9003:SD2:CBE	2.68	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:70:VAL:HG22	1:B:252:ILE:HD11	2.02	0.42
1:B:437:LEU:HD11	1:B:519:LEU:HD12	2.02	0.42
1:A:645:HIS:NE2	1:A:663:SER:HB3	2.34	0.42
1:B:56:LYS:C	1:B:58:ALA:N	2.73	0.42
1:A:686:HIS:C	1:A:686:HIS:CD2	2.93	0.42
1:A:469:ASN:H	1:A:469:ASN:ND2	2.15	0.42
1:A:159:ILE:HG23	1:A:259:LEU:HD11	2.01	0.42
1:B:416:ILE:HG22	1:B:420:ASP:OD1	2.20	0.42
1:B:60:GLU:C	1:B:62:LEU:N	2.72	0.42
1:A:725:LEU:HB2	1:A:736:PHE:HE1	1.83	0.42
1:A:366:ASN:H	1:A:367:PRO:CD	2.32	0.42
1:B:30:LYS:HG3	1:B:30:LYS:O	2.20	0.42
1:B:427:ILE:O	1:B:432:TYR:OH	2.35	0.42
1:A:70:VAL:HG12	1:A:252:ILE:HD11	2.01	0.42
1:A:693:ASP:C	1:A:693:ASP:OD2	2.58	0.42
1:B:657:GLY:HA2	1:B:667:LEU:O	2.20	0.42
1:A:403:SER:HB2	1:A:638:ASN:OD1	2.20	0.42
1:A:563:GLN:HE21	1:A:585:PHE:H	1.68	0.42
1:B:313:GLN:C	1:B:315:GLU:H	2.22	0.42
1:B:190:PHE:CB	1:B:194:LEU:HD23	2.50	0.42
1:B:659:TYR:CE2	1:B:661:PRO:HG3	2.55	0.42
1:B:578:LYS:O	1:B:579:TYR:HB2	2.20	0.42
1:B:498:ARG:HA	1:B:498:ARG:HD2	1.92	0.41
1:B:303:LYS:CD	1:B:304:LYS:HZ1	2.33	0.41
1:B:77:ILE:CG2	1:B:77:ILE:O	2.68	0.41
1:B:732:ASN:OD1	1:B:734:ALA:HB3	2.20	0.41
1:B:324:ILE:O	1:B:325:ASP:C	2.59	0.41
1:B:234:GLN:HB2	1:B:241:PHE:CD2	2.55	0.41
1:B:264:MET:O	1:B:266:SER:N	2.53	0.41
1:A:125:TYR:HA	1:B:268:TYR:HE2	1.86	0.41
1:A:560:GLN:O	1:A:561:GLU:C	2.59	0.41
1:A:96:ALA:O	1:A:97:LEU:C	2.59	0.41
1:A:567:ASN:O	1:A:569:GLU:N	2.49	0.41
1:B:529:ILE:N	1:B:529:ILE:CD1	2.83	0.41
1:B:45:LYS:HD2	1:B:82:TYR:HE2	1.80	0.41
1:B:619:THR:O	1:B:619:THR:HG22	2.19	0.41
1:B:206:LEU:HD23	1:B:213:VAL:HG21	2.03	0.41
1:A:394:ASP:HB3	1:A:635:THR:OG1	2.20	0.41
1:A:655:SER:HA	3:A:9002:SD2:CBE	2.51	0.41
1:A:618:VAL:O	1:A:621:TYR:HB3	2.20	0.41
1:A:369:SER:OG	1:A:372:GLU:CB	2.67	0.41
1:B:388:ILE:HG23	1:B:416:ILE:CD1	2.50	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:228:GLN:OE1	1:A:228:GLN:HA	2.19	0.41
1:A:733:GLU:HG2	1:A:734:ALA:N	2.35	0.41
1:B:420:ASP:CG	1:B:523:ARG:HH11	2.24	0.41
1:A:178:LYS:HG3	1:A:179:ASN:ND2	2.34	0.41
1:A:118:TYR:CE2	1:A:143:LYS:HB3	2.56	0.41
1:B:467:ILE:H	1:B:467:ILE:CD1	2.33	0.41
1:A:114:LEU:C	1:A:116:GLU:H	2.24	0.41
1:A:608:ASN:C	1:A:609:ASN:ND2	2.64	0.41
1:B:610:ILE:HG23	1:B:614:LEU:HD23	1.99	0.41
1:B:174:LEU:CD2	1:B:216:VAL:HG11	2.51	0.41
1:A:272:GLU:HA	1:A:275:LYS:HB3	2.01	0.41
1:B:114:LEU:HD22	1:B:120:TYR:HB2	2.01	0.41
1:A:175:ASN:O	1:A:178:LYS:HG2	2.21	0.41
1:B:468:PHE:CD2	1:B:534:ILE:HD11	2.56	0.41
1:B:401:SER:CB	1:B:638:ASN:ND2	2.75	0.41
1:A:247:PHE:CG	1:A:247:PHE:O	2.73	0.41
1:B:74:TYR:CE1	1:B:79:GLY:HA3	2.55	0.41
1:B:294:LYS:C	1:B:296:LEU:H	2.22	0.41
1:A:301:GLU:HA	1:A:302:PRO:HD3	1.84	0.41
1:B:540:LYS:HD3	1:B:542:TYR:CZ	2.55	0.41
1:A:563:GLN:NE2	1:A:585:PHE:H	2.17	0.41
1:B:755:VAL:HG12	1:B:756:GLN:N	2.34	0.41
1:B:257:GLU:HA	1:B:260:LYS:HD3	2.03	0.41
1:A:319:LEU:HD13	1:A:319:LEU:C	2.41	0.41
1:A:311:LEU:O	1:A:315:GLU:OE1	2.39	0.41
1:A:721:GLU:OE1	1:A:759:ALA:HA	2.20	0.41
1:A:235:LEU:HD23	1:A:236:TYR:CE2	2.56	0.41
1:A:121:ALA:HA	1:A:129:LEU:HA	2.02	0.41
1:B:473:LYS:O	1:B:474:ASN:HB2	2.20	0.41
1:B:743:LEU:O	1:B:744:MET:C	2.59	0.41
1:A:677:LEU:O	1:A:678:ARG:C	2.59	0.41
1:B:143:LYS:O	1:B:147:VAL:HG23	2.21	0.41
1:B:186:GLN:NE2	1:B:195:LYS:HB2	2.25	0.41
1:B:27:GLU:CG	1:B:27:GLU:O	2.63	0.41
1:A:391:ARG:CZ	1:A:395:THR:HG21	2.51	0.41
1:A:430:THR:O	1:A:431:LEU:HD23	2.21	0.41
1:A:427:ILE:HA	1:A:427:ILE:HD12	1.81	0.41
1:A:151:ILE:O	1:A:152:GLY:C	2.57	0.41
1:A:241:PHE:HD1	1:A:242:ASN:N	2.18	0.41
1:A:169:LYS:HE3	1:A:533:GLN:HB3	2.03	0.41
1:A:118:TYR:HE2	1:A:143:LYS:HB3	1.86	0.41
1:B:490:GLU:HG2	1:B:537:GLN:HE22	1.86	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:728:TYR:O	1:A:729:GLY:C	2.59	0.41
1:B:235:LEU:HD13	1:B:236:TYR:CD1	2.56	0.41
1:B:341:LEU:O	1:B:341:LEU:HD23	2.21	0.41
1:A:154:ILE:HG22	1:A:155:LEU:N	2.35	0.41
1:B:673:LYS:CG	1:B:673:LYS:O	2.68	0.41
1:A:522:GLN:HG3	1:A:523:ARG:N	2.36	0.41
1:B:113:LEU:H	1:B:116:GLU:CD	2.25	0.40
1:A:223:TYR:HB3	1:A:233:LEU:CD1	2.50	0.40
1:B:408:VAL:O	1:B:411:GLN:HB3	2.21	0.40
1:A:634:ILE:HD11	1:A:639:ILE:HD12	2.02	0.40
1:A:73:MET:SD	1:A:159:ILE:HG21	2.61	0.40
1:B:343:ILE:HG23	1:B:346:ARG:HD2	2.01	0.40
1:A:681:SER:O	1:A:684:PHE:HB3	2.21	0.40
1:A:511:ALA:HB2	1:A:521:LEU:HD23	2.03	0.40
1:B:106:ASP:OD2	1:B:110:LYS:HB2	2.21	0.40
1:B:234:GLN:HB2	1:B:241:PHE:CE2	2.57	0.40
1:A:467:ILE:N	1:A:467:ILE:HD12	2.36	0.40
1:A:478:SER:OG	1:A:590:ARG:HA	2.20	0.40
1:B:89:THR:HG21	1:B:97:LEU:CD1	2.52	0.40
1:A:640:ALA:O	1:A:644:THR:HG23	2.22	0.40
1:B:177:ILE:CG2	1:B:186:GLN:HA	2.51	0.40
1:B:303:LYS:NZ	1:B:304:LYS:HZ1	2.18	0.40
1:B:226:GLU:HA	1:B:227:PRO:HD3	1.94	0.40
1:B:256:LEU:O	1:B:257:GLU:C	2.59	0.40
1:A:749:HIS:O	1:A:750:ALA:C	2.60	0.40
1:A:266:SER:O	1:A:269:GLU:HB3	2.22	0.40
1:B:511:ALA:CB	1:B:521:LEU:HD23	2.51	0.40
1:B:510:ARG:HB2	1:B:522:GLN:OE1	2.22	0.40
1:B:202:SER:O	1:B:203:VAL:C	2.60	0.40
1:B:202:SER:C	1:B:204:GLU:H	2.25	0.40
1:B:322:ILE:O	1:B:342:GLN:NE2	2.53	0.40
1:A:278:TYR:C	1:A:280:HIS:N	2.75	0.40
1:A:721:GLU:HA	1:A:724:ASN:OD1	2.22	0.40
1:B:422:LEU:HD12	1:B:422:LEU:HA	1.81	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	728/776 (94%)	529 (73%)	144 (20%)	55 (8%)	2	23
1	B	730/776 (94%)	536 (73%)	143 (20%)	51 (7%)	2	26
All	All	1458/1552 (94%)	1065 (73%)	287 (20%)	106 (7%)	2	25

All (106) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	52	GLU
1	A	92	ILE
1	A	227	PRO
1	A	238	PRO
1	A	405	ASN
1	A	457	SER
1	A	473	LYS
1	A	539	GLU
1	A	675	VAL
1	A	678	ARG
1	A	702	LYS
1	A	720	GLU
1	B	33	GLU
1	B	95	GLU
1	B	211	ASN
1	B	310	SER
1	B	325	ASP
1	B	366	ASN
1	B	495	ASP
1	B	553	SER
1	B	731	THR
1	A	181	SER
1	A	279	GLN
1	A	336	GLU
1	A	369	SER
1	A	428	GLY
1	A	573	ALA

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Mol	Chain	Res	Type
1	A	590	ARG
1	A	615	ILE
1	A	647	ASP
1	A	676	GLU
1	B	35	HIS
1	B	96	ALA
1	B	157	ARG
1	B	168	GLN
1	B	203	VAL
1	B	210	SER
1	B	242	ASN
1	B	250	GLN
1	B	324	ILE
1	B	326	SER
1	B	367	PRO
1	B	370	GLU
1	B	417	GLN
1	B	515	GLU
1	B	592	ALA
1	B	593	SER
1	A	30	LYS
1	A	125	TYR
1	A	254	LEU
1	A	265	LEU
1	A	312	SER
1	A	460	ASN
1	A	509	THR
1	A	568	GLN
1	A	593	SER
1	A	741	PHE
1	A	760	PRO
1	B	48	VAL
1	B	52	GLU
1	B	123	GLU
1	B	187	ASP
1	B	531	ASP
1	B	767	ASN
1	A	114	LEU
1	A	198	PRO
1	A	264	MET
1	A	299	PRO
1	A	300	ILE

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Mol	Chain	Res	Type
1	A	329	PHE
1	A	492	PRO
1	A	682	GLU
1	B	53	ALA
1	B	180	ALA
1	B	200	ASP
1	B	468	PHE
1	B	474	ASN
1	B	666	ILE
1	B	732	ASN
1	A	77	ILE
1	A	164	ASN
1	A	402	PRO
1	A	731	THR
1	A	742	ARG
1	B	142	GLU
1	B	169	LYS
1	B	265	LEU
1	B	314	GLU
1	B	464	ASN
1	B	647	ASP
1	A	78	GLY
1	A	433	ASN
1	A	670	GLY
1	B	674	GLY
1	A	529	ILE
1	A	627	GLY
1	A	722	GLY
1	B	198	PRO
1	B	227	PRO
1	A	147	VAL
1	A	366	ASN
1	A	383	ILE
1	B	466	GLY
1	B	467	ILE
1	B	595	ILE
1	B	383	ILE

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	671/710 (94%)	607 (90%)	64 (10%)	12	51
1	B	673/710 (95%)	607 (90%)	66 (10%)	12	49
All	All	1344/1420 (95%)	1214 (90%)	130 (10%)	12	50

All (130) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	GLN
1	A	35	HIS
1	A	42	HIS
1	A	46	ILE
1	A	49	LYS
1	A	51	GLU
1	A	52	GLU
1	A	56	LYS
1	A	85	ASP
1	A	93	SER
1	A	100	ASP
1	A	101	LYS
1	A	104	ILE
1	A	107	ILE
1	A	113	LEU
1	A	118	TYR
1	A	193	GLN
1	A	199	THR
1	A	211	ASN
1	A	233	LEU
1	A	239	GLU
1	A	241	PHE
1	A	259	LEU
1	A	283	ASP
1	A	292	LEU
1	A	321	ARG
1	A	329	PHE
1	A	333	GLU
1	A	343	ILE
1	A	346	ARG
1	A	373	LYS
1	A	381	LEU
1	A	404	ILE

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Mol	Chain	Res	Type
1	A	426	SER
1	A	447	THR
1	A	449	THR
1	A	453	ASP
1	A	456	ASP
1	A	469	ASN
1	A	498	ARG
1	A	514	LEU
1	A	522	GLN
1	A	546	ASP
1	A	550	VAL
1	A	556	ASP
1	A	574	LEU
1	A	578	LYS
1	A	586	ASN
1	A	594	ASN
1	A	601	LEU
1	A	604	ASN
1	A	611	GLN
1	A	619	THR
1	A	620	ASN
1	A	658	LEU
1	A	693	ASP
1	A	710	ASN
1	A	712	LYS
1	A	716	ASP
1	A	725	LEU
1	A	727	SER
1	A	737	PHE
1	A	764	GLN
1	A	772	PHE
1	B	28	ARG
1	B	32	GLN
1	B	36	LEU
1	B	60	GLU
1	B	62	LEU
1	B	92	ILE
1	B	105	LYS
1	B	107	ILE
1	B	111	ASP
1	B	128	VAL
1	B	131	ILE

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Mol	Chain	Res	Type
1	B	136	ASP
1	B	140	ASN
1	B	178	LYS
1	B	193	GLN
1	B	197	HIS
1	B	199	THR
1	B	203	VAL
1	B	204	GLU
1	B	206	LEU
1	B	209	ASN
1	B	228	GLN
1	B	233	LEU
1	B	235	LEU
1	B	242	ASN
1	B	250	GLN
1	B	282	SER
1	B	296	LEU
1	B	297	GLN
1	B	304	LYS
1	B	309	HIS
1	B	323	GLN
1	B	343	ILE
1	B	344	ASP
1	B	346	ARG
1	B	366	ASN
1	B	381	LEU
1	B	384	GLN
1	B	398	LEU
1	B	407	ASP
1	B	408	VAL
1	B	433	ASN
1	B	445	ASN
1	B	449	THR
1	B	456	ASP
1	B	464	ASN
1	B	475	PHE
1	B	487	ASP
1	B	496	ASN
1	B	503	ILE
1	B	516	ASN
1	B	523	ARG
1	B	533	GLN

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Mol	Chain	Res	Type
1	B	556	ASP
1	B	571	ASN
1	B	580	THR
1	B	586	ASN
1	B	611	GLN
1	B	613	ASP
1	B	620	ASN
1	B	647	ASP
1	B	652	GLN
1	B	712	LYS
1	B	733	GLU
1	B	747	THR
1	B	753	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (60) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	29	ASN
1	A	32	GLN
1	A	132	GLN
1	A	140	ASN
1	A	164	ASN
1	A	179	ASN
1	A	186	GLN
1	A	193	GLN
1	A	197	HIS
1	A	214	GLN
1	A	276	GLN
1	A	323	GLN
1	A	440	ASN
1	A	444	ASN
1	A	460	ASN
1	A	469	ASN
1	A	496	ASN
1	A	504	GLN
1	A	524	ASN
1	A	563	GLN
1	A	571	ASN
1	A	589	ASN
1	A	608	ASN
1	A	609	ASN
1	A	611	GLN

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Mol	Chain	Res	Type
1	A	620	ASN
1	A	710	ASN
1	B	91	HIS
1	B	140	ASN
1	B	165	GLN
1	B	186	GLN
1	B	193	GLN
1	B	214	GLN
1	B	228	GLN
1	B	234	GLN
1	B	242	ASN
1	B	276	GLN
1	B	277	HIS
1	B	342	GLN
1	B	366	ASN
1	B	390	GLN
1	B	440	ASN
1	B	445	ASN
1	B	496	ASN
1	B	516	ASN
1	B	524	ASN
1	B	533	GLN
1	B	537	GLN
1	B	563	GLN
1	B	571	ASN
1	B	589	ASN
1	B	609	ASN
1	B	611	GLN
1	B	620	ASN
1	B	638	ASN
1	B	645	HIS
1	B	710	ASN
1	B	756	GLN
1	B	764	GLN
1	B	769	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 ⓘ

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	SD2	A	9002	2	33,33,33	0.89	1 (3%)	44,44,44	1.88	6 (13%)
3	SD2	B	9003	2	33,33,33	1.06	3 (9%)	44,44,44	2.21	6 (13%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SD2	A	9002	2	-	0/33/44/44	0/2/2/2
3	SD2	B	9003	2	-	0/33/44/44	0/2/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	9002	SD2	CBB-CBC	-3.36	1.37	1.51
3	B	9003	SD2	CBB-CBC	-3.17	1.38	1.51
3	B	9003	SD2	CAR-NAQ	2.26	1.51	1.47
3	B	9003	SD2	CBB-CAY	-2.10	1.48	1.53

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	9003	SD2	CAY-NAX-CAS	10.10	143.97	121.63
3	A	9002	SD2	CAY-NAX-CAS	7.25	137.67	121.63
3	A	9002	SD2	CBB-CAY-NAX	-5.75	99.87	110.83
3	B	9003	SD2	CAR-CAS-NAX	5.39	128.60	116.70
3	B	9003	SD2	CBB-CAY-NAX	5.01	120.38	110.83
3	A	9002	SD2	CAR-CAS-NAX	-4.66	106.44	116.70
3	A	9002	SD2	OAT-CAS-NAX	3.92	130.48	122.93
3	B	9003	SD2	OAT-CAS-NAX	-3.91	115.39	122.93
3	B	9003	SD2	CAS-CAR-NAQ	-2.92	105.42	112.71
3	A	9002	SD2	CBC-CBB-CAY	2.38	119.87	112.97
3	B	9003	SD2	CBB-CAY-CAZ	2.32	115.67	110.32
3	A	9002	SD2	CAZ-CAY-NAX	-2.22	106.02	111.28

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 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	732/776 (94%)	-0.09	0 100 100	13, 39, 88, 93	0
1	B	734/776 (94%)	-0.10	1 (0%) 93 84	11, 38, 84, 96	0
All	All	1466/1552 (94%)	-0.10	1 (0%) 93 84	11, 38, 86, 96	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	101	LYS	2.2

### 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 ⓘ

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

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	SD2	A	9002	32/32	0.24	1.09	21,23,30,41	0
3	SD2	B	9003	32/32	0.23	0.49	16,23,32,37	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	ZN	B	9002	1/1	0.12	-1.76	17,17,17,17	0
2	ZN	A	9001	1/1	0.12	-1.79	21,21,21,21	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.