



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 30, 2024 – 02:31 PM JST

PDB ID : 8I6Y  
Title : Crystal structure of Arabidopsis thaliana LOX1  
Authors : Liu, X.; Liu, L.  
Deposited on : 2023-01-30  
Resolution : 3.26 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4.02b-467  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

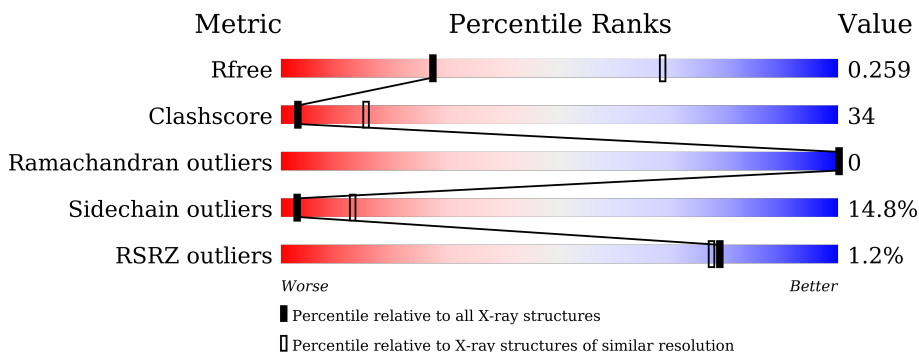
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.26 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1191 (3.30-3.22)
Clashscore	141614	1251 (3.30-3.22)
Ramachandran outliers	138981	1229 (3.30-3.22)
Sidechain outliers	138945	1228 (3.30-3.22)
RSRZ outliers	127900	1154 (3.30-3.22)

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 of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	859	
1	B	859	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 13633 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Linoleate 9S-lipoxygenase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	844	6810	4371	1132	1292	15	0	0	0
1	B	844	6810	4371	1132	1292	15	0	0	0

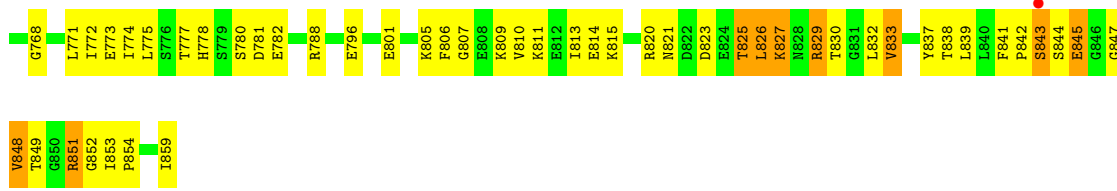
- Molecule 2 is FE (III) ION (three-letter code: FE) (formula: Fe).

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

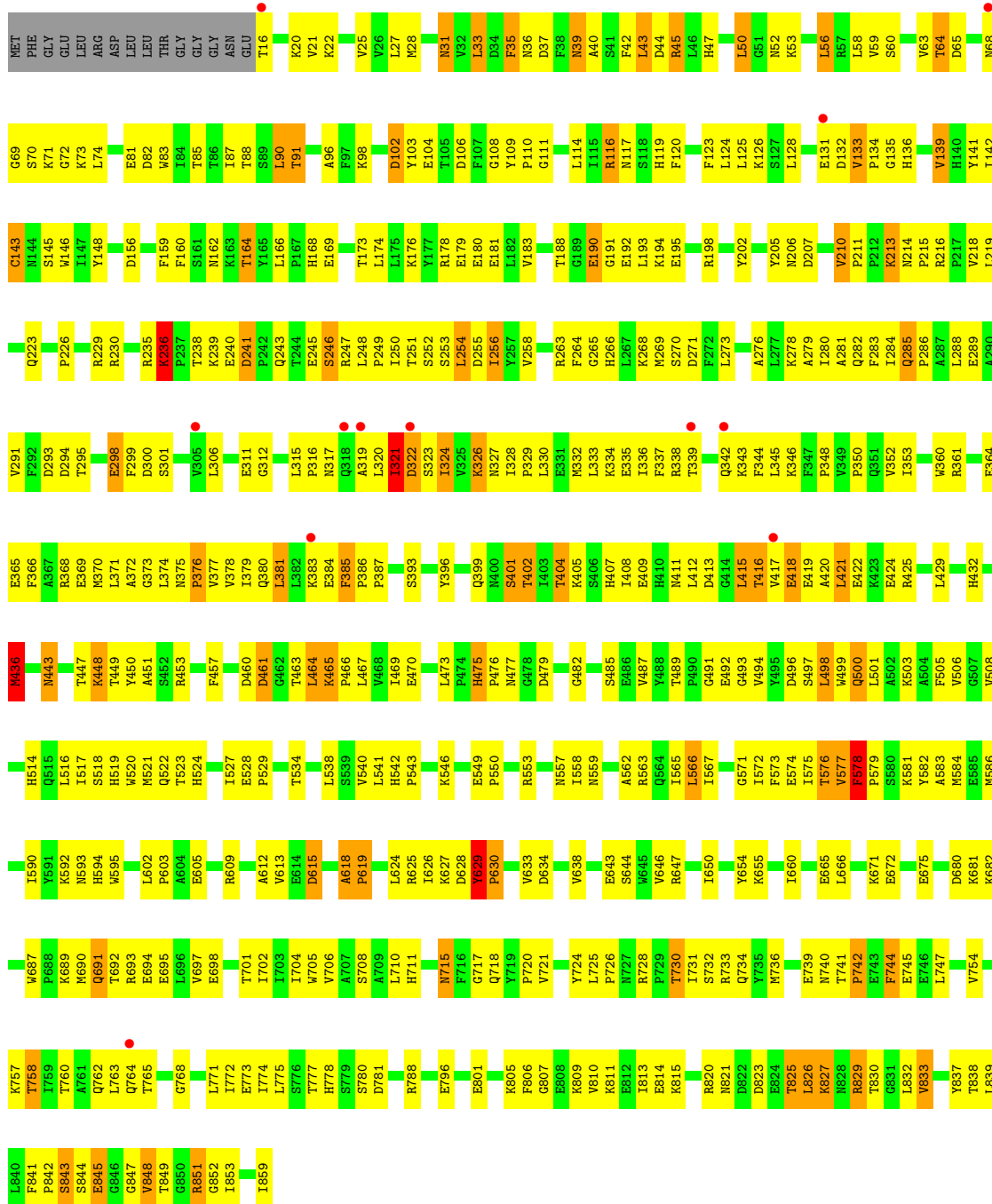
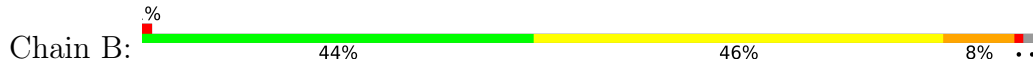
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	6	Total	O	0	0
			6	6		
3	B	5	Total	O	0	0
			5	5		





● Molecule 1: Linoleate 9S-lipoxygenase 1



## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	116.37Å 119.35Å 135.36Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	67.68 – 3.26 67.68 – 3.26	Depositor EDS
% Data completeness (in resolution range)	95.8 (67.68-3.26) 95.8 (67.68-3.26)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.36 (at 3.26Å)	Xtrriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, $R_{free}$	0.233 , 0.259 0.233 , 0.259	Depositor DCC
$R_{free}$ test set	1380 reflections (4.81%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	66.9	Xtrriage
Anisotropy	0.071	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 45.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.000 for k,h,-l	Xtrriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	13633	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	58.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 26.92 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.4147e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

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

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.80	6/6986 (0.1%)	0.83	27/9482 (0.3%)
1	B	0.80	7/6986 (0.1%)	0.83	27/9482 (0.3%)
All	All	0.80	13/13972 (0.1%)	0.83	54/18964 (0.3%)

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
1	B	0	1
All	All	0	2

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	376	PRO	N-CD	5.37	1.55	1.47
1	A	376	PRO	N-CD	5.34	1.55	1.47
1	B	619	PRO	N-CD	5.32	1.55	1.47
1	B	742	PRO	N-CD	5.29	1.55	1.47
1	A	215	PRO	N-CD	5.29	1.55	1.47
1	A	619	PRO	N-CD	5.29	1.55	1.47
1	A	742	PRO	N-CD	5.27	1.55	1.47
1	A	211	PRO	N-CD	5.07	1.54	1.47
1	A	630	PRO	N-CD	5.07	1.54	1.47
1	B	630	PRO	N-CD	5.04	1.54	1.47
1	B	543	PRO	N-CD	5.03	1.54	1.47
1	B	134	PRO	N-CD	5.01	1.54	1.47
1	B	466	PRO	N-CD	5.01	1.54	1.47

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	241	ASP	C-N-CD	6.39	141.81	128.40
1	A	241	ASP	C-N-CD	6.38	141.80	128.40
1	A	578	PHE	C-N-CD	6.17	141.35	128.40
1	B	578	PHE	C-N-CD	6.16	141.34	128.40
1	B	687	TRP	C-N-CD	6.13	141.26	128.40
1	A	687	TRP	C-N-CD	6.11	141.22	128.40
1	B	211	PRO	C-N-CD	6.08	141.18	128.40
1	A	473	LEU	C-N-CD	6.08	141.17	128.40
1	B	473	LEU	C-N-CD	6.08	141.17	128.40
1	A	248	LEU	C-N-CD	6.01	141.03	128.40
1	B	615	ASP	C-N-CD	6.01	141.03	128.40
1	B	248	LEU	C-N-CD	6.01	141.02	128.40
1	B	295	THR	C-N-CD	5.99	140.98	128.40
1	A	285	GLN	C-N-CD	5.98	140.96	128.40
1	B	285	GLN	C-N-CD	5.98	140.95	128.40
1	A	615	ASP	C-N-CD	5.97	140.94	128.40
1	A	295	THR	C-N-CD	5.96	140.92	128.40
1	A	236	LYS	C-N-CD	5.93	140.85	128.40
1	B	236	LYS	C-N-CD	5.93	140.85	128.40
1	A	133	VAL	C-N-CD	5.86	140.70	128.40
1	B	133	VAL	C-N-CD	5.85	140.69	128.40
1	A	853	ILE	C-N-CD	5.83	140.65	128.40
1	B	489	THR	C-N-CD	5.83	140.64	128.40
1	A	475	HIS	C-N-CD	5.83	140.63	128.40
1	A	489	THR	C-N-CD	5.83	140.63	128.40
1	B	853	ILE	C-N-CD	5.81	140.60	128.40
1	B	475	HIS	C-N-CD	5.81	140.60	128.40
1	A	436	MET	C-N-CD	5.80	140.59	128.40
1	B	436	MET	C-N-CD	5.80	140.57	128.40
1	B	214	ASN	C-N-CD	5.79	140.57	128.40
1	B	210	VAL	C-N-CD	5.76	140.50	128.40
1	A	210	VAL	C-N-CD	5.68	140.32	128.40
1	A	211	PRO	C-N-CD	5.67	140.32	128.40
1	B	728	ARG	C-N-CD	5.65	140.27	128.40
1	A	728	ARG	C-N-CD	5.65	140.26	128.40
1	B	465	LYS	C-N-CD	5.64	140.24	128.40
1	A	465	LYS	C-N-CD	5.63	140.22	128.40
1	B	741	THR	C-N-CD	5.63	140.22	128.40
1	A	741	THR	C-N-CD	5.61	140.18	128.40
1	B	618	ALA	C-N-CD	5.59	140.13	128.40
1	A	618	ALA	C-N-CD	5.57	140.10	128.40
1	A	542	HIS	C-N-CD	5.54	140.04	128.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	629	TYR	C-N-CD	5.54	140.04	128.40
1	A	321	ILE	C-N-CA	-5.54	107.86	121.70
1	B	629	TYR	C-N-CD	5.53	140.01	128.40
1	B	542	HIS	C-N-CD	5.52	140.00	128.40
1	B	321	ILE	C-N-CA	-5.52	107.91	121.70
1	A	214	ASN	C-N-CD	5.50	139.96	128.40
1	A	56	LEU	CA-CB-CG	5.37	127.64	115.30
1	B	56	LEU	CA-CB-CG	5.36	127.64	115.30
1	A	375	ASN	C-N-CD	5.36	139.65	128.40
1	B	375	ASN	C-N-CD	5.35	139.63	128.40
1	B	69	GLY	N-CA-C	-5.11	100.34	113.10
1	A	69	GLY	N-CA-C	-5.10	100.36	113.10

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	321	ILE	Mainchain
1	B	321	ILE	Mainchain

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6810	0	6696	451	2
1	B	6810	0	6696	476	2
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	6	0	0	1	0
3	B	5	0	0	4	0
All	All	13633	0	13392	927	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 34.

All (927) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:381:LEU:CD2	1:A:383:LYS:HE3	1.57	1.33
1:B:381:LEU:CD2	1:B:383:LYS:HE3	1.57	1.33
1:B:311:GLU:O	1:B:343:LYS:CB	1.79	1.28
1:A:573:PHE:O	1:A:577:VAL:HG23	1.32	1.26
1:A:823:ASP:OD1	1:A:825:THR:HG22	1.12	1.25
1:B:823:ASP:OD1	1:B:825:THR:HG22	1.12	1.25
1:B:385:PHE:CE2	1:B:408:ILE:HD11	1.74	1.21
1:B:823:ASP:OD1	1:B:825:THR:CG2	1.90	1.19
1:A:823:ASP:OD1	1:A:825:THR:CG2	1.90	1.17
1:B:321:ILE:HA	1:B:324:ILE:CD1	1.74	1.17
1:A:321:ILE:HA	1:A:324:ILE:CD1	1.74	1.16
1:A:381:LEU:HD21	1:A:383:LYS:CE	1.77	1.14
1:B:385:PHE:HE2	1:B:408:ILE:HD11	0.99	1.14
1:B:415:LEU:HD22	1:B:419:GLU:HB3	1.19	1.14
1:A:782:GLU:OE2	1:A:854:PRO:HG3	1.45	1.14
1:A:782:GLU:OE2	1:A:854:PRO:CG	1.97	1.12
1:B:381:LEU:HD21	1:B:383:LYS:CE	1.77	1.12
1:B:254:LEU:HD22	1:B:255:ASP:H	1.15	1.11
1:A:254:LEU:HD22	1:A:255:ASP:H	1.16	1.11
1:B:385:PHE:HE2	1:B:408:ILE:CD1	1.61	1.11
1:A:192:GLU:OE2	1:A:236:LYS:HE2	1.51	1.10
1:B:192:GLU:OE2	1:B:236:LYS:HE2	1.51	1.09
1:A:498:LEU:CD1	1:A:736:MET:HE1	1.84	1.08
1:A:498:LEU:HD12	1:A:736:MET:HE1	1.12	1.08
1:B:416:THR:HG23	1:B:419:GLU:H	1.08	1.07
1:A:321:ILE:O	1:A:322:ASP:C	1.88	1.06
1:B:263:ARG:HE	1:B:557:ASN:ND2	1.53	1.06
1:B:65:ASP:HB2	1:B:73:LYS:HA	1.38	1.05
1:A:263:ARG:HE	1:A:557:ASN:ND2	1.53	1.05
1:A:565:ILE:HD12	1:A:566:LEU:HD12	1.38	1.05
1:B:321:ILE:HA	1:B:324:ILE:HD13	1.37	1.05
1:A:634:ASP:OD1	1:A:829:ARG:NH2	1.90	1.04
1:B:416:THR:N	1:B:419:GLU:OE1	1.90	1.04
1:B:634:ASP:OD1	1:B:829:ARG:NH2	1.90	1.03
1:A:250:ILE:HD12	1:A:250:ILE:H	1.20	1.03
1:A:65:ASP:HB2	1:A:73:LYS:HA	1.38	1.02
1:A:321:ILE:HA	1:A:324:ILE:HD13	1.37	1.02
1:B:71:LYS:O	1:B:173:THR:O	1.77	1.02
1:A:498:LEU:HD12	1:A:736:MET:CE	1.90	1.01
1:A:385:PHE:HE2	1:A:408:ILE:HD11	1.26	1.01
1:B:250:ILE:HD12	1:B:250:ILE:H	1.20	1.01
1:B:573:PHE:O	1:B:577:VAL:HG23	1.58	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:71:LYS:O	1:A:173:THR:O	1.77	1.01
1:A:754:VAL:O	1:A:758:THR:OG1	1.79	1.01
1:B:50:LEU:HD21	1:B:81:GLU:O	1.61	1.01
1:A:324:ILE:HD12	1:A:324:ILE:H	1.22	1.01
1:B:565:ILE:HD12	1:B:566:LEU:HD12	1.39	1.01
1:B:321:ILE:O	1:B:322:ASP:C	1.88	1.00
1:B:324:ILE:HD12	1:B:324:ILE:H	1.22	1.00
1:B:754:VAL:O	1:B:758:THR:OG1	1.79	1.00
1:B:415:LEU:HD22	1:B:419:GLU:CB	1.93	0.99
1:B:689:LYS:HA	1:B:689:LYS:HE2	1.40	0.99
1:A:148:TYR:OH	1:A:195:GLU:OE2	1.81	0.99
1:B:45:ARG:HG2	1:B:45:ARG:HH11	1.29	0.97
1:A:425:ARG:NH2	1:A:460:ASP:OD1	1.97	0.97
1:B:425:ARG:NH2	1:B:460:ASP:OD1	1.97	0.97
1:B:143:CYS:HB3	1:B:159:PHE:CD1	2.00	0.97
1:B:148:TYR:OH	1:B:195:GLU:OE2	1.81	0.96
1:B:443:ASN:HD21	1:B:449:THR:H	1.12	0.96
1:A:143:CYS:HB3	1:A:159:PHE:CD1	2.00	0.96
1:B:823:ASP:CG	1:B:825:THR:CG2	2.33	0.96
1:A:45:ARG:HH11	1:A:45:ARG:HG2	1.29	0.96
1:A:823:ASP:CG	1:A:825:THR:CG2	2.33	0.95
1:A:374:LEU:HB2	1:A:721:VAL:HG21	1.48	0.95
1:A:271:ASP:OD2	1:A:780:SER:OG	1.84	0.94
1:B:271:ASP:OD2	1:B:780:SER:OG	1.84	0.94
1:B:374:LEU:HB2	1:B:721:VAL:HG21	1.48	0.94
1:B:416:THR:HG23	1:B:419:GLU:N	1.82	0.94
1:B:565:ILE:CD1	1:B:566:LEU:HD12	1.98	0.94
1:A:565:ILE:CD1	1:A:566:LEU:HD12	1.98	0.93
1:B:381:LEU:HD21	1:B:383:LYS:HE3	0.94	0.93
1:B:416:THR:HG22	1:B:419:GLU:CD	1.89	0.93
1:A:68:ASN:ND2	1:A:74:LEU:HD11	1.84	0.93
1:B:289:GLU:O	1:B:293:ASP:HB2	1.69	0.92
1:B:263:ARG:HE	1:B:557:ASN:HD21	1.07	0.92
1:B:68:ASN:ND2	1:B:74:LEU:HD11	1.84	0.92
1:A:381:LEU:HD21	1:A:383:LYS:HE3	0.94	0.92
1:A:289:GLU:O	1:A:293:ASP:HB2	1.69	0.91
1:B:692:THR:OG1	1:B:695:GLU:HG3	1.70	0.91
1:A:250:ILE:O	1:A:282:GLN:NE2	2.03	0.91
1:B:250:ILE:O	1:B:282:GLN:NE2	2.04	0.91
1:A:690:MET:HE2	1:A:690:MET:HA	1.50	0.91
1:A:263:ARG:NE	1:A:557:ASN:ND2	2.19	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:443:ASN:HD21	1:A:449:THR:H	1.12	0.90
1:A:263:ARG:HE	1:A:557:ASN:HD21	1.07	0.90
1:B:415:LEU:CD2	1:B:419:GLU:HB3	2.00	0.90
1:A:35:PHE:O	1:A:269:MET:HG2	1.71	0.90
1:A:68:ASN:ND2	1:A:74:LEU:CD1	2.35	0.90
1:A:475:HIS:HE1	1:A:477:ASN:HD22	1.15	0.90
1:B:35:PHE:O	1:B:269:MET:HG2	1.71	0.89
1:B:299:PHE:CZ	1:B:762:GLN:NE2	2.40	0.89
1:B:475:HIS:HE1	1:B:477:ASN:HD22	1.15	0.89
1:B:68:ASN:ND2	1:B:74:LEU:CD1	2.35	0.88
1:B:263:ARG:NE	1:B:557:ASN:ND2	2.19	0.88
1:B:321:ILE:HA	1:B:324:ILE:HD12	1.54	0.88
1:A:573:PHE:O	1:A:577:VAL:CG2	2.21	0.88
1:B:396:TYR:O	1:B:399:GLN:NE2	2.07	0.88
1:A:321:ILE:HA	1:A:324:ILE:HD12	1.54	0.88
1:A:299:PHE:CZ	1:A:762:GLN:NE2	2.40	0.87
1:A:298:GLU:OE1	1:A:733:ARG:NH2	2.07	0.87
1:A:396:TYR:O	1:A:399:GLN:NE2	2.07	0.87
1:A:263:ARG:HH21	1:A:557:ASN:ND2	1.72	0.87
1:B:116:ARG:HG2	1:B:116:ARG:HH11	1.39	0.87
1:A:266:HIS:ND1	1:A:781:ASP:OD2	2.08	0.87
1:B:263:ARG:HH21	1:B:557:ASN:ND2	1.72	0.87
1:B:28:MET:HE2	1:B:33:LEU:CD2	2.05	0.86
1:B:298:GLU:OE1	1:B:733:ARG:NH2	2.07	0.86
1:A:116:ARG:HH11	1:A:116:ARG:HG2	1.39	0.86
1:B:28:MET:HE2	1:B:33:LEU:HD21	1.57	0.86
1:B:68:ASN:HD22	1:B:74:LEU:CD1	1.89	0.86
1:A:28:MET:HE2	1:A:33:LEU:CD2	2.06	0.86
1:B:385:PHE:HD1	1:B:386:PRO:N	1.74	0.86
1:A:28:MET:HE2	1:A:33:LEU:HD21	1.57	0.86
1:A:28:MET:HE1	1:A:33:LEU:HD11	1.58	0.85
1:A:68:ASN:HD22	1:A:74:LEU:CD1	1.89	0.85
1:B:266:HIS:ND1	1:B:781:ASP:OD2	2.08	0.85
1:A:208:LEU:HD13	1:A:567:ILE:O	1.77	0.85
1:A:385:PHE:HD1	1:A:386:PRO:N	1.74	0.85
1:B:415:LEU:HD13	1:B:419:GLU:C	1.97	0.84
1:A:86:THR:O	1:A:89:SER:OG	1.95	0.84
1:B:28:MET:HE1	1:B:33:LEU:HD11	1.60	0.84
1:B:299:PHE:CE2	1:B:762:GLN:NE2	2.45	0.83
1:A:299:PHE:CE2	1:A:762:GLN:NE2	2.45	0.83
1:A:312:GLY:HA2	1:A:345:LEU:O	1.76	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:498:LEU:CD1	1:A:736:MET:CE	2.51	0.83
1:A:447:THR:O	1:A:448:LYS:HD2	1.79	0.83
1:B:249:PRO:HD2	1:B:252:SER:HB2	1.61	0.83
1:A:249:PRO:HD2	1:A:252:SER:HB2	1.61	0.83
1:A:385:PHE:CE2	1:A:408:ILE:HD11	2.13	0.83
1:B:415:LEU:HD13	1:B:420:ALA:N	1.93	0.83
1:B:447:THR:O	1:B:448:LYS:HD2	1.79	0.83
1:B:330:LEU:HD12	1:B:330:LEU:O	1.80	0.82
1:A:782:GLU:OE2	1:A:854:PRO:HG2	1.79	0.82
1:B:558:ILE:HD11	1:B:859:ILE:HD12	1.61	0.82
1:B:43:LEU:HD12	1:B:44:ASP:HA	1.61	0.82
1:A:254:LEU:HD22	1:A:255:ASP:N	1.95	0.81
1:B:823:ASP:OD2	1:B:825:THR:HG23	1.81	0.81
1:A:43:LEU:HD12	1:A:44:ASP:HA	1.61	0.81
1:A:461:ASP:OD2	1:A:463:THR:HG23	1.81	0.81
1:A:823:ASP:OD2	1:A:825:THR:HG23	1.81	0.81
1:A:558:ILE:HD11	1:A:859:ILE:HD12	1.61	0.81
1:B:254:LEU:HD22	1:B:255:ASP:N	1.95	0.80
1:A:86:THR:N	1:A:89:SER:OG	2.15	0.80
1:B:236:LYS:O	1:B:246:SER:OG	1.99	0.80
1:A:236:LYS:O	1:A:246:SER:OG	1.99	0.80
1:A:443:ASN:HD21	1:A:449:THR:N	1.80	0.80
1:A:733:ARG:N	1:A:758:THR:O	2.15	0.79
1:B:461:ASP:OD2	1:B:463:THR:HG23	1.81	0.79
1:A:823:ASP:OD2	1:A:825:THR:CG2	2.30	0.79
1:B:263:ARG:NH2	1:B:557:ASN:ND2	2.31	0.78
1:B:443:ASN:HD21	1:B:449:THR:N	1.80	0.78
1:B:733:ARG:N	1:B:758:THR:O	2.15	0.78
1:B:82:ASP:O	1:B:98:LYS:N	2.15	0.78
1:B:823:ASP:OD2	1:B:825:THR:CG2	2.30	0.78
1:B:263:ARG:NE	1:B:557:ASN:HD21	1.80	0.78
1:A:263:ARG:NH2	1:A:557:ASN:ND2	2.31	0.78
1:A:660:ILE:HD12	1:A:693:ARG:HA	1.64	0.78
1:A:689:LYS:HA	1:A:689:LYS:CE	2.13	0.77
1:A:45:ARG:HG2	1:A:45:ARG:NH1	1.99	0.77
1:B:256:ILE:HD11	1:B:563:ARG:HH21	1.49	0.77
1:B:312:GLY:HA3	1:B:343:LYS:CB	2.13	0.77
1:A:312:GLY:CA	1:A:345:LEU:O	2.33	0.77
1:A:39:ASN:H	1:A:42:PHE:HD2	1.33	0.77
1:B:39:ASN:H	1:B:42:PHE:HD2	1.33	0.76
1:B:190:GLU:HG2	1:B:191:GLY:N	2.00	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:739:GLU:HA	1:B:744:PHE:CD2	2.20	0.76
1:A:493:GLY:O	1:A:496:ASP:HB3	1.85	0.76
1:A:739:GLU:HA	1:A:744:PHE:CD2	2.20	0.76
1:B:449:THR:HG22	1:B:450:TYR:H	1.51	0.76
1:A:832:LEU:N	1:A:832:LEU:HD12	2.01	0.75
1:A:190:GLU:HG2	1:A:191:GLY:N	2.00	0.75
1:A:256:ILE:HD11	1:A:563:ARG:HH21	1.49	0.75
1:B:36:ASN:HB2	3:B:1003:HOH:O	1.84	0.75
1:A:449:THR:HG22	1:A:450:TYR:H	1.52	0.75
1:A:324:ILE:CD1	1:A:324:ILE:H	1.99	0.75
1:A:690:MET:HA	1:A:690:MET:CE	2.17	0.75
1:B:385:PHE:CE2	1:B:408:ILE:CD1	2.51	0.75
1:A:582:TYR:O	1:A:586:MET:HG3	1.86	0.75
1:B:374:LEU:HD11	1:B:718:GLN:HA	1.69	0.75
1:B:582:TYR:O	1:B:586:MET:HG3	1.86	0.75
1:B:321:ILE:CA	1:B:324:ILE:HD13	2.16	0.74
1:B:832:LEU:HD12	1:B:832:LEU:N	2.01	0.74
1:A:254:LEU:CD2	1:A:255:ASP:H	1.97	0.74
1:A:263:ARG:NE	1:A:557:ASN:HD21	1.80	0.74
1:A:321:ILE:CA	1:A:324:ILE:HD13	2.17	0.74
1:A:689:LYS:HA	1:A:689:LYS:HE2	1.67	0.74
1:B:109:TYR:HD2	1:B:136:HIS:CD2	2.05	0.74
1:B:324:ILE:CD1	1:B:324:ILE:H	1.99	0.74
1:B:385:PHE:CD1	1:B:386:PRO:N	2.56	0.74
1:B:254:LEU:CD2	1:B:255:ASP:H	1.97	0.74
1:B:432:HIS:HA	1:B:451:ALA:HB1	1.70	0.74
1:A:517:ILE:HD11	1:A:590:ILE:HD12	1.69	0.73
1:A:381:LEU:HD23	1:A:383:LYS:HE3	1.69	0.73
1:B:424:GLU:OE1	1:B:625:ARG:NH1	2.21	0.73
1:A:374:LEU:HD11	1:A:718:GLN:HA	1.69	0.73
1:A:385:PHE:HE2	1:A:408:ILE:CD1	2.00	0.73
1:B:558:ILE:CD1	1:B:859:ILE:HD12	2.18	0.73
1:A:671:LYS:NZ	1:A:675:GLU:OE1	2.20	0.73
1:A:143:CYS:CB	1:A:159:PHE:CD1	2.72	0.73
1:B:143:CYS:CB	1:B:159:PHE:CD1	2.72	0.73
1:A:558:ILE:CD1	1:A:859:ILE:HD12	2.18	0.72
1:A:823:ASP:CG	1:A:825:THR:HG23	2.10	0.72
1:B:517:ILE:HD11	1:B:590:ILE:HD12	1.69	0.72
1:B:47:HIS:O	1:B:50:LEU:HB2	1.89	0.72
1:A:385:PHE:CD1	1:A:386:PRO:N	2.56	0.72
1:A:47:HIS:O	1:A:50:LEU:HB2	1.89	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:416:THR:HG22	1:B:419:GLU:CG	2.20	0.72
1:A:109:TYR:HD2	1:A:136:HIS:CD2	2.05	0.72
1:B:16:THR:OG1	1:B:104:GLU:HG2	1.90	0.72
1:A:432:HIS:HA	1:A:451:ALA:HB1	1.70	0.72
1:B:814:GLU:OE2	1:B:843:SER:OG	2.08	0.72
1:B:116:ARG:HG2	1:B:116:ARG:NH1	2.04	0.71
1:B:823:ASP:CG	1:B:825:THR:HG23	2.09	0.71
1:A:16:THR:OG1	1:A:104:GLU:HG2	1.90	0.71
1:A:475:HIS:CE1	1:A:477:ASN:HD22	2.05	0.71
1:B:660:ILE:HD12	1:B:693:ARG:HA	1.71	0.71
1:B:321:ILE:O	1:B:322:ASP:O	2.08	0.71
1:A:208:LEU:CD1	1:A:567:ILE:O	2.38	0.71
1:A:342:GLN:HG3	1:A:342:GLN:O	1.91	0.71
1:A:416:THR:HG23	1:A:419:GLU:HB2	1.72	0.71
1:B:72:GLY:HA3	1:B:173:THR:HB	1.73	0.71
1:A:814:GLU:OE2	1:A:843:SER:OG	2.08	0.70
1:B:475:HIS:CE1	1:B:477:ASN:HD22	2.05	0.70
1:A:321:ILE:O	1:A:322:ASP:O	2.08	0.70
1:A:72:GLY:HA3	1:A:173:THR:HB	1.73	0.70
1:B:82:ASP:O	1:B:98:LYS:HB2	1.90	0.70
1:A:133:VAL:HG21	1:A:139:VAL:CG1	2.22	0.70
1:B:45:ARG:HG2	1:B:45:ARG:NH1	1.99	0.70
1:B:133:VAL:HG21	1:B:139:VAL:CG1	2.22	0.70
1:B:20:LYS:HD3	1:B:102:ASP:OD1	1.93	0.69
1:B:321:ILE:HG22	1:B:324:ILE:HD13	1.74	0.69
1:B:572:ILE:O	1:B:576:THR:OG1	2.10	0.69
1:A:84:ILE:C	1:A:84:ILE:HD12	2.13	0.69
1:A:116:ARG:HG2	1:A:116:ARG:NH1	2.04	0.69
1:B:324:ILE:HD12	1:B:324:ILE:N	2.04	0.69
1:B:322:ASP:O	1:B:326:LYS:HB2	1.91	0.69
1:B:827:LYS:N	1:B:827:LYS:HD3	2.08	0.69
1:A:321:ILE:HG22	1:A:324:ILE:HD13	1.74	0.69
1:A:322:ASP:O	1:A:326:LYS:HB2	1.91	0.69
1:B:517:ILE:O	1:B:522:GLN:HG3	1.93	0.69
1:B:216:ARG:NH2	1:B:574:GLU:OE2	2.20	0.68
1:A:517:ILE:O	1:A:522:GLN:HG3	1.93	0.68
1:A:572:ILE:O	1:A:576:THR:OG1	2.11	0.68
1:B:273:LEU:HD22	1:B:777:THR:OG1	1.93	0.68
1:A:143:CYS:HB3	1:A:159:PHE:HD1	1.56	0.68
1:A:250:ILE:H	1:A:250:ILE:CD1	1.96	0.68
1:A:263:ARG:CZ	1:A:557:ASN:ND2	2.57	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:827:LYS:HD3	1:A:827:LYS:N	2.08	0.68
1:B:43:LEU:HD12	1:B:44:ASP:CA	2.24	0.68
1:B:660:ILE:CD1	1:B:693:ARG:HA	2.24	0.68
1:A:20:LYS:HD3	1:A:102:ASP:OD1	1.93	0.68
1:B:387:PRO:O	1:B:401:SER:OG	2.12	0.68
1:B:250:ILE:H	1:B:250:ILE:CD1	1.96	0.68
1:A:273:LEU:HD22	1:A:777:THR:OG1	1.93	0.68
1:B:263:ARG:CZ	1:B:557:ASN:ND2	2.57	0.68
1:A:50:LEU:HD21	1:A:81:GLU:O	1.93	0.67
1:B:671:LYS:NZ	1:B:675:GLU:OE1	2.20	0.67
1:B:381:LEU:HD23	1:B:383:LYS:HE3	1.69	0.67
1:A:43:LEU:HD12	1:A:44:ASP:CA	2.24	0.67
1:B:498:LEU:CD1	1:B:747:LEU:HD21	2.24	0.67
1:B:50:LEU:CD2	1:B:81:GLU:O	2.40	0.67
1:A:387:PRO:O	1:A:401:SER:OG	2.12	0.66
1:B:385:PHE:CD1	1:B:386:PRO:CA	2.78	0.66
1:B:64:THR:HA	1:B:72:GLY:HA2	1.78	0.66
1:B:566:LEU:O	1:B:573:PHE:HB2	1.94	0.66
1:A:660:ILE:CD1	1:A:693:ARG:HA	2.25	0.66
1:B:278:LYS:O	1:B:282:GLN:HG3	1.96	0.66
1:A:178:ARG:HH21	1:A:665:GLU:CD	1.99	0.66
1:B:178:ARG:HH21	1:B:665:GLU:CD	1.99	0.66
1:A:278:LYS:O	1:A:282:GLN:HG3	1.96	0.66
1:A:306:LEU:HD21	1:A:353:ILE:HD11	1.78	0.66
1:B:415:LEU:HD22	1:B:419:GLU:CG	2.25	0.66
1:A:385:PHE:CD1	1:A:386:PRO:CA	2.78	0.65
1:B:306:LEU:HD21	1:B:353:ILE:HD11	1.78	0.65
1:A:43:LEU:HD12	1:A:43:LEU:C	2.17	0.65
1:B:519:HIS:O	1:B:523:THR:OG1	2.14	0.65
1:A:273:LEU:CD2	1:A:777:THR:OG1	2.45	0.65
1:A:64:THR:HA	1:A:72:GLY:HA2	1.77	0.65
1:B:43:LEU:HD12	1:B:43:LEU:C	2.17	0.65
1:B:814:GLU:CD	1:B:843:SER:OG	2.35	0.65
1:A:28:MET:CE	1:A:33:LEU:HD11	2.26	0.64
1:A:71:LYS:NZ	1:A:180:GLU:OE1	2.30	0.64
1:A:814:GLU:CD	1:A:843:SER:OG	2.35	0.64
1:A:519:HIS:O	1:A:523:THR:OG1	2.14	0.64
1:A:338:ARG:HB2	1:A:346:LYS:HB3	1.80	0.64
1:B:71:LYS:NZ	1:B:180:GLU:OE1	2.30	0.64
1:B:273:LEU:CD2	1:B:777:THR:OG1	2.45	0.64
1:A:374:LEU:HD13	1:A:721:VAL:HG22	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:704:ILE:O	1:A:708:SER:OG	2.12	0.64
1:B:143:CYS:HB3	1:B:159:PHE:HD1	1.56	0.64
1:B:28:MET:CE	1:B:33:LEU:HD11	2.26	0.64
1:A:336:ILE:HG12	1:A:774:ILE:HD11	1.80	0.64
1:B:385:PHE:CD1	1:B:386:PRO:HA	2.33	0.64
1:B:448:LYS:O	1:B:732:SER:OG	2.16	0.64
1:A:814:GLU:HG3	1:A:842:PRO:HD2	1.80	0.64
1:B:374:LEU:HD13	1:B:721:VAL:HG22	1.79	0.63
1:A:385:PHE:CD1	1:A:386:PRO:HA	2.32	0.63
1:A:841:PHE:O	1:A:852:GLY:HA2	1.98	0.63
1:A:216:ARG:NH1	1:A:581:LYS:HG3	2.14	0.63
1:A:312:GLY:CA	1:A:343:LYS:CB	2.76	0.63
1:B:250:ILE:HD12	1:B:250:ILE:N	2.04	0.63
1:A:206:ASN:OD1	1:A:206:ASN:N	2.32	0.63
1:A:448:LYS:O	1:A:732:SER:OG	2.16	0.63
1:A:103:TYR:OH	1:A:108:GLY:O	2.17	0.63
1:A:39:ASN:ND2	1:A:40:ALA:H	1.96	0.63
1:A:571:GLY:O	1:A:575:ILE:HG12	1.99	0.63
1:B:336:ILE:HG12	1:B:774:ILE:HD11	1.80	0.63
1:A:324:ILE:HD12	1:A:324:ILE:N	2.04	0.62
1:A:235:ARG:HB2	1:A:245:GLU:OE2	1.99	0.62
1:A:660:ILE:HD11	1:A:693:ARG:HG2	1.81	0.62
1:B:39:ASN:ND2	1:B:40:ALA:H	1.96	0.62
1:B:841:PHE:O	1:B:852:GLY:HA2	1.98	0.62
1:B:814:GLU:HG3	1:B:842:PRO:HD2	1.80	0.62
1:B:206:ASN:OD1	1:B:206:ASN:N	2.32	0.62
1:A:43:LEU:HD12	1:A:44:ASP:N	2.15	0.62
1:A:241:ASP:OD1	1:A:243:GLN:HG2	2.00	0.62
1:B:43:LEU:HD12	1:B:44:ASP:N	2.15	0.62
1:B:416:THR:N	1:B:419:GLU:HB2	2.14	0.62
1:B:235:ARG:HB2	1:B:245:GLU:OE2	1.99	0.61
1:A:250:ILE:HD12	1:A:250:ILE:N	2.04	0.61
1:A:405:LYS:O	1:A:409:GLU:HB3	2.00	0.61
1:B:103:TYR:OH	1:B:108:GLY:O	2.17	0.61
1:B:241:ASP:OD1	1:B:243:GLN:HG2	2.00	0.61
1:B:321:ILE:CA	1:B:324:ILE:CD1	2.66	0.61
1:B:689:LYS:HE2	1:B:689:LYS:CA	2.21	0.61
1:A:693:ARG:O	1:A:697:VAL:HG23	2.01	0.61
1:B:162:ASN:O	1:B:546:LYS:NZ	2.35	0.60
1:A:216:ARG:NH1	1:A:581:LYS:HE3	2.16	0.60
1:A:162:ASN:O	1:A:546:LYS:NZ	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:126:LYS:O	1:B:143:CYS:O	2.19	0.60
1:B:571:GLY:O	1:B:575:ILE:HG12	2.01	0.60
1:A:402:THR:HG21	1:A:485:SER:HB2	1.84	0.60
1:A:126:LYS:O	1:A:143:CYS:O	2.19	0.60
1:B:374:LEU:HB2	1:B:721:VAL:CG2	2.28	0.60
1:A:84:ILE:HD12	1:A:84:ILE:O	2.01	0.60
1:A:214:ASN:OD1	1:A:214:ASN:N	2.35	0.60
1:A:374:LEU:HB2	1:A:721:VAL:CG2	2.28	0.60
1:B:558:ILE:HD13	1:B:859:ILE:HA	1.84	0.60
1:A:229:ARG:NH1	1:A:680:ASP:OD2	2.26	0.59
1:A:447:THR:C	1:A:448:LYS:HD2	2.22	0.59
1:B:315:LEU:HD21	1:B:345:LEU:HD11	1.84	0.59
1:B:593:ASN:CB	1:B:594:HIS:CD2	2.85	0.59
1:A:92:ALA:HA	1:A:267:LEU:HD21	1.84	0.59
1:A:593:ASN:CB	1:A:594:HIS:CD2	2.85	0.59
1:A:312:GLY:HA3	1:A:343:LYS:CB	2.33	0.59
1:A:832:LEU:HD12	1:A:832:LEU:H	1.68	0.59
1:B:65:ASP:CB	1:B:73:LYS:HA	2.25	0.59
1:B:447:THR:C	1:B:448:LYS:HD2	2.22	0.59
1:B:704:ILE:O	1:B:708:SER:OG	2.12	0.59
1:A:366:PHE:HZ	1:A:506:VAL:HG21	1.68	0.59
1:B:725:LEU:HB3	1:B:726:PRO:HD3	1.85	0.59
1:B:366:PHE:HZ	1:B:506:VAL:HG21	1.68	0.59
1:A:494:VAL:O	1:A:497:SER:HB2	2.03	0.58
1:B:402:THR:HG21	1:B:485:SER:HB2	1.84	0.58
1:B:312:GLY:CA	1:B:343:LYS:CB	2.80	0.58
1:B:581:LYS:CE	3:B:1004:HOH:O	2.51	0.58
1:B:832:LEU:HD12	1:B:832:LEU:H	1.68	0.58
1:A:245:GLU:HG3	3:A:1005:HOH:O	2.03	0.58
1:B:133:VAL:HG21	1:B:139:VAL:HG13	1.85	0.58
1:B:436:MET:HE2	1:B:436:MET:HA	1.83	0.58
1:B:764:GLN:N	1:B:764:GLN:OE1	2.37	0.58
1:A:436:MET:HA	1:A:436:MET:HE2	1.85	0.58
1:A:558:ILE:HD13	1:A:859:ILE:HA	1.84	0.58
1:B:166:LEU:HB2	1:B:169:GLU:HG2	1.85	0.58
1:A:133:VAL:HG21	1:A:139:VAL:HG13	1.85	0.58
1:B:229:ARG:NH1	1:B:680:ASP:OD2	2.26	0.58
1:B:654:TYR:CD1	1:B:660:ILE:HG12	2.39	0.58
1:A:206:ASN:HB3	1:A:218:VAL:HG13	1.85	0.58
1:A:523:THR:OG1	1:A:524:HIS:N	2.35	0.58
1:A:763:LEU:HB3	1:A:764:GLN:OE1	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:848:VAL:HG22	1:A:848:VAL:O	2.03	0.58
1:B:475:HIS:HE1	1:B:477:ASN:ND2	1.96	0.58
1:B:593:ASN:CB	1:B:594:HIS:HD2	2.17	0.58
1:A:654:TYR:CD1	1:A:660:ILE:HG12	2.39	0.58
1:B:321:ILE:HG21	1:B:344:PHE:CD2	2.39	0.58
1:A:417:VAL:HG23	1:A:418:GLU:N	2.18	0.58
1:B:33:LEU:O	1:B:265:GLY:HA3	2.04	0.58
1:A:65:ASP:CB	1:A:73:LYS:HA	2.25	0.57
1:A:216:ARG:NH2	1:A:574:GLU:OE2	2.36	0.57
1:B:206:ASN:HB3	1:B:218:VAL:HG13	1.85	0.57
1:B:848:VAL:HG22	1:B:848:VAL:O	2.03	0.57
1:A:166:LEU:HB2	1:A:169:GLU:HG2	1.85	0.57
1:B:763:LEU:HB3	1:B:764:GLN:OE1	2.04	0.57
1:B:210:VAL:HB	1:B:213:LYS:O	2.04	0.57
1:B:379:ILE:O	1:B:609:ARG:HD2	2.05	0.57
1:A:33:LEU:O	1:A:265:GLY:HA3	2.04	0.57
1:A:725:LEU:HB3	1:A:726:PRO:HD3	1.85	0.57
1:B:594:HIS:CD2	1:B:594:HIS:N	2.73	0.57
1:A:379:ILE:O	1:A:609:ARG:HD2	2.04	0.57
1:A:764:GLN:OE1	1:A:764:GLN:N	2.37	0.57
1:A:469:ILE:HG13	1:A:499:TRP:CZ3	2.40	0.57
1:B:288:LEU:HB3	1:B:763:LEU:CD1	2.35	0.57
1:A:288:LEU:HB3	1:A:763:LEU:CD1	2.35	0.57
1:A:594:HIS:CD2	1:A:594:HIS:N	2.73	0.57
1:A:814:GLU:HG2	1:A:841:PHE:CZ	2.40	0.57
1:B:469:ILE:HG13	1:B:499:TRP:CZ3	2.40	0.57
1:A:706:VAL:HG13	1:A:710:LEU:HD23	1.87	0.56
1:B:109:TYR:CD2	1:B:136:HIS:CD2	2.92	0.56
1:B:117:ASN:ND2	1:B:123:PHE:CE1	2.73	0.56
1:B:706:VAL:HG13	1:B:710:LEU:HD23	1.87	0.56
1:A:240:GLU:CD	1:A:240:GLU:H	2.09	0.56
1:A:321:ILE:CA	1:A:324:ILE:CD1	2.66	0.56
1:A:593:ASN:CB	1:A:594:HIS:HD2	2.17	0.56
1:B:181:GLU:OE2	1:B:198:ARG:NH2	2.28	0.56
1:B:814:GLU:HG2	1:B:841:PHE:CZ	2.40	0.56
1:A:283:PHE:CE2	1:A:327:ASN:HB3	2.40	0.56
1:A:607:LYS:HE3	1:A:614:GLU:OE1	2.05	0.56
1:B:453:ARG:NH1	1:B:470:GLU:OE2	2.37	0.56
1:A:230:ARG:HD3	1:A:563:ARG:CZ	2.36	0.56
1:B:523:THR:OG1	1:B:524:HIS:N	2.35	0.56
1:B:283:PHE:CE2	1:B:327:ASN:HB3	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:ASN:OD1	1:A:31:ASN:N	2.33	0.56
1:B:207:ASP:O	1:B:247:ARG:HD2	2.06	0.56
1:B:230:ARG:HD3	1:B:563:ARG:CZ	2.36	0.56
1:B:572:ILE:HG21	1:B:771:LEU:HD13	1.88	0.56
1:A:117:ASN:ND2	1:A:123:PHE:CE1	2.73	0.56
1:B:114:LEU:HD22	1:B:156:ASP:HB2	1.88	0.56
1:B:263:ARG:NH2	1:B:557:ASN:HD22	2.03	0.56
1:B:505:PHE:HZ	1:B:734:GLN:O	1.89	0.56
1:A:50:LEU:CD2	1:A:81:GLU:O	2.54	0.56
1:A:282:GLN:O	1:A:286:PRO:HG2	2.05	0.56
1:B:282:GLN:O	1:B:286:PRO:HG2	2.05	0.56
1:A:35:PHE:O	1:A:269:MET:CG	2.51	0.55
1:B:581:LYS:HE3	3:B:1004:HOH:O	2.06	0.55
1:B:742:PRO:O	1:B:745:GLU:HB2	2.06	0.55
1:A:744:PHE:HD1	1:A:744:PHE:O	1.90	0.55
1:B:385:PHE:HE2	1:B:408:ILE:HD13	1.65	0.55
1:A:146:TRP:HE1	1:A:264:PHE:HD2	1.54	0.55
1:A:742:PRO:O	1:A:745:GLU:HB2	2.06	0.55
1:B:823:ASP:CG	1:B:825:THR:HG22	2.00	0.55
1:A:374:LEU:CD1	1:A:718:GLN:HA	2.37	0.55
1:B:415:LEU:CD1	1:B:420:ALA:HA	2.36	0.55
1:B:146:TRP:HE1	1:B:264:PHE:HD2	1.53	0.55
1:B:240:GLU:H	1:B:240:GLU:CD	2.09	0.55
1:B:689:LYS:HA	1:B:689:LYS:CE	2.25	0.55
1:A:505:PHE:HZ	1:A:734:GLN:O	1.89	0.55
1:B:241:ASP:OD1	1:B:243:GLN:N	2.39	0.55
1:B:744:PHE:HD1	1:B:744:PHE:O	1.90	0.55
1:A:114:LEU:HD22	1:A:156:ASP:HB2	1.88	0.55
1:B:202:TYR:HE2	1:B:672:GLU:OE1	1.90	0.55
1:A:109:TYR:HD2	1:A:136:HIS:HD2	1.51	0.54
1:A:572:ILE:HG21	1:A:771:LEU:HD13	1.87	0.54
1:A:202:TYR:HE2	1:A:672:GLU:OE1	1.90	0.54
1:A:207:ASP:O	1:A:247:ARG:HD2	2.06	0.54
1:A:494:VAL:O	1:A:497:SER:N	2.39	0.54
1:B:366:PHE:CZ	1:B:506:VAL:HG21	2.43	0.54
1:B:693:ARG:O	1:B:697:VAL:HG23	2.07	0.54
1:A:28:MET:HE1	1:A:33:LEU:CD1	2.34	0.54
1:A:39:ASN:HD22	1:A:40:ALA:H	1.56	0.54
1:B:31:ASN:N	1:B:31:ASN:OD1	2.33	0.54
1:B:416:THR:H	1:B:419:GLU:HB2	1.73	0.54
1:A:453:ARG:NH1	1:A:470:GLU:OE2	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:181:GLU:OE2	1:A:198:ARG:NH2	2.28	0.54
1:A:443:ASN:O	1:A:448:LYS:HE3	2.08	0.54
1:A:739:GLU:HA	1:A:744:PHE:HD2	1.71	0.54
1:B:321:ILE:CG2	1:B:324:ILE:HD13	2.38	0.54
1:A:520:TRP:CZ2	1:A:567:ILE:HD13	2.43	0.54
1:A:28:MET:CE	1:A:33:LEU:HD21	2.34	0.53
1:A:366:PHE:CZ	1:A:506:VAL:HG21	2.43	0.53
1:A:498:LEU:CG	1:A:736:MET:HE1	2.38	0.53
1:A:607:LYS:CE	1:A:614:GLU:OE2	2.56	0.53
1:A:216:ARG:CZ	1:A:581:LYS:HG3	2.39	0.53
1:A:689:LYS:HA	1:A:689:LYS:HE3	1.89	0.53
1:B:21:VAL:HG13	1:B:131:GLU:O	2.09	0.53
1:B:415:LEU:HD13	1:B:419:GLU:HB3	1.90	0.53
1:A:91:THR:O	1:A:92:ALA:HB3	2.08	0.53
1:A:821:ASN:OD1	1:A:829:ARG:HG2	2.08	0.53
1:B:520:TRP:CZ2	1:B:567:ILE:HD13	2.43	0.53
1:B:821:ASN:OD1	1:B:829:ARG:HG2	2.08	0.53
1:A:263:ARG:CZ	1:A:557:ASN:HD22	2.22	0.53
1:B:160:PHE:HB3	1:B:541:LEU:HD21	1.91	0.53
1:A:494:VAL:HG13	1:A:495:TYR:N	2.23	0.53
1:A:607:LYS:HE3	1:A:614:GLU:OE2	2.08	0.53
1:B:190:GLU:HG2	1:B:191:GLY:H	1.74	0.53
1:B:374:LEU:CD1	1:B:718:GLN:HA	2.37	0.53
1:B:634:ASP:CG	1:B:829:ARG:NH2	2.61	0.53
1:A:21:VAL:HG13	1:A:131:GLU:O	2.09	0.53
1:A:321:ILE:CG2	1:A:324:ILE:HD13	2.38	0.53
1:B:39:ASN:HD22	1:B:40:ALA:H	1.56	0.53
1:B:90:LEU:O	1:B:90:LEU:HD12	2.09	0.53
1:B:416:THR:HG22	1:B:419:GLU:OE1	2.09	0.53
1:A:160:PHE:HB3	1:A:541:LEU:HD21	1.91	0.53
1:B:491:GLY:O	1:B:496:ASP:HB2	2.09	0.53
1:B:595:TRP:O	1:B:681:LYS:HE2	2.09	0.53
1:B:807:GLY:O	1:B:811:LYS:HG3	2.09	0.53
1:B:28:MET:CE	1:B:33:LEU:CD1	2.87	0.52
1:B:417:VAL:HG23	1:B:418:GLU:OE2	2.08	0.52
1:A:111:GLY:HA3	1:A:174:LEU:HD11	1.91	0.52
1:A:263:ARG:NH2	1:A:557:ASN:HD22	2.03	0.52
1:B:443:ASN:O	1:B:448:LYS:HE3	2.08	0.52
1:B:28:MET:HE1	1:B:33:LEU:CD1	2.35	0.52
1:B:207:ASP:O	1:B:247:ARG:CD	2.58	0.52
1:B:263:ARG:CZ	1:B:557:ASN:HD22	2.22	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:424:GLU:CD	1:B:625:ARG:HH11	2.13	0.52
1:A:28:MET:CE	1:A:33:LEU:CD1	2.86	0.52
1:A:218:VAL:O	1:A:219:LEU:HD23	2.09	0.52
1:A:595:TRP:O	1:A:681:LYS:HE2	2.09	0.52
1:A:634:ASP:OD1	1:A:820:ARG:NH2	2.43	0.52
1:B:111:GLY:HA3	1:B:174:LEU:HD11	1.91	0.52
1:A:109:TYR:CD2	1:A:136:HIS:CD2	2.92	0.52
1:A:593:ASN:HB2	1:A:594:HIS:HD2	1.75	0.52
1:B:109:TYR:HD2	1:B:136:HIS:HD2	1.51	0.52
1:B:28:MET:CE	1:B:33:LEU:HD21	2.34	0.52
1:B:534:THR:HG23	1:B:538:LEU:HD12	1.92	0.52
1:B:825:THR:O	1:B:827:LYS:NZ	2.29	0.52
1:A:241:ASP:OD1	1:A:243:GLN:N	2.40	0.52
1:B:218:VAL:O	1:B:219:LEU:HD23	2.09	0.52
1:A:190:GLU:HG2	1:A:191:GLY:H	1.74	0.52
1:A:317:ASN:HD22	1:A:319:ALA:HB3	1.75	0.52
1:B:35:PHE:O	1:B:269:MET:CG	2.51	0.52
1:B:68:ASN:HD21	1:B:74:LEU:HD11	1.73	0.52
1:A:207:ASP:O	1:A:247:ARG:CD	2.58	0.52
1:A:807:GLY:O	1:A:811:LYS:HG3	2.09	0.52
1:A:312:GLY:C	1:A:343:LYS:CB	2.79	0.51
1:A:717:GLY:C	1:A:720:PRO:HD2	2.31	0.51
1:B:565:ILE:HD11	1:B:566:LEU:HD12	1.89	0.51
1:A:254:LEU:HD13	1:A:255:ASP:O	2.10	0.51
1:A:634:ASP:CG	1:A:829:ARG:NH2	2.61	0.51
1:B:317:ASN:HD22	1:B:319:ALA:HB3	1.75	0.51
1:A:825:THR:O	1:A:827:LYS:NZ	2.29	0.51
1:B:634:ASP:OD1	1:B:820:ARG:NH2	2.43	0.51
1:A:33:LEU:HB3	1:A:265:GLY:HA3	1.92	0.51
1:B:254:LEU:HD13	1:B:255:ASP:O	2.10	0.51
1:A:534:THR:HG23	1:A:538:LEU:HD12	1.92	0.51
1:A:832:LEU:N	1:A:832:LEU:CD1	2.73	0.51
1:B:717:GLY:C	1:B:720:PRO:HD2	2.31	0.51
1:A:408:ILE:HB	1:A:467:LEU:HD13	1.93	0.51
1:B:33:LEU:HB3	1:B:265:GLY:HA3	1.92	0.51
1:B:739:GLU:HA	1:B:744:PHE:HD2	1.71	0.51
1:B:832:LEU:N	1:B:832:LEU:CD1	2.73	0.51
1:A:109:TYR:CD2	1:A:136:HIS:HD2	2.28	0.51
1:A:89:SER:HA	1:A:94:GLU:O	2.11	0.51
1:B:65:ASP:OD2	1:B:68:ASN:HB2	2.11	0.51
1:B:87:ILE:O	1:B:91:THR:HG23	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:369:GLU:O	1:B:373:GLY:HA3	2.11	0.51
1:B:593:ASN:HB2	1:B:594:HIS:HD2	1.75	0.51
1:A:332:MET:HA	1:A:335:GLU:HG3	1.94	0.50
1:A:369:GLU:O	1:A:373:GLY:HA3	2.11	0.50
1:B:164:THR:OG1	1:B:796:GLU:OE2	2.29	0.50
1:B:281:ALA:HB2	1:B:572:ILE:HD11	1.92	0.50
1:A:593:ASN:HB3	1:A:594:HIS:CD2	2.47	0.50
1:B:179:GLU:O	1:B:183:VAL:HG23	2.11	0.50
1:B:385:PHE:CD1	1:B:385:PHE:C	2.85	0.50
1:A:179:GLU:O	1:A:183:VAL:HG23	2.11	0.50
1:A:475:HIS:HE1	1:A:477:ASN:ND2	1.96	0.50
1:A:690:MET:CE	1:A:690:MET:CA	2.86	0.50
1:B:251:THR:O	1:B:251:THR:OG1	2.28	0.50
1:B:374:LEU:HD11	1:B:718:GLN:CA	2.38	0.50
1:A:416:THR:CG2	1:A:419:GLU:HB2	2.41	0.50
1:A:65:ASP:OD2	1:A:68:ASN:HB2	2.11	0.50
1:A:164:THR:OG1	1:A:796:GLU:OE2	2.29	0.50
1:B:263:ARG:NE	1:B:557:ASN:HD22	2.08	0.50
1:B:330:LEU:HD12	1:B:330:LEU:C	2.32	0.50
1:B:416:THR:CG2	1:B:419:GLU:HB2	2.41	0.50
1:B:494:VAL:O	1:B:497:SER:N	2.44	0.50
1:A:284:ILE:CD1	1:A:337:PHE:CE2	2.95	0.50
1:A:578:PHE:C	1:A:578:PHE:CD2	2.85	0.50
1:B:416:THR:HG22	1:B:419:GLU:CB	2.40	0.50
1:B:647:ARG:NH1	1:B:694:GLU:OE1	2.35	0.50
1:B:372:ALA:HB2	1:B:630:PRO:HG2	1.94	0.49
1:A:374:LEU:HD11	1:A:718:GLN:CA	2.39	0.49
1:B:344:PHE:CD1	1:B:344:PHE:C	2.85	0.49
1:A:412:LEU:O	1:A:413:ASP:HB2	2.10	0.49
1:A:417:VAL:CG2	1:A:418:GLU:N	2.74	0.49
1:B:352:VAL:HB	1:B:721:VAL:HA	1.94	0.49
1:B:408:ILE:HG22	1:B:467:LEU:HB3	1.94	0.49
1:B:593:ASN:HB3	1:B:594:HIS:CD2	2.47	0.49
1:A:207:ASP:O	1:A:247:ARG:CG	2.61	0.49
1:B:109:TYR:CD2	1:B:136:HIS:HD2	2.28	0.49
1:B:660:ILE:HD11	1:B:693:ARG:HG2	1.92	0.49
1:B:844:SER:OG	1:B:845:GLU:N	2.45	0.49
1:A:352:VAL:HB	1:A:721:VAL:HA	1.94	0.49
1:B:284:ILE:CD1	1:B:337:PHE:CE2	2.95	0.49
1:B:524:HIS:O	1:B:559:ASN:ND2	2.44	0.49
1:A:372:ALA:HB2	1:A:630:PRO:HG2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:837:TYR:HE2	1:A:839:LEU:HD12	1.77	0.49
1:B:332:MET:HA	1:B:335:GLU:HG3	1.94	0.49
1:B:578:PHE:C	1:B:578:PHE:CD2	2.85	0.49
1:A:63:VAL:HG12	1:A:64:THR:N	2.27	0.49
1:A:470:GLU:HB2	1:A:487:VAL:HG22	1.95	0.49
1:A:498:LEU:HD13	1:A:747:LEU:HD21	1.95	0.49
1:A:602:LEU:HD22	1:A:705:TRP:CH2	2.47	0.49
1:B:660:ILE:HG23	1:B:666:LEU:HD23	1.95	0.49
1:A:119:HIS:CE1	1:A:120:PHE:CD2	3.01	0.49
1:A:385:PHE:CE2	1:A:408:ILE:CD1	2.87	0.49
1:A:646:VAL:O	1:A:650:ILE:HG12	2.13	0.49
1:B:63:VAL:HG12	1:B:64:THR:N	2.27	0.49
1:A:844:SER:OG	1:A:845:GLU:N	2.45	0.49
1:B:493:GLY:O	1:B:496:ASP:HB3	2.13	0.49
1:B:562:ALA:HA	1:B:566:LEU:HB2	1.95	0.49
1:B:778:HIS:NE2	1:B:851:ARG:O	2.45	0.49
1:A:323:SER:OG	1:A:324:ILE:HD12	2.13	0.48
1:A:385:PHE:CD1	1:A:385:PHE:C	2.85	0.48
1:B:119:HIS:CE1	1:B:120:PHE:CD2	3.01	0.48
1:B:164:THR:HG23	1:B:546:LYS:CE	2.43	0.48
1:B:323:SER:OG	1:B:324:ILE:HD12	2.13	0.48
1:B:411:ASN:C	1:B:412:LEU:HD23	2.33	0.48
1:B:806:PHE:O	1:B:810:VAL:HG23	2.13	0.48
1:A:164:THR:HG23	1:A:546:LYS:CE	2.43	0.48
1:B:715:ASN:ND2	1:B:775:LEU:O	2.46	0.48
1:B:572:ILE:O	1:B:572:ILE:HG22	2.12	0.48
1:A:806:PHE:O	1:A:810:VAL:HG23	2.13	0.48
1:B:602:LEU:HD22	1:B:705:TRP:CH2	2.47	0.48
1:A:615:ASP:O	1:A:618:ALA:HB3	2.13	0.48
1:B:470:GLU:HB2	1:B:487:VAL:HG22	1.95	0.48
1:B:646:VAL:O	1:B:650:ILE:HG12	2.13	0.48
1:B:837:TYR:HE2	1:B:839:LEU:HD12	1.77	0.48
1:A:28:MET:HE2	1:A:33:LEU:HD22	1.92	0.48
1:A:517:ILE:CD1	1:A:590:ILE:HD12	2.42	0.48
1:A:524:HIS:O	1:A:559:ASN:ND2	2.44	0.48
1:A:715:ASN:ND2	1:A:775:LEU:O	2.46	0.48
1:B:207:ASP:O	1:B:247:ARG:CG	2.60	0.48
1:B:469:ILE:HG13	1:B:499:TRP:CH2	2.48	0.48
1:B:615:ASP:O	1:B:618:ALA:HB3	2.13	0.48
1:A:469:ILE:HG13	1:A:499:TRP:CH2	2.48	0.48
1:A:660:ILE:HG23	1:A:666:LEU:HD23	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:283:PHE:C	1:A:286:PRO:HD2	2.34	0.48
1:A:562:ALA:HA	1:A:566:LEU:HB2	1.96	0.48
1:B:385:PHE:HD1	1:B:385:PHE:C	2.17	0.48
1:B:516:LEU:HD21	1:B:573:PHE:HE1	1.79	0.48
1:B:692:THR:OG1	1:B:695:GLU:CG	2.53	0.48
1:B:27:LEU:HD22	1:B:123:PHE:CD2	2.49	0.48
1:B:566:LEU:O	1:B:573:PHE:CB	2.61	0.48
1:A:711:HIS:CE1	1:A:859:ILE:O	2.67	0.47
1:B:612:ALA:HB2	1:B:624:LEU:HD23	1.96	0.47
1:B:706:VAL:HA	1:B:710:LEU:HB3	1.97	0.47
1:B:711:HIS:CE1	1:B:859:ILE:O	2.67	0.47
1:A:405:LYS:HE2	1:A:417:VAL:CG2	2.44	0.47
1:A:550:PRO:HG2	1:A:788:ARG:CZ	2.44	0.47
1:B:413:ASP:N	1:B:413:ASP:OD1	2.46	0.47
1:A:86:THR:O	1:A:89:SER:N	2.47	0.47
1:A:321:ILE:O	1:A:323:SER:N	2.47	0.47
1:A:39:ASN:ND2	1:A:40:ALA:N	2.62	0.47
1:A:58:LEU:HD13	1:A:110:PRO:HB3	1.96	0.47
1:A:71:LYS:O	1:A:173:THR:C	2.52	0.47
1:A:607:LYS:HE3	1:A:614:GLU:CD	2.35	0.47
1:B:374:LEU:HD13	1:B:721:VAL:CG2	2.44	0.47
1:B:517:ILE:CD1	1:B:590:ILE:HD12	2.42	0.47
1:B:226:PRO:CG	1:B:592:LYS:HB2	2.45	0.47
1:B:698:GLU:O	1:B:702:ILE:HG13	2.15	0.47
1:B:725:LEU:HB3	1:B:726:PRO:CD	2.44	0.47
1:A:27:LEU:HD22	1:A:123:PHE:CD2	2.49	0.47
1:A:119:HIS:CE1	1:A:120:PHE:CE2	3.03	0.47
1:A:306:LEU:CD2	1:A:353:ILE:HD11	2.44	0.47
1:A:602:LEU:HB3	1:A:603:PRO:HD3	1.97	0.47
1:A:605:GLU:OE1	1:A:609:ARG:NE	2.39	0.47
1:A:725:LEU:HB3	1:A:726:PRO:CD	2.44	0.47
1:B:475:HIS:ND1	1:B:476:PRO:HD2	2.30	0.47
1:B:550:PRO:HG2	1:B:788:ARG:CZ	2.44	0.47
1:B:579:PRO:HB2	1:B:583:ALA:HA	1.97	0.47
1:B:142:ILE:HG23	1:B:142:ILE:O	2.15	0.47
1:B:334:LYS:HG2	1:B:339:THR:HG23	1.96	0.47
1:A:226:PRO:CG	1:A:592:LYS:HB2	2.45	0.47
1:A:475:HIS:CE1	1:A:476:PRO:HD2	2.50	0.47
1:A:698:GLU:O	1:A:702:ILE:HG13	2.15	0.47
1:B:365:GLU:CD	1:B:368:ARG:HE	2.18	0.47
1:A:475:HIS:ND1	1:A:476:PRO:HD2	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:527:ILE:HD13	1:B:527:ILE:HA	1.74	0.47
1:A:377:VAL:HA	1:A:609:ARG:NH2	2.30	0.46
1:A:612:ALA:HB2	1:A:624:LEU:HD23	1.96	0.46
1:B:475:HIS:CE1	1:B:476:PRO:HD2	2.50	0.46
1:A:413:ASP:OD2	1:A:459:LYS:HE3	2.15	0.46
1:A:579:PRO:HB2	1:A:583:ALA:HA	1.97	0.46
1:A:643:GLU:OE1	1:A:698:GLU:OE1	2.33	0.46
1:B:283:PHE:C	1:B:286:PRO:HD2	2.34	0.46
1:B:628:ASP:OD2	1:B:826:LEU:HB3	2.15	0.46
1:B:643:GLU:OE1	1:B:698:GLU:OE1	2.33	0.46
1:B:838:THR:HB	1:B:851:ARG:HB3	1.98	0.46
1:A:567:ILE:HD12	1:A:584:MET:HE1	1.97	0.46
1:A:847:GLY:O	1:A:849:THR:HG23	2.16	0.46
1:B:415:LEU:HD12	1:B:420:ALA:HA	1.97	0.46
1:B:796:GLU:OE2	1:B:796:GLU:N	2.49	0.46
1:A:352:VAL:O	1:A:833:VAL:HG11	2.16	0.46
1:A:706:VAL:HA	1:A:710:LEU:HB3	1.96	0.46
1:B:58:LEU:HD13	1:B:110:PRO:HB3	1.96	0.46
1:B:83:TRP:HB2	1:B:96:ALA:O	2.15	0.46
1:B:377:VAL:HA	1:B:609:ARG:NH2	2.30	0.46
1:B:593:ASN:HB2	1:B:594:HIS:CD2	2.51	0.46
1:A:25:VAL:HG22	1:A:128:LEU:HD13	1.98	0.46
1:A:365:GLU:CD	1:A:368:ARG:HE	2.18	0.46
1:A:374:LEU:HD13	1:A:721:VAL:CG2	2.44	0.46
1:A:447:THR:HG23	1:A:731:ILE:HG23	1.98	0.46
1:A:565:ILE:HD11	1:A:566:LEU:HD12	1.89	0.46
1:B:254:LEU:HD13	1:B:255:ASP:N	2.31	0.46
1:B:447:THR:HG23	1:B:731:ILE:HG23	1.98	0.46
1:A:508:VAL:HG13	1:A:730:THR:O	2.16	0.46
1:A:164:THR:HG23	1:A:546:LYS:HD2	1.98	0.46
1:B:28:MET:HE2	1:B:33:LEU:HD22	1.92	0.46
1:B:416:THR:HG22	1:B:419:GLU:HB2	1.97	0.46
1:B:164:THR:HG23	1:B:546:LYS:HD2	1.98	0.46
1:B:514:HIS:HA	1:B:518:SER:HB2	1.98	0.46
1:B:602:LEU:HB3	1:B:603:PRO:HD3	1.97	0.46
1:A:142:ILE:HG23	1:A:142:ILE:O	2.15	0.46
1:A:443:ASN:ND2	1:A:448:LYS:HA	2.31	0.46
1:A:628:ASP:OD2	1:A:826:LEU:HB3	2.15	0.46
1:A:796:GLU:OE2	1:A:796:GLU:N	2.49	0.46
1:A:827:LYS:HD3	1:A:827:LYS:H	1.80	0.46
1:B:469:ILE:HD13	1:B:506:VAL:HG11	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:508:VAL:HG13	1:B:730:THR:O	2.16	0.46
1:A:514:HIS:HA	1:A:518:SER:HB2	1.98	0.46
1:A:838:THR:HB	1:A:851:ARG:HB3	1.98	0.46
1:B:415:LEU:CG	1:B:419:GLU:HB3	2.46	0.46
1:B:567:ILE:HD12	1:B:584:MET:HE1	1.98	0.46
1:A:68:ASN:HD21	1:A:74:LEU:HD11	1.72	0.45
1:A:256:ILE:HD11	1:A:563:ARG:NH2	2.25	0.45
1:A:593:ASN:HB2	1:A:594:HIS:CD2	2.51	0.45
1:A:655:LYS:O	1:A:693:ARG:NH1	2.49	0.45
1:B:119:HIS:CE1	1:B:120:PHE:CE2	3.03	0.45
1:B:352:VAL:O	1:B:833:VAL:HG11	2.15	0.45
1:A:633:VAL:HG11	1:A:829:ARG:HH12	1.82	0.45
1:B:25:VAL:HG22	1:B:128:LEU:HD13	1.98	0.45
1:B:71:LYS:O	1:B:173:THR:C	2.52	0.45
1:B:847:GLY:O	1:B:849:THR:HG23	2.16	0.45
1:B:39:ASN:ND2	1:B:40:ALA:N	2.62	0.45
1:B:124:LEU:HD12	1:B:125:LEU:N	2.32	0.45
1:A:124:LEU:HD12	1:A:125:LEU:N	2.32	0.45
1:B:82:ASP:H	1:B:98:LYS:HB2	1.80	0.45
1:B:288:LEU:HB3	1:B:763:LEU:HD11	1.98	0.45
1:A:258:VAL:HG22	1:A:263:ARG:NH1	2.31	0.45
1:A:469:ILE:HD13	1:A:506:VAL:HG11	1.97	0.45
1:A:288:LEU:HB3	1:A:763:LEU:HD11	1.98	0.45
1:A:317:ASN:ND2	1:A:319:ALA:HB3	2.32	0.45
1:A:491:GLY:O	1:A:496:ASP:HB2	2.17	0.45
1:A:254:LEU:HD13	1:A:255:ASP:N	2.31	0.45
1:A:778:HIS:NE2	1:A:851:ARG:O	2.45	0.45
1:A:698:GLU:HA	1:A:701:THR:HG22	1.99	0.45
1:B:59:VAL:HG12	1:B:60:SER:N	2.32	0.45
1:B:258:VAL:HG22	1:B:263:ARG:NH1	2.31	0.45
1:B:317:ASN:ND2	1:B:319:ALA:HB3	2.32	0.45
1:B:691:GLN:HE21	1:B:691:GLN:HB3	1.60	0.45
1:A:371:LEU:HB3	1:A:629:TYR:CD2	2.52	0.45
1:A:634:ASP:O	1:A:638:VAL:HG23	2.17	0.45
1:A:837:TYR:CE2	1:A:839:LEU:HD12	2.52	0.45
1:B:103:TYR:CE1	1:B:104:GLU:O	2.70	0.45
1:B:768:GLY:O	1:B:772:ILE:HG12	2.17	0.45
1:A:827:LYS:N	1:A:827:LYS:CD	2.79	0.44
1:B:98:LYS:HA	1:B:98:LYS:HD3	1.71	0.44
1:B:306:LEU:CD2	1:B:353:ILE:HD11	2.44	0.44
1:B:634:ASP:O	1:B:638:VAL:HG23	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:176:LYS:O	1:B:180:GLU:HG3	2.18	0.44
1:B:498:LEU:HD12	1:B:747:LEU:HD21	1.97	0.44
1:B:731:ILE:HG22	1:B:732:SER:N	2.32	0.44
1:B:744:PHE:O	1:B:744:PHE:CD1	2.70	0.44
1:A:98:LYS:HD3	1:A:98:LYS:HA	1.71	0.44
1:A:103:TYR:CE1	1:A:104:GLU:O	2.70	0.44
1:B:581:LYS:HE2	3:B:1004:HOH:O	2.13	0.44
1:A:276:ALA:O	1:A:279:ALA:HB3	2.18	0.44
1:A:330:LEU:O	1:A:333:LEU:N	2.50	0.44
1:A:443:ASN:HD22	1:A:443:ASN:HA	1.60	0.44
1:A:567:ILE:HB	1:A:584:MET:SD	2.58	0.44
1:B:415:LEU:HD22	1:B:419:GLU:HG2	1.97	0.44
1:B:315:LEU:HD21	1:B:345:LEU:CD1	2.48	0.44
1:B:383:LYS:HA	1:B:421:LEU:HD23	1.99	0.44
1:B:417:VAL:HG23	1:B:418:GLU:N	2.32	0.44
1:B:633:VAL:HG11	1:B:829:ARG:HH12	1.82	0.44
1:A:59:VAL:HG12	1:A:60:SER:N	2.32	0.44
1:A:116:ARG:NH1	1:A:116:ARG:CG	2.73	0.44
1:A:449:THR:HG22	1:A:450:TYR:N	2.26	0.44
1:B:139:VAL:HG22	1:B:141:TYR:CE2	2.52	0.44
1:B:256:ILE:HD11	1:B:563:ARG:NH2	2.25	0.44
1:B:443:ASN:ND2	1:B:448:LYS:HA	2.31	0.44
1:A:139:VAL:HG22	1:A:141:TYR:CE2	2.53	0.44
1:A:505:PHE:CZ	1:A:734:GLN:O	2.70	0.44
1:A:731:ILE:HG22	1:A:732:SER:N	2.32	0.44
1:B:44:ASP:O	1:B:45:ARG:HB2	2.18	0.44
1:B:68:ASN:HD22	1:B:74:LEU:HD12	1.78	0.44
1:B:344:PHE:CD1	1:B:344:PHE:O	2.70	0.44
1:B:416:THR:CG2	1:B:419:GLU:CB	2.95	0.44
1:B:605:GLU:OE1	1:B:609:ARG:NE	2.39	0.44
1:A:374:LEU:CD1	1:A:717:GLY:C	2.87	0.44
1:A:385:PHE:HD1	1:A:385:PHE:C	2.17	0.44
1:A:593:ASN:C	1:A:594:HIS:CD2	2.92	0.44
1:A:768:GLY:O	1:A:772:ILE:HG12	2.17	0.43
1:B:837:TYR:CE2	1:B:839:LEU:HD12	2.52	0.43
1:A:148:TYR:CZ	1:A:195:GLU:OE2	2.68	0.43
1:A:744:PHE:O	1:A:744:PHE:CD1	2.70	0.43
1:B:205:TYR:HB2	1:B:219:LEU:HB2	2.00	0.43
1:B:276:ALA:O	1:B:279:ALA:HB3	2.18	0.43
1:B:567:ILE:HB	1:B:584:MET:SD	2.58	0.43
1:A:263:ARG:NE	1:A:557:ASN:HD22	2.08	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:377:VAL:O	1:A:609:ARG:NE	2.52	0.43
1:B:43:LEU:C	1:B:43:LEU:CD1	2.85	0.43
1:A:193:LEU:HA	1:A:193:LEU:HD23	1.78	0.43
1:B:178:ARG:NH2	1:B:665:GLU:OE1	2.51	0.43
1:B:377:VAL:O	1:B:609:ARG:NE	2.52	0.43
1:B:498:LEU:CD1	1:B:747:LEU:CD2	2.96	0.43
1:B:593:ASN:C	1:B:594:HIS:CD2	2.92	0.43
1:A:475:HIS:HB2	1:A:482:GLY:C	2.39	0.43
1:A:773:GLU:O	1:A:777:THR:HG23	2.19	0.43
1:B:374:LEU:CD1	1:B:717:GLY:C	2.87	0.43
1:B:449:THR:HG22	1:B:450:TYR:N	2.26	0.43
1:B:773:GLU:O	1:B:777:THR:HG23	2.19	0.43
1:A:370:MET:SD	1:A:429:LEU:HD22	2.59	0.43
1:B:71:LYS:O	1:B:173:THR:CA	2.67	0.43
1:B:312:GLY:CA	1:B:345:LEU:O	2.66	0.43
1:B:371:LEU:HB3	1:B:629:TYR:CD2	2.52	0.43
1:B:385:PHE:HB2	1:B:421:LEU:HD11	2.00	0.43
1:B:415:LEU:CD1	1:B:419:GLU:HB3	2.48	0.43
1:B:415:LEU:CD1	1:B:420:ALA:CA	2.96	0.43
1:B:475:HIS:HB2	1:B:482:GLY:C	2.39	0.43
1:A:205:TYR:HB2	1:A:219:LEU:HB2	2.00	0.43
1:A:849:THR:O	1:A:851:ARG:HG2	2.19	0.43
1:A:405:LYS:CE	1:A:418:GLU:OE2	2.67	0.43
1:B:630:PRO:HB3	1:B:837:TYR:CD1	2.54	0.43
1:B:698:GLU:HA	1:B:701:THR:HG22	1.99	0.43
1:A:45:ARG:NH1	1:A:45:ARG:CG	2.73	0.43
1:A:215:PRO:C	1:A:216:ARG:HD3	2.39	0.43
1:A:411:ASN:HB3	1:A:467:LEU:HD22	2.01	0.43
1:B:320:LEU:O	1:B:324:ILE:CD1	2.67	0.43
1:B:443:ASN:ND2	1:B:449:THR:H	1.96	0.43
1:A:25:VAL:HG22	1:A:128:LEU:CD1	2.49	0.42
1:A:84:ILE:C	1:A:84:ILE:CD1	2.85	0.42
1:A:321:ILE:C	1:A:323:SER:N	2.65	0.42
1:A:660:ILE:CD1	1:A:693:ARG:HG2	2.46	0.42
1:A:732:SER:HA	1:A:758:THR:O	2.19	0.42
1:B:148:TYR:CZ	1:B:195:GLU:OE2	2.68	0.42
1:B:312:GLY:HA2	1:B:345:LEU:O	2.19	0.42
1:B:56:LEU:HA	1:B:114:LEU:O	2.19	0.42
1:B:82:ASP:O	1:B:98:LYS:CB	2.65	0.42
1:B:732:SER:HA	1:B:758:THR:O	2.19	0.42
1:B:801:GLU:O	1:B:805:LYS:HG2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:348:PRO:O	1:A:350:PRO:HD3	2.20	0.42
1:B:25:VAL:HG22	1:B:128:LEU:CD1	2.49	0.42
1:A:56:LEU:HA	1:A:114:LEU:O	2.19	0.42
1:A:71:LYS:O	1:A:173:THR:CA	2.67	0.42
1:A:320:LEU:O	1:A:324:ILE:CD1	2.67	0.42
1:A:405:LYS:HE2	1:A:417:VAL:HG22	2.00	0.42
1:B:464:LEU:HD21	1:B:626:ILE:CD1	2.49	0.42
1:A:328:ILE:HA	1:A:329:PRO:HD2	1.80	0.42
1:B:194:LYS:HE2	1:B:194:LYS:HB2	1.82	0.42
1:B:348:PRO:O	1:B:350:PRO:HD3	2.20	0.42
1:B:370:MET:SD	1:B:429:LEU:HD22	2.59	0.42
1:A:44:ASP:O	1:A:45:ARG:HB2	2.18	0.42
1:A:135:GLY:C	1:A:136:HIS:ND1	2.73	0.42
1:A:402:THR:CG2	1:A:485:SER:HB2	2.49	0.42
1:B:240:GLU:CD	1:B:240:GLU:N	2.73	0.42
1:B:338:ARG:HB2	1:B:346:LYS:HG2	2.02	0.42
1:B:416:THR:O	1:B:419:GLU:HB2	2.19	0.42
1:A:215:PRO:O	1:A:216:ARG:HD2	2.20	0.42
1:A:528:GLU:HB3	1:A:529:PRO:HD3	2.02	0.42
1:A:801:GLU:O	1:A:805:LYS:HG2	2.19	0.42
1:B:135:GLY:C	1:B:136:HIS:ND1	2.73	0.42
1:B:402:THR:CG2	1:B:485:SER:HB2	2.49	0.42
1:B:457:PHE:HB2	1:B:467:LEU:HD11	2.02	0.42
1:B:689:LYS:CA	1:B:689:LYS:CE	2.92	0.42
1:B:809:LYS:HE3	1:B:813:ILE:HD11	2.02	0.42
1:A:361:ARG:NH2	1:A:500:GLN:HG2	2.35	0.42
1:A:457:PHE:HB2	1:A:467:LEU:HD11	2.02	0.42
1:A:809:LYS:HE3	1:A:813:ILE:HD11	2.02	0.42
1:B:128:LEU:HB3	1:B:141:TYR:HB2	2.02	0.42
1:B:832:LEU:H	1:B:832:LEU:CD1	2.33	0.42
1:B:849:THR:O	1:B:851:ARG:HG2	2.19	0.42
1:A:207:ASP:OD1	1:A:207:ASP:N	2.50	0.42
1:A:360:TRP:NE1	1:A:724:TYR:HE1	2.18	0.42
1:A:630:PRO:HB3	1:A:837:TYR:CD1	2.54	0.42
1:B:827:LYS:N	1:B:827:LYS:CD	2.79	0.42
1:A:178:ARG:NH2	1:A:665:GLU:OE1	2.51	0.41
1:A:832:LEU:H	1:A:832:LEU:CD1	2.33	0.41
1:A:464:LEU:HD21	1:A:626:ILE:CD1	2.50	0.41
1:B:284:ILE:HD11	1:B:337:PHE:CE2	2.55	0.41
1:B:360:TRP:NE1	1:B:724:TYR:HE1	2.19	0.41
1:B:361:ARG:NH2	1:B:500:GLN:HG2	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:501:LEU:HD23	1:B:501:LEU:HA	1.84	0.41
1:A:291:VAL:HG13	1:A:316:PRO:HD3	2.02	0.41
1:A:68:ASN:HD22	1:A:74:LEU:HD12	1.78	0.41
1:A:176:LYS:O	1:A:180:GLU:HG3	2.20	0.41
1:A:240:GLU:CD	1:A:240:GLU:N	2.73	0.41
1:A:284:ILE:HD11	1:A:337:PHE:CE2	2.55	0.41
1:B:553:ARG:HE	1:B:553:ARG:HB2	1.65	0.41
1:A:607:LYS:HE2	1:A:614:GLU:OE2	2.19	0.41
1:A:660:ILE:HD12	1:A:693:ARG:CA	2.42	0.41
1:B:116:ARG:NH1	1:B:116:ARG:CG	2.73	0.41
1:B:494:VAL:O	1:B:497:SER:HB2	2.21	0.41
1:B:573:PHE:O	1:B:577:VAL:CG2	2.48	0.41
1:B:827:LYS:HD3	1:B:827:LYS:H	1.80	0.41
1:A:63:VAL:CG1	1:A:64:THR:N	2.83	0.41
1:A:128:LEU:HB3	1:A:141:TYR:HB2	2.02	0.41
1:A:553:ARG:HE	1:A:553:ARG:HB2	1.65	0.41
1:A:689:LYS:HE2	1:A:689:LYS:CA	2.39	0.41
1:A:517:ILE:N	1:A:517:ILE:HD13	2.36	0.41
1:A:527:ILE:HA	1:A:527:ILE:HD13	1.74	0.41
1:B:164:THR:HG1	1:B:796:GLU:CD	2.24	0.41
1:B:517:ILE:HG23	1:B:521:MET:CE	2.51	0.41
1:A:71:LYS:O	1:A:173:THR:HB	2.21	0.41
1:A:258:VAL:HG22	1:A:263:ARG:CZ	2.51	0.41
1:A:448:LYS:HD2	1:A:448:LYS:N	2.32	0.41
1:A:494:VAL:CG1	1:A:495:TYR:N	2.83	0.41
1:A:517:ILE:HG23	1:A:521:MET:CE	2.51	0.41
1:A:778:HIS:HB2	1:A:847:GLY:O	2.20	0.41
1:B:283:PHE:O	1:B:286:PRO:HD2	2.21	0.41
1:B:503:LYS:HB2	1:B:503:LYS:HE3	1.94	0.41
1:B:505:PHE:CZ	1:B:734:GLN:O	2.70	0.41
1:B:757:LYS:HB3	1:B:757:LYS:HE3	1.83	0.41
1:A:50:LEU:HD21	1:A:82:ASP:HA	2.02	0.41
1:B:63:VAL:CG1	1:B:64:THR:N	2.83	0.41
1:B:71:LYS:O	1:B:173:THR:HB	2.21	0.41
1:B:258:VAL:HG22	1:B:263:ARG:CZ	2.51	0.41
1:B:276:ALA:O	1:B:280:ILE:HG13	2.21	0.41
1:B:291:VAL:HG13	1:B:316:PRO:HD3	2.02	0.41
1:B:725:LEU:HD22	1:B:765:THR:OG1	2.21	0.41
1:B:778:HIS:HB2	1:B:847:GLY:O	2.20	0.41
1:A:166:LEU:H	1:A:169:GLU:CG	2.33	0.40
1:B:22:LYS:HE2	1:B:22:LYS:HB2	1.89	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:45:ARG:NH1	1:B:45:ARG:CG	2.73	0.40
1:B:215:PRO:C	1:B:216:ARG:HD3	2.42	0.40
1:B:528:GLU:HB3	1:B:529:PRO:HD3	2.02	0.40
1:B:328:ILE:HA	1:B:329:PRO:HD2	1.80	0.40
1:B:517:ILE:HD13	1:B:517:ILE:N	2.36	0.40
1:B:675:GLU:HA	1:B:682:LYS:HE2	2.03	0.40
1:A:43:LEU:C	1:A:43:LEU:CD1	2.85	0.40
1:A:565:ILE:CD1	1:A:566:LEU:CD1	2.86	0.40
1:B:35:PHE:HD1	1:B:35:PHE:HA	1.78	0.40
1:B:404:THR:OG1	1:B:407:HIS:ND1	2.49	0.40
1:A:572:ILE:O	1:A:572:ILE:HG22	2.21	0.40
1:A:675:GLU:HA	1:A:682:LYS:HE2	2.04	0.40
1:B:103:TYR:CD1	1:B:103:TYR:C	2.95	0.40
1:B:166:LEU:H	1:B:169:GLU:CG	2.34	0.40
1:B:190:GLU:CG	1:B:191:GLY:N	2.79	0.40
1:B:263:ARG:HH11	1:B:263:ARG:HD2	1.75	0.40
1:B:516:LEU:CD2	1:B:573:PHE:HE1	2.34	0.40
1:B:579:PRO:HB2	1:B:583:ALA:CA	2.52	0.40
1:A:276:ALA:O	1:A:280:ILE:HG13	2.21	0.40
1:A:579:PRO:HB2	1:A:583:ALA:CA	2.52	0.40
1:A:730:THR:HB	1:A:731:ILE:HG13	2.03	0.40
1:B:193:LEU:HD23	1:B:193:LEU:HA	1.78	0.40
1:B:436:MET:HE2	1:B:436:MET:CA	2.52	0.40
1:B:443:ASN:HD22	1:B:443:ASN:HA	1.60	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:691:GLN:CG	1:B:190:GLU:OE1[2_384]	1.87	0.33
1:A:211:PRO:O	1:B:85:THR:O[4_488]	1.99	0.21

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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



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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	842/859 (98%)	823 (98%)	19 (2%)	0	100	100
1	B	842/859 (98%)	822 (98%)	20 (2%)	0	100	100
All	All	1684/1718 (98%)	1645 (98%)	39 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

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	745/759 (98%)	632 (85%)	113 (15%)	3	12
1	B	745/759 (98%)	638 (86%)	107 (14%)	3	14
All	All	1490/1518 (98%)	1270 (85%)	220 (15%)	3	13

All (220) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	ASN
1	A	33	LEU
1	A	35	PHE
1	A	37	ASP
1	A	39	ASN
1	A	43	LEU
1	A	45	ARG
1	A	50	LEU
1	A	52	ASN
1	A	53	LYS
1	A	64	THR
1	A	70	SER
1	A	86	THR
1	A	89	SER
1	A	91	THR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	95	SER
1	A	102	ASP
1	A	106	ASP
1	A	116	ARG
1	A	132	ASP
1	A	139	VAL
1	A	143	CYS
1	A	145	SER
1	A	164	THR
1	A	168	HIS
1	A	188	THR
1	A	190	GLU
1	A	208	LEU
1	A	210	VAL
1	A	213	LYS
1	A	214	ASN
1	A	223	GLN
1	A	236	LYS
1	A	238	THR
1	A	239	LYS
1	A	246	SER
1	A	253	SER
1	A	254	LEU
1	A	256	ILE
1	A	268	LYS
1	A	270	SER
1	A	285	GLN
1	A	294	ASP
1	A	298	GLU
1	A	300	ASP
1	A	301	SER
1	A	322	ASP
1	A	324	ILE
1	A	326	LYS
1	A	333	LEU
1	A	338	ARG
1	A	340	ASP
1	A	342	GLN
1	A	364	GLU
1	A	376	PRO
1	A	378	VAL
1	A	380	GLN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	381	LEU
1	A	384	GLU
1	A	385	PHE
1	A	393	SER
1	A	401	SER
1	A	402	THR
1	A	404	THR
1	A	405	LYS
1	A	416	THR
1	A	419	GLU
1	A	421	LEU
1	A	422	GLU
1	A	423	LYS
1	A	424	GLU
1	A	436	MET
1	A	443	ASN
1	A	448	LYS
1	A	461	ASP
1	A	464	LEU
1	A	465	LYS
1	A	479	ASP
1	A	492	GLU
1	A	498	LEU
1	A	500	GLN
1	A	540	VAL
1	A	549	GLU
1	A	566	LEU
1	A	576	THR
1	A	577	VAL
1	A	578	PHE
1	A	613	VAL
1	A	619	PRO
1	A	627	LYS
1	A	629	TYR
1	A	644	SER
1	A	655	LYS
1	A	690	MET
1	A	691	GLN
1	A	715	ASN
1	A	730	THR
1	A	736	MET
1	A	740	ASN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	744	PHE
1	A	758	THR
1	A	760	THR
1	A	815	LYS
1	A	825	THR
1	A	826	LEU
1	A	827	LYS
1	A	829	ARG
1	A	830	THR
1	A	833	VAL
1	A	843	SER
1	A	845	GLU
1	A	848	VAL
1	A	851	ARG
1	B	31	ASN
1	B	33	LEU
1	B	35	PHE
1	B	37	ASP
1	B	39	ASN
1	B	43	LEU
1	B	45	ARG
1	B	50	LEU
1	B	52	ASN
1	B	53	LYS
1	B	64	THR
1	B	70	SER
1	B	88	THR
1	B	90	LEU
1	B	91	THR
1	B	102	ASP
1	B	106	ASP
1	B	116	ARG
1	B	132	ASP
1	B	139	VAL
1	B	143	CYS
1	B	145	SER
1	B	164	THR
1	B	168	HIS
1	B	188	THR
1	B	190	GLU
1	B	213	LYS
1	B	223	GLN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	236	LYS
1	B	238	THR
1	B	239	LYS
1	B	246	SER
1	B	253	SER
1	B	254	LEU
1	B	256	ILE
1	B	268	LYS
1	B	270	SER
1	B	285	GLN
1	B	294	ASP
1	B	298	GLU
1	B	300	ASP
1	B	301	SER
1	B	322	ASP
1	B	324	ILE
1	B	326	LYS
1	B	333	LEU
1	B	342	GLN
1	B	364	GLU
1	B	376	PRO
1	B	378	VAL
1	B	380	GLN
1	B	381	LEU
1	B	384	GLU
1	B	385	PHE
1	B	393	SER
1	B	401	SER
1	B	402	THR
1	B	404	THR
1	B	405	LYS
1	B	409	GLU
1	B	415	LEU
1	B	416	THR
1	B	418	GLU
1	B	421	LEU
1	B	422	GLU
1	B	436	MET
1	B	443	ASN
1	B	448	LYS
1	B	461	ASP
1	B	464	LEU

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Mol	Chain	Res	Type
1	B	465	LYS
1	B	479	ASP
1	B	492	GLU
1	B	498	LEU
1	B	500	GLN
1	B	540	VAL
1	B	549	GLU
1	B	566	LEU
1	B	576	THR
1	B	577	VAL
1	B	578	PHE
1	B	613	VAL
1	B	619	PRO
1	B	627	LYS
1	B	629	TYR
1	B	644	SER
1	B	655	LYS
1	B	690	MET
1	B	691	GLN
1	B	715	ASN
1	B	730	THR
1	B	736	MET
1	B	740	ASN
1	B	744	PHE
1	B	758	THR
1	B	760	THR
1	B	815	LYS
1	B	825	THR
1	B	826	LEU
1	B	827	LYS
1	B	829	ARG
1	B	830	THR
1	B	833	VAL
1	B	843	SER
1	B	845	GLU
1	B	848	VAL
1	B	851	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	ASN

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Mol	Chain	Res	Type
1	A	52	ASN
1	A	68	ASN
1	A	342	GLN
1	A	380	GLN
1	A	443	ASN
1	A	477	ASN
1	A	557	ASN
1	A	593	ASN
1	A	594	HIS
1	A	828	ASN
1	B	39	ASN
1	B	52	ASN
1	B	68	ASN
1	B	342	GLN
1	B	380	GLN
1	B	443	ASN
1	B	477	ASN
1	B	557	ASN
1	B	593	ASN
1	B	594	HIS
1	B	691	GLN
1	B	828	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.



## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	844/859 (98%)	0.04	8 (0%) 84 84	32, 53, 86, 126	0
1	B	844/859 (98%)	0.16	12 (1%) 75 74	36, 58, 91, 126	0
All	All	1688/1718 (98%)	0.10	20 (1%) 79 77	32, 55, 89, 126	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	68	ASN	9.4
1	A	67	GLU	3.5
1	B	68	ASN	3.4
1	A	69	GLY	3.3
1	B	318	GLN	3.3
1	B	319	ALA	3.1
1	B	322	ASP	3.0
1	B	16	THR	2.9
1	A	843	SER	2.6
1	A	322	ASP	2.6
1	B	305	VAL	2.6
1	A	239	LYS	2.4
1	B	764	GLN	2.4
1	A	316	PRO	2.4
1	B	342	GLN	2.3
1	B	417	VAL	2.3
1	B	383	LYS	2.2
1	B	131	GLU	2.2
1	A	292	PHE	2.1
1	B	339	THR	2.1

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

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	FE	A	901	1/1	0.96	0.06	35,35,35,35	0
2	FE	B	901	1/1	0.96	0.07	42,42,42,42	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.