Full wwPDB X-ray Structure Validation Report ⓘ

Oct 11, 2021 – 04:03 AM EDT

PDB ID	:	3BG9
Title	:	Crystal Structure of Human Pyruvate Carboxylase (missing the biotin carboxylase domain at the N-terminus) F1077A Mutant
Authors	:	Xiang, S.; Tong, L.
Deposited on	:	2007-11-26
Resolution	:	3.00 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

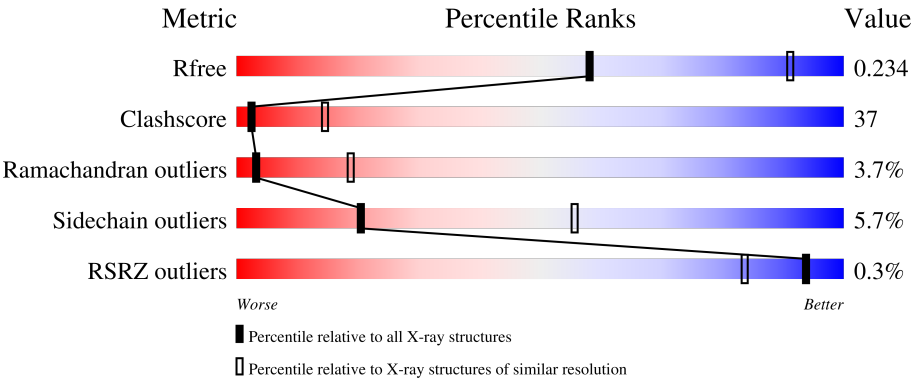
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

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 3.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=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 <=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	718	38% 41% 5% 16%
1	B	718	37% 42% 5% 16%
1	C	718	35% 44% . 16%
1	D	718	39% 40% . 16%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 18516 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 Pyruvate carboxylase, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	601	Total	C	N	O	S	0	0	0
			4628	2937	798	865	28			
1	B	601	Total	C	N	O	S	0	0	0
			4628	2937	798	865	28			
1	C	601	Total	C	N	O	S	0	0	0
			4628	2937	798	865	28			
1	D	601	Total	C	N	O	S	0	0	0
			4628	2937	798	865	28			

There are 88 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	461	MET	-	expression tag	UNP P11498
A	462	GLY	-	expression tag	UNP P11498
A	463	SER	-	expression tag	UNP P11498
A	464	SER	-	expression tag	UNP P11498
A	465	HIS	-	expression tag	UNP P11498
A	466	HIS	-	expression tag	UNP P11498
A	467	HIS	-	expression tag	UNP P11498
A	468	HIS	-	expression tag	UNP P11498
A	469	HIS	-	expression tag	UNP P11498
A	470	HIS	-	expression tag	UNP P11498
A	471	SER	-	expression tag	UNP P11498
A	472	SER	-	expression tag	UNP P11498
A	473	GLY	-	expression tag	UNP P11498
A	474	LEU	-	expression tag	UNP P11498
A	475	VAL	-	expression tag	UNP P11498
A	476	PRO	-	expression tag	UNP P11498
A	477	ARG	-	expression tag	UNP P11498
A	478	GLY	-	expression tag	UNP P11498
A	479	SER	-	expression tag	UNP P11498
A	480	HIS	-	expression tag	UNP P11498
A	481	MET	-	expression tag	UNP P11498

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1077	ALA	PHE	engineered mutation	UNP P11498
B	461	MET	-	expression tag	UNP P11498
B	462	GLY	-	expression tag	UNP P11498
B	463	SER	-	expression tag	UNP P11498
B	464	SER	-	expression tag	UNP P11498
B	465	HIS	-	expression tag	UNP P11498
B	466	HIS	-	expression tag	UNP P11498
B	467	HIS	-	expression tag	UNP P11498
B	468	HIS	-	expression tag	UNP P11498
B	469	HIS	-	expression tag	UNP P11498
B	470	HIS	-	expression tag	UNP P11498
B	471	SER	-	expression tag	UNP P11498
B	472	SER	-	expression tag	UNP P11498
B	473	GLY	-	expression tag	UNP P11498
B	474	LEU	-	expression tag	UNP P11498
B	475	VAL	-	expression tag	UNP P11498
B	476	PRO	-	expression tag	UNP P11498
B	477	ARG	-	expression tag	UNP P11498
B	478	GLY	-	expression tag	UNP P11498
B	479	SER	-	expression tag	UNP P11498
B	480	HIS	-	expression tag	UNP P11498
B	481	MET	-	expression tag	UNP P11498
B	1077	ALA	PHE	engineered mutation	UNP P11498
C	461	MET	-	expression tag	UNP P11498
C	462	GLY	-	expression tag	UNP P11498
C	463	SER	-	expression tag	UNP P11498
C	464	SER	-	expression tag	UNP P11498
C	465	HIS	-	expression tag	UNP P11498
C	466	HIS	-	expression tag	UNP P11498
C	467	HIS	-	expression tag	UNP P11498
C	468	HIS	-	expression tag	UNP P11498
C	469	HIS	-	expression tag	UNP P11498
C	470	HIS	-	expression tag	UNP P11498
C	471	SER	-	expression tag	UNP P11498
C	472	SER	-	expression tag	UNP P11498
C	473	GLY	-	expression tag	UNP P11498
C	474	LEU	-	expression tag	UNP P11498
C	475	VAL	-	expression tag	UNP P11498
C	476	PRO	-	expression tag	UNP P11498
C	477	ARG	-	expression tag	UNP P11498
C	478	GLY	-	expression tag	UNP P11498
C	479	SER	-	expression tag	UNP P11498

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Chain	Residue	Modelled	Actual	Comment	Reference
C	480	HIS	-	expression tag	UNP P11498
C	481	MET	-	expression tag	UNP P11498
C	1077	ALA	PHE	engineered mutation	UNP P11498
D	461	MET	-	expression tag	UNP P11498
D	462	GLY	-	expression tag	UNP P11498
D	463	SER	-	expression tag	UNP P11498
D	464	SER	-	expression tag	UNP P11498
D	465	HIS	-	expression tag	UNP P11498
D	466	HIS	-	expression tag	UNP P11498
D	467	HIS	-	expression tag	UNP P11498
D	468	HIS	-	expression tag	UNP P11498
D	469	HIS	-	expression tag	UNP P11498
D	470	HIS	-	expression tag	UNP P11498
D	471	SER	-	expression tag	UNP P11498
D	472	SER	-	expression tag	UNP P11498
D	473	GLY	-	expression tag	UNP P11498
D	474	LEU	-	expression tag	UNP P11498
D	475	VAL	-	expression tag	UNP P11498
D	476	PRO	-	expression tag	UNP P11498
D	477	ARG	-	expression tag	UNP P11498
D	478	GLY	-	expression tag	UNP P11498
D	479	SER	-	expression tag	UNP P11498
D	480	HIS	-	expression tag	UNP P11498
D	481	MET	-	expression tag	UNP P11498
D	1077	ALA	PHE	engineered mutation	UNP P11498

- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

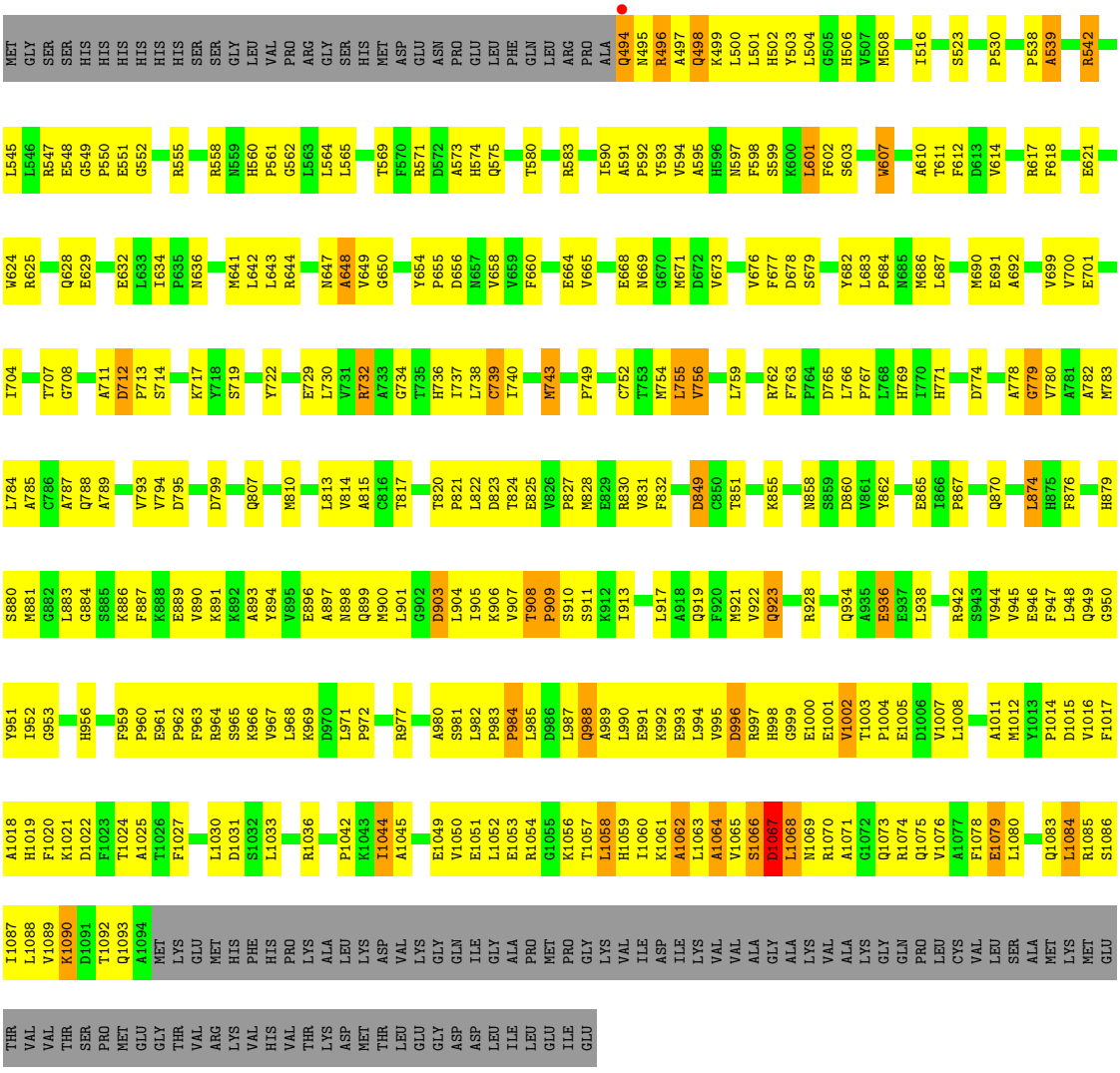
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Mn 1 1	0	0
2	B	1	Total Mn 1 1	0	0
2	C	1	Total Mn 1 1	0	0
2	D	1	Total Mn 1 1	0	0

3 Residue-property plots (i)

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

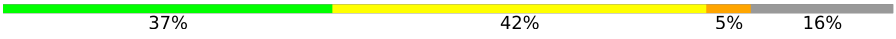
• Molecule 1: Pyruvate carboxylase, mitochondrial

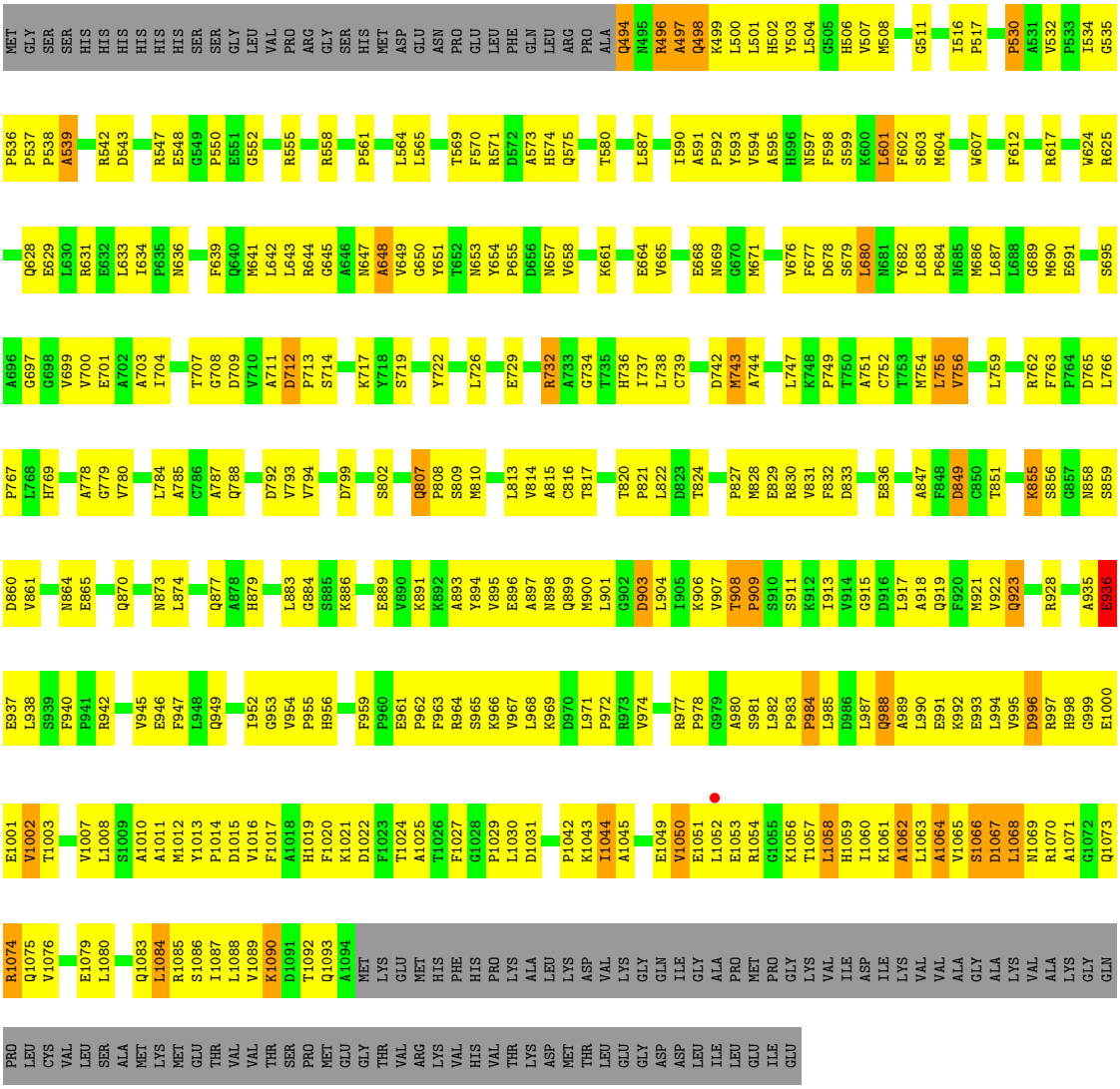
Chain A:



• Molecule 1: Pyruvate carboxylase, mitochondrial

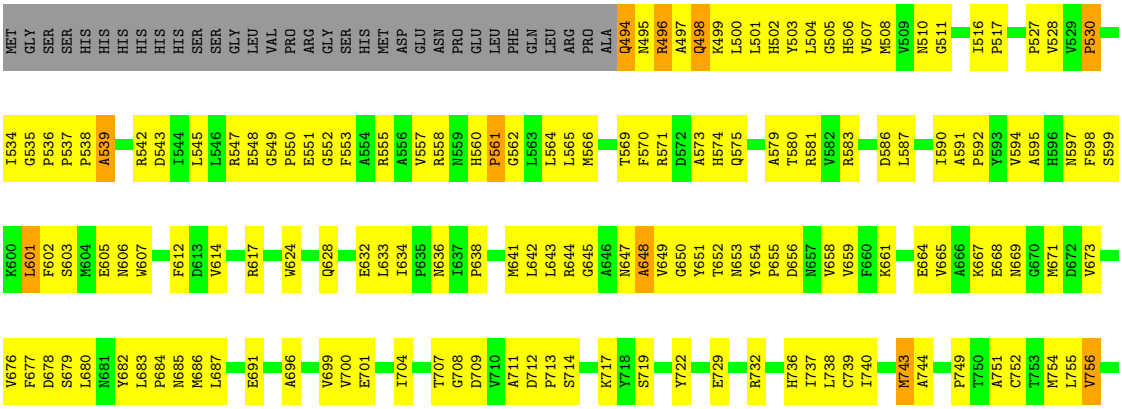
Chain B:

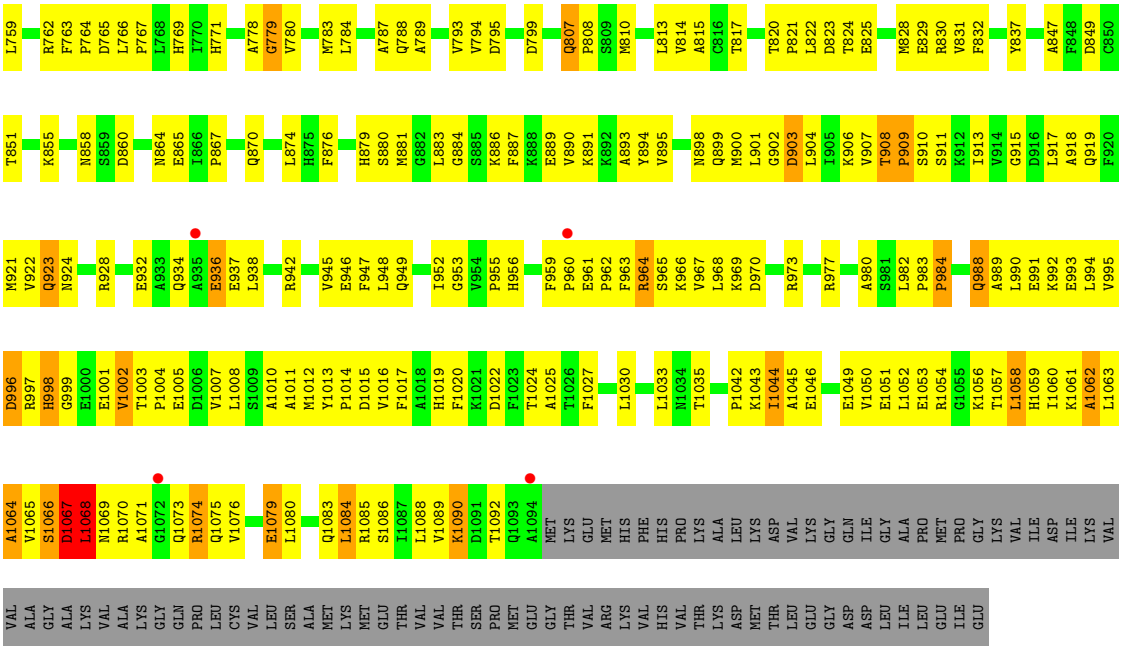




• Molecule 1: Pyruvate carboxylase, mitochondrial

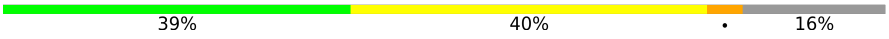
Chain C:

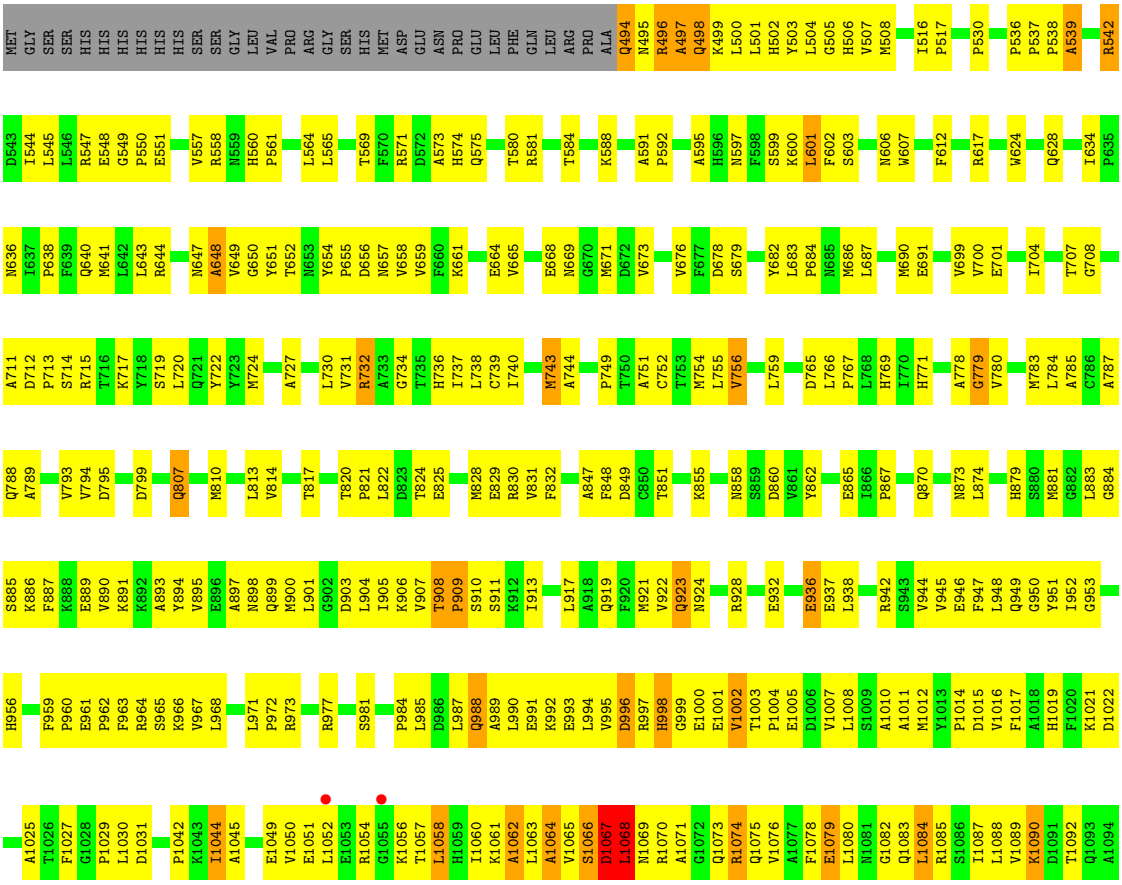




• Molecule 1: Pyruvate carboxylase, mitochondrial

Chain D:





MET LYS GLU MET HIS PHE HIS PRO LYS ALA LEU LYS ASP VAL LYS GLY GLN ILE GLY ALA PRO MET PRO GLY LYS VAL ILE ASP ILE LYS VAL VAL ALA GLY ALA LYS VAL ALA LYS GLY GLN PRO LEU CYS VAL LEU SER ALA MET LYS MET GLU THR VAL VAL THR SER PRO MET GLU

GLY THR VAL ARG LYS VAL HIS VAL THR LYS ASP MET THR LEU GLU GLY ASP ASP LEU ILE LEU GLU ILE GLU

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	107.54Å 107.54Å 524.47Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 3.00 29.77 – 3.01	Depositor EDS
% Data completeness (in resolution range)	80.8 (30.00-3.00) 88.9 (29.77-3.01)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	0.12	Depositor
$< I/\sigma(I) >$ [1]	3.38 (at 3.00Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.189 , 0.236 0.193 , 0.234	Depositor DCC
R_{free} test set	2799 reflections (4.42%)	wwPDB-VP
Wilson B-factor (Å^2)	58.6	Xtriage
Anisotropy	0.258	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 26.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.38$, $< L^2 > = 0.21$	Xtriage
Estimated twinning fraction	0.370 for -h,-k,l	Xtriage
Reported twinning fraction	0.366 for -h,-k,l	Depositor
Outliers	0 of 63285 reflections	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	18516	wwPDB-VP
Average B, all atoms (Å^2)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.14% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.47	0/4736	0.68	0/6428
1	B	0.49	0/4736	0.68	0/6428
1	C	0.48	0/4736	0.68	0/6428
1	D	0.49	0/4736	0.68	1/6428 (0.0%)
All	All	0.48	0/18944	0.68	1/25712 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	1068	LEU	CA-CB-CG	5.03	126.86	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4628	0	4579	349	1
1	B	4628	0	4579	354	0
1	C	4628	0	4579	363	1
1	D	4628	0	4579	328	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	1	0	0	0	0
2	D	1	0	0	0	0
All	All	18516	0	18316	1380	1

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 37.

All (1380) 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:C:496:ARG:HB3	1:C:1052:LEU:HD11	1.27	1.12
1:D:1044:ILE:H	1:D:1044:ILE:HD12	1.18	1.07
1:D:496:ARG:HB3	1:D:1052:LEU:HD11	1.37	1.06
1:A:496:ARG:HB3	1:A:1052:LEU:HD11	1.38	1.02
1:A:700:VAL:H	1:A:736:HIS:HD2	1.11	0.98
1:B:665:VAL:HG21	1:B:1008:LEU:HD11	1.45	0.96
1:B:1044:ILE:HD12	1:B:1044:ILE:H	1.28	0.95
1:B:700:VAL:H	1:B:736:HIS:HD2	1.14	0.94
1:B:496:ARG:HB3	1:B:1052:LEU:HD11	1.49	0.94
1:A:732:ARG:HH11	1:A:732:ARG:HB2	1.33	0.93
1:A:1044:ILE:HD12	1:A:1044:ILE:H	1.32	0.92
1:A:752:CYS:O	1:A:756:VAL:HG12	1.71	0.91
1:A:1068:LEU:HD13	1:A:1074:ARG:NH2	1.85	0.91
1:D:700:VAL:H	1:D:736:HIS:HD2	1.15	0.91
1:B:1068:LEU:HD13	1:B:1074:ARG:NH2	1.85	0.90
1:C:913:ILE:HD13	1:C:947:PHE:HB2	1.54	0.89
1:A:571:ARG:HH11	1:A:575:GLN:NE2	1.70	0.88
1:A:913:ILE:HD13	1:A:947:PHE:HB2	1.56	0.88
1:D:1068:LEU:HD13	1:D:1074:ARG:NH2	1.89	0.88
1:C:1065:VAL:HG13	1:C:1076:VAL:HG12	1.56	0.88
1:D:991:GLU:O	1:D:995:VAL:HG23	1.74	0.88
1:B:913:ILE:HD13	1:B:947:PHE:HB2	1.56	0.87
1:D:732:ARG:HH11	1:D:732:ARG:HB2	1.40	0.87
1:C:679:SER:HB3	1:C:909:PRO:HD2	1.59	0.85
1:B:870:GLN:O	1:B:874:LEU:HD13	1.77	0.85
1:A:571:ARG:HH11	1:A:575:GLN:HE22	1.24	0.84
1:C:665:VAL:HG21	1:C:1008:LEU:HD11	1.57	0.84
1:B:624:TRP:O	1:B:628:GLN:HG3	1.77	0.84
1:B:732:ARG:HB2	1:B:732:ARG:HH11	1.42	0.84
1:C:564:LEU:HB2	1:C:793:VAL:HG22	1.60	0.84
1:C:1068:LEU:HD13	1:C:1074:ARG:NH2	1.92	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:679:SER:HB3	1:D:909:PRO:HD2	1.60	0.83
1:C:1044:ILE:HD12	1:C:1044:ILE:H	1.44	0.83
1:D:665:VAL:HG21	1:D:1008:LEU:HD11	1.60	0.83
1:A:649:VAL:H	1:A:1012:MET:HE1	1.44	0.82
1:D:496:ARG:CB	1:D:1052:LEU:HD11	2.09	0.82
1:D:870:GLN:O	1:D:874:LEU:HD13	1.79	0.82
1:A:991:GLU:O	1:A:995:VAL:HG23	1.80	0.82
1:C:989:ALA:O	1:C:993:GLU:HB2	1.80	0.82
1:B:571:ARG:HH11	1:B:575:GLN:HE22	1.27	0.82
1:C:870:GLN:O	1:C:874:LEU:HD13	1.80	0.82
1:C:1066:SER:O	1:C:1068:LEU:HD23	1.80	0.82
1:D:752:CYS:O	1:D:756:VAL:HG12	1.80	0.81
1:A:989:ALA:O	1:A:993:GLU:HB2	1.79	0.81
1:C:601:LEU:HD22	1:C:603:SER:O	1.81	0.81
1:B:571:ARG:HH11	1:B:575:GLN:NE2	1.78	0.81
1:B:900:MET:HE2	1:B:928:ARG:HG3	1.62	0.81
1:B:539:ALA:HA	1:B:636:ASN:HB2	1.63	0.80
1:C:700:VAL:H	1:C:736:HIS:HD2	1.28	0.80
1:C:995:VAL:HG22	1:C:1002:VAL:CG2	2.11	0.80
1:A:900:MET:HE2	1:A:928:ARG:HG3	1.64	0.80
1:C:612:PHE:CB	1:C:649:VAL:HG11	2.12	0.80
1:C:571:ARG:HH11	1:C:575:GLN:HE22	1.29	0.79
1:D:913:ILE:HD13	1:D:947:PHE:HB2	1.62	0.79
1:C:942:ARG:O	1:C:945:VAL:HG22	1.82	0.79
1:A:732:ARG:HB2	1:A:732:ARG:NH1	1.97	0.79
1:C:571:ARG:HH11	1:C:575:GLN:NE2	1.80	0.79
1:D:649:VAL:H	1:D:1012:MET:HE1	1.46	0.79
1:A:496:ARG:CB	1:A:1052:LEU:HD11	2.11	0.78
1:C:624:TRP:O	1:C:628:GLN:HG3	1.83	0.78
1:C:504:LEU:HD22	1:C:1042:PRO:HD3	1.63	0.78
1:B:1066:SER:O	1:B:1068:LEU:HD23	1.84	0.78
1:C:900:MET:HE2	1:C:928:ARG:HG3	1.66	0.78
1:C:991:GLU:O	1:C:995:VAL:HG23	1.84	0.78
1:B:595:ALA:HB2	1:B:634:ILE:HG23	1.64	0.77
1:B:989:ALA:O	1:B:993:GLU:HB2	1.84	0.77
1:B:849:ASP:HB3	1:B:851:THR:HG22	1.65	0.77
1:D:992:LYS:O	1:D:996:ASP:HB3	1.84	0.77
1:D:989:ALA:O	1:D:993:GLU:HB2	1.84	0.77
1:B:991:GLU:O	1:B:995:VAL:HG23	1.85	0.77
1:C:591:ALA:HB3	1:C:592:PRO:HD3	1.65	0.77
1:A:1051:GLU:OE1	1:A:1057:THR:HG23	1.85	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:571:ARG:HH11	1:D:575:GLN:NE2	1.83	0.77
1:A:679:SER:HB3	1:A:909:PRO:HD2	1.67	0.76
1:B:564:LEU:HB2	1:B:793:VAL:HG22	1.67	0.76
1:C:977:ARG:HH11	1:C:977:ARG:HB3	1.50	0.76
1:D:612:PHE:CB	1:D:649:VAL:HG11	2.15	0.76
1:A:655:PRO:O	1:A:658:VAL:HG22	1.84	0.76
1:D:1022:ASP:O	1:D:1025:ALA:HB3	1.85	0.76
1:A:995:VAL:HG22	1:A:1002:VAL:CG2	2.16	0.76
1:B:898:ASN:HD21	1:B:904:LEU:H	1.34	0.76
1:A:992:LYS:O	1:A:996:ASP:HB3	1.86	0.76
1:C:995:VAL:HG22	1:C:1002:VAL:HG21	1.66	0.76
1:B:649:VAL:H	1:B:1012:MET:HE1	1.50	0.76
1:A:665:VAL:HG21	1:A:1008:LEU:HD11	1.67	0.75
1:C:498:GLN:HA	1:C:501:LEU:HD12	1.67	0.75
1:D:732:ARG:HB2	1:D:732:ARG:NH1	2.01	0.75
1:A:849:ASP:HB3	1:A:851:THR:HG22	1.66	0.75
1:C:687:LEU:O	1:C:691:GLU:HG2	1.87	0.75
1:D:784:LEU:O	1:D:788:GLN:HG2	1.86	0.75
1:B:752:CYS:O	1:B:756:VAL:HG12	1.87	0.75
1:D:655:PRO:O	1:D:658:VAL:HG22	1.85	0.74
1:A:908:THR:HB	1:A:909:PRO:HD3	1.68	0.74
1:C:641:MET:HB3	1:C:671:MET:CE	2.17	0.74
1:A:995:VAL:HG22	1:A:1002:VAL:HG21	1.68	0.74
1:B:1054:ARG:O	1:B:1054:ARG:HD3	1.87	0.74
1:C:977:ARG:HB3	1:C:977:ARG:NH1	2.02	0.74
1:B:886:LYS:HA	1:B:889:GLU:OE1	1.87	0.74
1:C:496:ARG:CB	1:C:1052:LEU:HD11	2.11	0.74
1:D:719:SER:O	1:D:722:TYR:HB3	1.88	0.73
1:B:732:ARG:HB2	1:B:732:ARG:NH1	2.03	0.73
1:B:898:ASN:ND2	1:B:904:LEU:H	1.85	0.73
1:D:886:LYS:HA	1:D:889:GLU:OE1	1.87	0.73
1:B:612:PHE:CB	1:B:649:VAL:HG11	2.17	0.73
1:B:711:ALA:O	1:B:713:PRO:HD3	1.88	0.73
1:C:883:LEU:O	1:C:886:LYS:HB2	1.88	0.73
1:A:687:LEU:O	1:A:691:GLU:HG2	1.88	0.73
1:D:624:TRP:O	1:D:628:GLN:HG3	1.88	0.73
1:D:498:GLN:HA	1:D:501:LEU:HD12	1.69	0.73
1:A:883:LEU:O	1:A:886:LYS:HB2	1.89	0.72
1:A:899:GLN:HA	1:A:899:GLN:NE2	2.04	0.72
1:C:539:ALA:HA	1:C:636:ASN:HB2	1.71	0.72
1:C:1045:ALA:CA	1:C:1063:LEU:HG	2.19	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:571:ARG:HH11	1:D:575:GLN:HE22	1.35	0.72
1:D:1065:VAL:HG13	1:D:1076:VAL:HG12	1.70	0.72
1:B:1045:ALA:CA	1:B:1063:LEU:HG	2.19	0.72
1:D:504:LEU:O	1:D:508:MET:HG3	1.90	0.72
1:D:1044:ILE:H	1:D:1044:ILE:CD1	1.91	0.72
1:B:995:VAL:HG22	1:B:1002:VAL:CG2	2.20	0.72
1:B:601:LEU:HD22	1:B:603:SER:O	1.89	0.72
1:D:936:GLU:HB3	1:D:966:LYS:NZ	2.04	0.72
1:A:898:ASN:ND2	1:A:904:LEU:H	1.87	0.72
1:B:784:LEU:O	1:B:788:GLN:HG2	1.90	0.71
1:A:612:PHE:CB	1:A:649:VAL:HG11	2.20	0.71
1:B:923:GLN:O	1:B:923:GLN:HG2	1.89	0.71
1:C:1051:GLU:OE1	1:C:1057:THR:HG23	1.90	0.71
1:A:601:LEU:HD22	1:A:603:SER:O	1.90	0.71
1:C:1003:THR:O	1:C:1007:VAL:HG23	1.91	0.71
1:D:883:LEU:O	1:D:886:LYS:HB2	1.90	0.71
1:A:539:ALA:HA	1:A:636:ASN:HB2	1.72	0.71
1:B:687:LEU:O	1:B:691:GLU:HG2	1.89	0.71
1:B:988:GLN:N	1:B:988:GLN:CD	2.43	0.71
1:A:575:GLN:HG3	1:A:580:THR:OG1	1.90	0.71
1:A:612:PHE:HB2	1:A:649:VAL:HG11	1.72	0.71
1:C:817:THR:HG21	1:C:824:THR:HG23	1.73	0.71
1:A:1065:VAL:HG13	1:A:1076:VAL:HG12	1.72	0.71
1:D:538:PRO:HG2	1:D:599:SER:HB3	1.73	0.70
1:A:644:ARG:HD2	1:A:647:ASN:OD1	1.91	0.70
1:C:992:LYS:O	1:C:996:ASP:HB3	1.92	0.70
1:C:906:LYS:C	1:C:911:SER:HB3	2.11	0.70
1:D:942:ARG:O	1:D:945:VAL:HG22	1.91	0.70
1:D:505:GLY:O	1:D:508:MET:HB2	1.91	0.70
1:C:643:LEU:CD1	1:C:648:ALA:HA	2.21	0.70
1:B:897:ALA:HB2	1:B:921:MET:HE2	1.72	0.70
1:D:1067:ASP:OD2	1:D:1067:ASP:N	2.22	0.70
1:A:569:THR:HA	1:A:573:ALA:HB3	1.74	0.70
1:B:1065:VAL:HG22	1:B:1076:VAL:HG12	1.74	0.70
1:A:988:GLN:CD	1:A:988:GLN:N	2.46	0.70
1:A:886:LYS:HA	1:A:889:GLU:OE1	1.92	0.69
1:A:498:GLN:HA	1:A:501:LEU:HD12	1.72	0.69
1:B:591:ALA:HB3	1:B:592:PRO:HD3	1.73	0.69
1:C:810:MET:O	1:C:814:VAL:HG23	1.91	0.69
1:A:494:GLN:HG2	1:A:1056:LYS:NZ	2.08	0.69
1:A:591:ALA:HB3	1:A:592:PRO:HD3	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:904:LEU:N	1:B:904:LEU:HD12	2.07	0.69
1:C:1089:VAL:HG12	1:C:1090:LYS:H	1.58	0.69
1:D:641:MET:HB3	1:D:671:MET:CE	2.22	0.69
1:C:936:GLU:HB3	1:C:966:LYS:NZ	2.05	0.69
1:A:564:LEU:HB2	1:A:793:VAL:HG22	1.73	0.69
1:B:496:ARG:CB	1:B:1052:LEU:HD11	2.22	0.69
1:C:550:PRO:HB3	1:C:699:VAL:HG22	1.74	0.69
1:C:617:ARG:HH21	1:C:1016:VAL:HG21	1.57	0.69
1:C:1089:VAL:HG12	1:C:1090:LYS:N	2.07	0.69
1:A:898:ASN:HD21	1:A:904:LEU:H	1.40	0.69
1:C:1027:PHE:HB3	1:C:1030:LEU:HD21	1.75	0.69
1:C:598:PHE:O	1:C:601:LEU:HB2	1.93	0.68
1:D:664:GLU:O	1:D:668:GLU:HG3	1.92	0.68
1:A:682:TYR:CE1	1:A:684:PRO:HB2	2.27	0.68
1:B:679:SER:HB3	1:B:909:PRO:HD2	1.74	0.68
1:C:649:VAL:HG12	1:C:649:VAL:O	1.93	0.68
1:C:1083:GLN:CD	1:C:1085:ARG:HH21	1.97	0.68
1:B:906:LYS:C	1:B:911:SER:HB3	2.14	0.68
1:A:1076:VAL:O	1:A:1086:SER:HB2	1.94	0.68
1:B:612:PHE:HB3	1:B:649:VAL:HG11	1.73	0.68
1:C:649:VAL:H	1:C:1012:MET:HE1	1.59	0.68
1:A:649:VAL:HG12	1:A:649:VAL:O	1.94	0.68
1:A:995:VAL:HA	1:A:999:GLY:O	1.94	0.68
1:C:597:ASN:HB3	1:C:830:ARG:HD3	1.76	0.68
1:A:1067:ASP:OD2	1:A:1067:ASP:N	2.27	0.68
1:B:1003:THR:O	1:B:1007:VAL:HG23	1.93	0.68
1:B:899:GLN:HA	1:B:899:GLN:NE2	2.06	0.68
1:C:977:ARG:NH1	1:C:980:ALA:HB2	2.07	0.68
1:B:1073:GLN:HB3	1:B:1089:VAL:O	1.94	0.67
1:C:737:ILE:HG23	1:C:767:PRO:HB2	1.75	0.67
1:C:977:ARG:HH12	1:C:980:ALA:HB2	1.58	0.67
1:D:810:MET:O	1:D:814:VAL:HG23	1.94	0.67
1:A:504:LEU:HD22	1:A:1042:PRO:HD3	1.76	0.67
1:A:538:PRO:HG2	1:A:599:SER:HB3	1.76	0.67
1:A:906:LYS:C	1:A:911:SER:HB3	2.14	0.67
1:D:1065:VAL:O	1:D:1066:SER:HB3	1.94	0.67
1:D:601:LEU:HD22	1:D:603:SER:O	1.93	0.67
1:A:717:LYS:NZ	1:A:956:HIS:O	2.27	0.67
1:B:499:LYS:NZ	1:B:1025:ALA:O	2.22	0.67
1:C:612:PHE:HB2	1:C:649:VAL:HG11	1.76	0.67
1:B:1089:VAL:HG12	1:B:1090:LYS:N	2.09	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:612:PHE:HB2	1:D:649:VAL:HG11	1.76	0.67
1:D:737:ILE:HG23	1:D:767:PRO:HB2	1.75	0.66
1:D:988:GLN:N	1:D:988:GLN:CD	2.48	0.66
1:D:1003:THR:O	1:D:1007:VAL:HG23	1.96	0.66
1:C:595:ALA:HB2	1:C:634:ILE:HG23	1.77	0.66
1:C:752:CYS:O	1:C:756:VAL:HG12	1.95	0.66
1:C:1045:ALA:HA	1:C:1063:LEU:HG	1.77	0.66
1:A:569:THR:HA	1:A:573:ALA:CB	2.25	0.66
1:B:504:LEU:HD22	1:B:1042:PRO:HD3	1.76	0.66
1:D:591:ALA:HB3	1:D:592:PRO:HD3	1.76	0.66
1:C:784:LEU:O	1:C:788:GLN:HG2	1.96	0.66
1:A:1066:SER:C	1:A:1068:LEU:H	1.99	0.66
1:B:936:GLU:HB3	1:B:966:LYS:NZ	2.11	0.66
1:A:1089:VAL:HG12	1:A:1090:LYS:N	2.10	0.66
1:B:737:ILE:HG23	1:B:767:PRO:HB2	1.77	0.66
1:B:922:VAL:HG23	1:B:923:GLN:N	2.11	0.66
1:B:1065:VAL:HG22	1:B:1076:VAL:CG1	2.26	0.66
1:C:612:PHE:HB3	1:C:649:VAL:HG11	1.76	0.66
1:D:1090:LYS:H	1:D:1090:LYS:HD2	1.59	0.66
1:B:550:PRO:HB3	1:B:699:VAL:HG22	1.78	0.66
1:B:644:ARG:HD2	1:B:647:ASN:OD1	1.95	0.66
1:B:992:LYS:O	1:B:996:ASP:HB3	1.95	0.66
1:D:612:PHE:HB3	1:D:649:VAL:HG11	1.77	0.66
1:D:901:LEU:HB2	1:D:904:LEU:HD11	1.78	0.66
1:A:683:LEU:O	1:A:687:LEU:HG	1.96	0.66
1:C:908:THR:HB	1:C:909:PRO:HD3	1.76	0.65
1:B:995:VAL:HG22	1:B:1002:VAL:HG21	1.77	0.65
1:C:901:LEU:HB2	1:C:904:LEU:HD11	1.78	0.65
1:A:700:VAL:H	1:A:736:HIS:CD2	2.03	0.65
1:A:1044:ILE:HA	1:A:1062:ALA:HB3	1.78	0.65
1:B:641:MET:HB3	1:B:671:MET:CE	2.27	0.65
1:B:649:VAL:HG12	1:B:649:VAL:O	1.97	0.65
1:B:1089:VAL:HG12	1:B:1090:LYS:H	1.60	0.65
1:C:849:ASP:HB3	1:C:851:THR:HG22	1.78	0.65
1:C:1065:VAL:O	1:C:1066:SER:HB3	1.97	0.65
1:A:624:TRP:O	1:A:628:GLN:HG3	1.97	0.65
1:A:963:PHE:O	1:A:967:VAL:HG23	1.96	0.65
1:B:1022:ASP:O	1:B:1025:ALA:HB3	1.97	0.65
1:D:687:LEU:O	1:D:691:GLU:HG2	1.96	0.65
1:C:612:PHE:HB3	1:C:649:VAL:CG1	2.27	0.65
1:C:1044:ILE:HG22	1:C:1063:LEU:HD23	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1051:GLU:OE1	1:B:1057:THR:HG23	1.97	0.65
1:D:1060:ILE:N	1:D:1060:ILE:HD12	2.11	0.65
1:B:1045:ALA:HA	1:B:1063:LEU:HG	1.76	0.65
1:D:995:VAL:HA	1:D:999:GLY:O	1.97	0.65
1:D:1051:GLU:OE1	1:D:1057:THR:HG23	1.97	0.64
1:D:1065:VAL:HG22	1:D:1076:VAL:HG12	1.78	0.64
1:C:1066:SER:C	1:C:1068:LEU:H	2.00	0.64
1:A:784:LEU:O	1:A:788:GLN:HG2	1.96	0.64
1:B:538:PRO:HG2	1:B:599:SER:HB3	1.78	0.64
1:A:1003:THR:O	1:A:1007:VAL:HG23	1.97	0.64
1:B:908:THR:HB	1:B:909:PRO:HD3	1.80	0.64
1:D:900:MET:HE2	1:D:928:ARG:HG3	1.80	0.64
1:A:719:SER:O	1:A:722:TYR:HB3	1.97	0.64
1:A:1054:ARG:O	1:A:1054:ARG:HD3	1.98	0.64
1:B:643:LEU:O	1:B:676:VAL:HA	1.97	0.64
1:D:923:GLN:O	1:D:923:GLN:HG2	1.96	0.64
1:B:1044:ILE:H	1:B:1044:ILE:CD1	1.98	0.64
1:B:617:ARG:HH21	1:B:1016:VAL:HG21	1.63	0.64
1:B:1060:ILE:N	1:B:1060:ILE:HD12	2.13	0.64
1:C:886:LYS:HA	1:C:889:GLU:OE1	1.97	0.64
1:D:1065:VAL:O	1:D:1066:SER:CB	2.45	0.64
1:D:682:TYR:CE1	1:D:684:PRO:HB2	2.33	0.64
1:A:1066:SER:O	1:A:1068:LEU:HD23	1.97	0.64
1:A:922:VAL:HG23	1:A:923:GLN:N	2.12	0.63
1:A:947:PHE:HD1	1:A:952:ILE:HD11	1.61	0.63
1:A:1065:VAL:O	1:A:1066:SER:CB	2.45	0.63
1:B:942:ARG:O	1:B:945:VAL:HG22	1.97	0.63
1:C:899:GLN:HA	1:C:899:GLN:NE2	2.12	0.63
1:C:923:GLN:HG2	1:C:923:GLN:O	1.98	0.63
1:A:947:PHE:CD1	1:A:952:ILE:HD11	2.34	0.63
1:A:1067:ASP:OD1	1:A:1075:GLN:HB3	1.98	0.63
1:A:1065:VAL:O	1:A:1066:SER:HB3	1.99	0.63
1:B:707:THR:HG22	1:B:708:GLY:N	2.14	0.63
1:B:1058:LEU:HB3	1:B:1060:ILE:HD11	1.81	0.63
1:C:494:GLN:HG2	1:C:1056:LYS:NZ	2.14	0.63
1:D:995:VAL:HG22	1:D:1002:VAL:CG2	2.28	0.63
1:A:595:ALA:HB2	1:A:634:ILE:HG23	1.80	0.63
1:C:569:THR:HA	1:C:573:ALA:HB3	1.80	0.63
1:D:550:PRO:HB3	1:D:699:VAL:HG22	1.79	0.63
1:B:883:LEU:O	1:B:886:LYS:HB2	1.98	0.63
1:D:1044:ILE:O	1:D:1045:ALA:HB3	1.97	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1066:SER:C	1:D:1068:LEU:H	2.01	0.63
1:A:1027:PHE:HB3	1:A:1030:LEU:HD21	1.80	0.62
1:B:1073:GLN:O	1:B:1074:ARG:HB2	1.98	0.62
1:C:643:LEU:HD12	1:C:648:ALA:HA	1.81	0.62
1:C:988:GLN:CD	1:C:988:GLN:N	2.52	0.62
1:D:678:ASP:HB2	1:D:686:MET:HG3	1.80	0.62
1:B:506:HIS:HD2	1:B:1090:LYS:HE2	1.62	0.62
1:B:990:LEU:O	1:B:994:LEU:HG	2.00	0.62
1:A:558:ARG:O	1:A:558:ARG:NH1	2.31	0.62
1:B:963:PHE:O	1:B:967:VAL:HG23	1.98	0.62
1:B:865:GLU:HB2	1:B:906:LYS:NZ	2.14	0.62
1:C:778:ALA:O	1:C:780:VAL:N	2.32	0.62
1:A:711:ALA:O	1:A:713:PRO:HD3	2.00	0.62
1:D:496:ARG:NH1	1:D:1056:LYS:NZ	2.47	0.62
1:D:539:ALA:HA	1:D:636:ASN:HB2	1.82	0.62
1:D:1073:GLN:HB3	1:D:1089:VAL:O	1.99	0.62
1:B:1044:ILE:HG22	1:B:1063:LEU:HD23	1.80	0.62
1:B:1083:GLN:CD	1:B:1085:ARG:HH21	2.03	0.62
1:C:780:VAL:HG13	1:C:813:LEU:HD22	1.82	0.62
1:A:900:MET:CE	1:A:928:ARG:HG3	2.29	0.61
1:C:1067:ASP:OD2	1:C:1067:ASP:N	2.32	0.61
1:D:569:THR:HA	1:D:573:ALA:HB3	1.82	0.61
1:D:778:ALA:O	1:D:780:VAL:N	2.33	0.61
1:C:1062:ALA:O	1:C:1063:LEU:HB2	1.99	0.61
1:D:711:ALA:O	1:D:713:PRO:HD3	2.01	0.61
1:A:778:ALA:O	1:A:780:VAL:N	2.33	0.61
1:B:1067:ASP:N	1:B:1067:ASP:OD2	2.33	0.61
1:C:1060:ILE:HD12	1:C:1060:ILE:N	2.15	0.61
1:B:766:LEU:HD12	1:B:767:PRO:HD2	1.82	0.61
1:C:907:VAL:N	1:C:911:SER:HB3	2.16	0.61
1:C:1065:VAL:O	1:C:1066:SER:CB	2.48	0.61
1:D:820:THR:HB	1:D:821:PRO:HD2	1.83	0.61
1:B:1065:VAL:O	1:B:1066:SER:CB	2.49	0.61
1:C:1022:ASP:O	1:C:1025:ALA:HB3	2.01	0.61
1:A:1065:VAL:HG22	1:A:1076:VAL:HG12	1.82	0.61
1:B:644:ARG:HH11	1:B:644:ARG:HB3	1.65	0.61
1:D:574:HIS:CD2	1:D:580:THR:HA	2.36	0.61
1:D:1092:THR:HG22	1:D:1092:THR:O	2.00	0.61
1:C:1044:ILE:O	1:C:1045:ALA:HB3	2.01	0.61
1:A:1060:ILE:N	1:A:1060:ILE:HD12	2.16	0.61
1:B:575:GLN:HG3	1:B:580:THR:OG1	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:644:ARG:HH11	1:C:644:ARG:HB3	1.65	0.60
1:D:644:ARG:HB3	1:D:644:ARG:HH11	1.64	0.60
1:D:1045:ALA:CA	1:D:1063:LEU:HG	2.30	0.60
1:C:732:ARG:HH11	1:C:732:ARG:HB2	1.66	0.60
1:C:738:LEU:HD12	1:C:739:CYS:N	2.16	0.60
1:C:1044:ILE:HA	1:C:1062:ALA:HB3	1.81	0.60
1:D:564:LEU:HB2	1:D:793:VAL:HG22	1.83	0.60
1:A:1044:ILE:O	1:A:1045:ALA:HB3	2.01	0.60
1:A:1045:ALA:CA	1:A:1063:LEU:HG	2.32	0.60
1:D:612:PHE:HB3	1:D:649:VAL:CG1	2.32	0.60
1:D:717:LYS:NZ	1:D:956:HIS:O	2.28	0.60
1:D:922:VAL:HG23	1:D:923:GLN:N	2.16	0.60
1:A:494:GLN:HA	1:A:496:ARG:NH2	2.17	0.60
1:A:560:HIS:CD2	1:A:564:LEU:HD21	2.37	0.60
1:B:1044:ILE:HA	1:B:1062:ALA:HB3	1.82	0.60
1:C:538:PRO:HG2	1:C:599:SER:HB3	1.84	0.60
1:D:977:ARG:NH1	1:D:977:ARG:HB3	2.17	0.60
1:A:860:ASP:HA	1:B:832:PHE:CZ	2.36	0.60
1:D:849:ASP:HB3	1:D:851:THR:HG22	1.82	0.60
1:D:1083:GLN:CD	1:D:1085:ARG:HH21	2.05	0.60
1:B:508:MET:SD	1:B:1042:PRO:HG2	2.42	0.60
1:B:1065:VAL:HG13	1:B:1076:VAL:HG12	1.84	0.60
1:C:1076:VAL:O	1:C:1086:SER:HB2	2.01	0.60
1:C:502:HIS:HE1	1:C:1090:LYS:NZ	2.00	0.60
1:C:709:ASP:OD1	1:C:751:ALA:HB2	2.01	0.60
1:D:1008:LEU:O	1:D:1011:ALA:HB3	2.02	0.60
1:A:828:MET:O	1:A:831:VAL:HG22	2.01	0.59
1:D:683:LEU:O	1:D:687:LEU:HG	2.02	0.59
1:C:655:PRO:O	1:C:658:VAL:HG22	2.02	0.59
1:C:711:ALA:O	1:C:713:PRO:HD3	2.01	0.59
1:D:1089:VAL:HG12	1:D:1090:LYS:N	2.17	0.59
1:B:595:ALA:CB	1:B:634:ILE:HG23	2.33	0.59
1:B:612:PHE:HB2	1:B:649:VAL:HG11	1.83	0.59
1:B:743:MET:SD	1:B:907:VAL:HG22	2.43	0.59
1:A:516:ILE:O	1:A:516:ILE:HG13	2.03	0.59
1:B:665:VAL:HG12	1:B:669:ASN:ND2	2.17	0.59
1:D:947:PHE:CD1	1:D:952:ILE:HD11	2.37	0.59
1:A:1083:GLN:CD	1:A:1085:ARG:HH21	2.05	0.59
1:B:787:ALA:HB1	1:B:822:LEU:HD13	1.83	0.59
1:C:766:LEU:HD12	1:C:767:PRO:HD2	1.84	0.59
1:D:947:PHE:HD1	1:D:952:ILE:HD11	1.65	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1069:ASN:O	1:D:1071:ALA:N	2.35	0.59
1:D:990:LEU:O	1:D:994:LEU:HG	2.01	0.59
1:C:642:LEU:HD11	1:C:677:PHE:CD2	2.38	0.59
1:C:977:ARG:HH11	1:C:977:ARG:CB	2.16	0.59
1:A:1089:VAL:HG12	1:A:1090:LYS:H	1.67	0.59
1:B:1067:ASP:OD1	1:B:1075:GLN:HB3	2.03	0.59
1:C:539:ALA:HB1	1:C:543:ASP:OD2	2.01	0.59
1:C:560:HIS:CD2	1:C:564:LEU:HD21	2.38	0.59
1:D:495:ASN:OD1	1:D:499:LYS:HE3	2.02	0.59
1:D:707:THR:HG22	1:D:708:GLY:N	2.17	0.59
1:A:1065:VAL:HG22	1:A:1076:VAL:CG1	2.32	0.59
1:A:1069:ASN:O	1:A:1071:ALA:N	2.35	0.59
1:B:612:PHE:HB3	1:B:649:VAL:CG1	2.32	0.59
1:C:719:SER:O	1:C:722:TYR:HB3	2.02	0.59
1:A:550:PRO:HB3	1:A:699:VAL:HG22	1.84	0.59
1:A:1015:ASP:HB3	1:A:1019:HIS:NE2	2.18	0.59
1:D:780:VAL:HG13	1:D:813:LEU:HD22	1.85	0.59
1:D:952:ILE:HG13	1:D:953:GLY:N	2.18	0.59
1:A:1058:LEU:HB3	1:A:1060:ILE:HD11	1.85	0.58
1:C:678:ASP:HB2	1:C:686:MET:HG3	1.85	0.58
1:C:865:GLU:HB2	1:C:906:LYS:HZ2	1.66	0.58
1:C:565:LEU:O	1:C:602:PHE:HB3	2.02	0.58
1:A:952:ILE:HG13	1:A:953:GLY:N	2.19	0.58
1:B:574:HIS:CD2	1:B:580:THR:HA	2.38	0.58
1:C:936:GLU:OE2	1:C:937:GLU:N	2.36	0.58
1:A:664:GLU:O	1:A:668:GLU:HG3	2.03	0.58
1:A:936:GLU:HB3	1:A:966:LYS:NZ	2.17	0.58
1:B:498:GLN:HA	1:B:501:LEU:HD12	1.84	0.58
1:B:807:GLN:H	1:B:807:GLN:NE2	2.01	0.58
1:C:1069:ASN:O	1:C:1071:ALA:N	2.37	0.58
1:D:756:VAL:HG11	1:D:789:ALA:HB3	1.85	0.58
1:D:907:VAL:N	1:D:911:SER:HB3	2.17	0.58
1:A:499:LYS:NZ	1:A:1025:ALA:O	2.27	0.58
1:A:917:LEU:O	1:A:921:MET:HG3	2.03	0.58
1:B:590:ILE:O	1:B:594:VAL:HG23	2.03	0.58
1:D:814:VAL:O	1:D:817:THR:HG22	2.03	0.58
1:A:949:GLN:HG3	1:A:968:LEU:CD2	2.34	0.58
1:A:1045:ALA:HA	1:A:1063:LEU:HG	1.85	0.58
1:B:749:PRO:O	1:B:752:CYS:HB2	2.04	0.58
1:D:644:ARG:HB3	1:D:644:ARG:NH1	2.19	0.58
1:D:1045:ALA:HA	1:D:1063:LEU:HG	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1065:VAL:HG22	1:A:1076:VAL:HB	1.85	0.58
1:B:955:PRO:HD2	1:B:959:PHE:CE1	2.39	0.58
1:D:917:LEU:O	1:D:921:MET:HG3	2.03	0.58
1:A:650:GLY:HA3	1:A:654:TYR:OH	2.04	0.58
1:A:832:PHE:CZ	1:B:860:ASP:HA	2.39	0.58
1:A:977:ARG:HB3	1:A:977:ARG:NH1	2.18	0.58
1:B:597:ASN:HB3	1:B:830:ARG:HD3	1.86	0.57
1:D:498:GLN:NE2	1:D:498:GLN:C	2.57	0.57
1:B:570:PHE:CD2	1:B:587:LEU:HD22	2.38	0.57
1:D:498:GLN:C	1:D:498:GLN:HE21	2.07	0.57
1:D:597:ASN:HB3	1:D:830:ARG:HD3	1.85	0.57
1:A:1022:ASP:O	1:A:1025:ALA:HB3	2.03	0.57
1:B:661:LYS:O	1:B:665:VAL:HG23	2.04	0.57
1:B:996:ASP:OD1	1:B:997:ARG:N	2.38	0.57
1:B:1068:LEU:HA	1:B:1074:ARG:HE	1.68	0.57
1:A:665:VAL:HG12	1:A:669:ASN:ND2	2.18	0.57
1:C:570:PHE:CD2	1:C:587:LEU:HD22	2.40	0.57
1:C:655:PRO:HB2	1:C:984:PRO:HA	1.87	0.57
1:D:494:GLN:HA	1:D:496:ARG:NH2	2.18	0.57
1:D:649:VAL:O	1:D:649:VAL:HG12	2.04	0.57
1:A:495:ASN:OD1	1:A:499:LYS:HE3	2.04	0.57
1:B:678:ASP:OD1	1:B:682:TYR:HB3	2.04	0.57
1:B:1044:ILE:CG2	1:B:1063:LEU:HA	2.34	0.57
1:C:807:GLN:H	1:C:807:GLN:NE2	2.02	0.57
1:D:1027:PHE:HB3	1:D:1030:LEU:HD21	1.86	0.57
1:B:762:ARG:HG3	1:B:763:PHE:CE1	2.40	0.57
1:B:1044:ILE:HD12	1:B:1044:ILE:N	2.09	0.57
1:B:711:ALA:HA	1:B:754:MET:CE	2.35	0.57
1:B:1044:ILE:O	1:B:1045:ALA:HB3	2.04	0.57
1:C:641:MET:HB3	1:C:671:MET:HE3	1.86	0.57
1:A:899:GLN:HA	1:A:899:GLN:HE21	1.68	0.57
1:B:949:GLN:HG3	1:B:968:LEU:CD2	2.35	0.57
1:C:575:GLN:HG3	1:C:580:THR:OG1	2.05	0.57
1:C:711:ALA:HA	1:C:754:MET:CE	2.35	0.57
1:C:963:PHE:O	1:C:967:VAL:HG23	2.05	0.57
1:D:504:LEU:HD22	1:D:1042:PRO:HD3	1.86	0.57
1:D:904:LEU:HD12	1:D:904:LEU:N	2.20	0.57
1:C:820:THR:HB	1:C:821:PRO:HD2	1.87	0.57
1:C:898:ASN:HD22	1:C:906:LYS:HD3	1.70	0.57
1:C:1080:LEU:HD23	1:C:1085:ARG:CZ	2.35	0.57
1:D:908:THR:HB	1:D:909:PRO:HD3	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:961:GLU:OE1	1:C:964:ARG:HD3	2.05	0.56
1:D:1065:VAL:HG22	1:D:1076:VAL:CG1	2.35	0.56
1:B:700:VAL:H	1:B:736:HIS:CD2	2.06	0.56
1:B:1065:VAL:O	1:B:1066:SER:HB3	2.05	0.56
1:D:617:ARG:HH21	1:D:1016:VAL:HG21	1.70	0.56
1:A:1044:ILE:H	1:A:1044:ILE:CD1	2.01	0.56
1:B:952:ILE:HG13	1:B:953:GLY:N	2.21	0.56
1:C:504:LEU:O	1:C:508:MET:HG3	2.05	0.56
1:D:644:ARG:NH1	1:D:644:ARG:CB	2.68	0.56
1:D:995:VAL:HG22	1:D:1002:VAL:HG21	1.86	0.56
1:D:1044:ILE:HD12	1:D:1044:ILE:N	2.03	0.56
1:C:707:THR:HG22	1:C:708:GLY:N	2.21	0.56
1:C:952:ILE:HG13	1:C:953:GLY:N	2.20	0.56
1:D:1067:ASP:O	1:D:1069:ASN:N	2.39	0.56
1:B:817:THR:HG21	1:B:824:THR:HG23	1.87	0.56
1:C:653:ASN:HB3	1:C:982:LEU:HD11	1.87	0.56
1:C:701:GLU:HG3	1:C:737:ILE:HB	1.85	0.56
1:A:1065:VAL:HG22	1:A:1076:VAL:CB	2.36	0.56
1:B:919:GLN:HA	1:B:922:VAL:HG22	1.86	0.56
1:B:1044:ILE:HG22	1:B:1063:LEU:HA	1.86	0.56
1:D:743:MET:SD	1:D:907:VAL:HG22	2.46	0.56
1:C:1058:LEU:HB3	1:C:1060:ILE:HD11	1.88	0.56
1:C:1060:ILE:HG22	1:C:1061:LYS:N	2.20	0.56
1:C:1065:VAL:CG1	1:C:1076:VAL:HG12	2.33	0.56
1:D:600:LYS:HE3	1:D:825:GLU:HB3	1.88	0.56
1:A:907:VAL:HG12	1:A:908:THR:H	1.70	0.56
1:A:1090:LYS:H	1:A:1090:LYS:HD2	1.70	0.56
1:B:778:ALA:O	1:B:780:VAL:N	2.39	0.56
1:C:644:ARG:HD2	1:C:647:ASN:OD1	2.05	0.56
1:C:1044:ILE:CG2	1:C:1063:LEU:HA	2.36	0.56
1:D:542:ARG:H	1:D:638:PRO:HD3	1.71	0.56
1:D:558:ARG:O	1:D:558:ARG:NH1	2.38	0.56
1:C:500:LEU:O	1:C:503:TYR:HB3	2.06	0.56
1:C:647:ASN:ND2	1:C:650:GLY:O	2.39	0.56
1:D:649:VAL:N	1:D:1012:MET:HE1	2.17	0.56
1:D:727:ALA:O	1:D:731:VAL:HG23	2.05	0.56
1:D:766:LEU:HD12	1:D:767:PRO:HD2	1.88	0.56
1:D:1063:LEU:O	1:D:1064:ALA:CB	2.53	0.56
1:A:881:MET:O	1:A:883:LEU:HG	2.05	0.56
1:C:1068:LEU:HA	1:C:1074:ARG:HE	1.70	0.56
1:D:1068:LEU:HA	1:D:1074:ARG:HE	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1066:SER:C	1:B:1068:LEU:H	2.09	0.55
1:C:922:VAL:HG23	1:C:923:GLN:N	2.22	0.55
1:D:565:LEU:O	1:D:602:PHE:HB3	2.06	0.55
1:A:961:GLU:OE1	1:A:964:ARG:HD3	2.06	0.55
1:B:569:THR:HA	1:B:573:ALA:HB3	1.87	0.55
1:B:655:PRO:O	1:B:658:VAL:HG22	2.06	0.55
1:D:547:ARG:C	1:D:548:GLU:HG3	2.26	0.55
1:D:936:GLU:HB3	1:D:966:LYS:HZ1	1.69	0.55
1:A:990:LEU:O	1:A:994:LEU:HG	2.07	0.55
1:B:539:ALA:HA	1:B:636:ASN:CB	2.34	0.55
1:B:995:VAL:HA	1:B:999:GLY:O	2.07	0.55
1:A:707:THR:HG22	1:A:708:GLY:N	2.21	0.55
1:A:949:GLN:HG3	1:A:968:LEU:HD22	1.89	0.55
1:D:700:VAL:H	1:D:736:HIS:CD2	2.08	0.55
1:D:968:LEU:O	1:D:971:LEU:HD12	2.06	0.55
1:A:502:HIS:HE1	1:A:1090:LYS:NZ	2.04	0.55
1:A:649:VAL:N	1:A:1012:MET:HE1	2.16	0.55
1:B:649:VAL:N	1:B:1012:MET:HE1	2.21	0.55
1:C:1065:VAL:HG22	1:C:1076:VAL:HB	1.87	0.55
1:A:502:HIS:CE1	1:A:1090:LYS:NZ	2.75	0.55
1:B:665:VAL:HG21	1:B:1008:LEU:CD1	2.27	0.55
1:B:908:THR:HG22	1:B:909:PRO:N	2.21	0.55
1:B:1065:VAL:HG22	1:B:1076:VAL:CB	2.37	0.55
1:C:558:ARG:O	1:C:558:ARG:NH1	2.36	0.55
1:D:949:GLN:HG3	1:D:968:LEU:CD2	2.36	0.55
1:A:995:VAL:HG13	1:A:1000:GLU:HA	1.87	0.55
1:A:1068:LEU:HA	1:A:1074:ARG:HE	1.71	0.55
1:C:961:GLU:OE2	1:C:965:SER:HB3	2.07	0.55
1:D:917:LEU:HB2	1:D:944:VAL:HG21	1.88	0.55
1:A:665:VAL:HG12	1:A:669:ASN:HD22	1.72	0.55
1:A:907:VAL:N	1:A:911:SER:HB3	2.21	0.55
1:B:494:GLN:HG2	1:B:1056:LYS:NZ	2.22	0.55
1:B:644:ARG:HB3	1:B:644:ARG:NH1	2.22	0.55
1:B:917:LEU:O	1:B:921:MET:HG3	2.07	0.55
1:B:1065:VAL:HG22	1:B:1076:VAL:HB	1.89	0.55
1:C:494:GLN:HA	1:C:496:ARG:NH2	2.21	0.55
1:C:983:PRO:O	1:C:984:PRO:O	2.25	0.55
1:D:898:ASN:ND2	1:D:904:LEU:H	2.04	0.55
1:A:780:VAL:HG13	1:A:813:LEU:HD22	1.88	0.55
1:A:810:MET:O	1:A:814:VAL:HG23	2.07	0.55
1:B:907:VAL:N	1:B:911:SER:HB3	2.22	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:643:LEU:HD11	1:C:648:ALA:HA	1.89	0.55
1:B:900:MET:HE1	1:B:921:MET:SD	2.46	0.54
1:B:682:TYR:CE1	1:B:684:PRO:HB2	2.42	0.54
1:B:945:VAL:HG23	1:B:946:GLU:N	2.22	0.54
1:C:569:THR:HA	1:C:573:ALA:CB	2.37	0.54
1:C:1052:LEU:HD23	1:C:1053:GLU:HB2	1.89	0.54
1:A:644:ARG:HH11	1:A:644:ARG:HB3	1.72	0.54
1:A:1092:THR:HG22	1:A:1092:THR:O	2.07	0.54
1:B:569:THR:HA	1:B:573:ALA:CB	2.37	0.54
1:C:1008:LEU:O	1:C:1011:ALA:HB3	2.08	0.54
1:C:1044:ILE:HG22	1:C:1063:LEU:HA	1.89	0.54
1:D:678:ASP:HB2	1:D:686:MET:CG	2.38	0.54
1:A:787:ALA:HB1	1:A:822:LEU:HD13	1.90	0.54
1:C:894:TYR:CE2	1:C:906:LYS:HD2	2.42	0.54
1:C:945:VAL:HG23	1:C:946:GLU:N	2.22	0.54
1:A:571:ARG:NH1	1:A:575:GLN:NE2	2.50	0.54
1:A:817:THR:HG21	1:A:824:THR:HG23	1.90	0.54
1:A:899:GLN:HE22	1:A:903:ASP:HB2	1.72	0.54
1:A:952:ILE:HG13	1:A:953:GLY:H	1.73	0.54
1:B:558:ARG:O	1:B:558:ARG:NH1	2.37	0.54
1:C:502:HIS:CE1	1:C:1090:LYS:NZ	2.75	0.54
1:C:919:GLN:HA	1:C:922:VAL:HG22	1.89	0.54
1:C:1090:LYS:H	1:C:1090:LYS:HD2	1.72	0.54
1:A:612:PHE:HB3	1:A:649:VAL:HG11	1.89	0.54
1:A:1049:GLU:HA	1:A:1058:LEU:O	2.08	0.54
1:B:974:VAL:HG11	1:B:978:PRO:HG3	1.88	0.54
1:B:1020:PHE:O	1:B:1024:THR:HG23	2.08	0.54
1:C:955:PRO:HD2	1:C:959:PHE:CE1	2.42	0.54
1:D:595:ALA:HB2	1:D:634:ILE:HG23	1.89	0.54
1:B:719:SER:O	1:B:722:TYR:HB3	2.08	0.54
1:C:887:PHE:CE2	1:C:891:LYS:HE3	2.43	0.54
1:A:1063:LEU:O	1:A:1064:ALA:CB	2.55	0.54
1:D:494:GLN:HG2	1:D:1056:LYS:NZ	2.23	0.54
1:D:516:ILE:O	1:D:516:ILE:HG13	2.08	0.54
1:A:598:PHE:O	1:A:601:LEU:HB2	2.08	0.54
1:A:678:ASP:HB2	1:A:686:MET:HG3	1.90	0.54
1:B:502:HIS:HE1	1:B:1090:LYS:NZ	2.05	0.54
1:B:686:MET:O	1:B:690:MET:HG3	2.08	0.54
1:D:901:LEU:HA	1:D:960:PRO:HG3	1.90	0.54
1:A:643:LEU:CD1	1:A:648:ALA:HA	2.38	0.53
1:B:849:ASP:CB	1:B:851:THR:HG22	2.36	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:595:ALA:CB	1:C:634:ILE:HG23	2.37	0.53
1:C:902:GLY:O	1:C:903:ASP:O	2.24	0.53
1:D:749:PRO:O	1:D:752:CYS:HB2	2.08	0.53
1:A:621:GLU:HG2	1:A:1031:ASP:HB3	1.90	0.53
1:A:942:ARG:O	1:A:945:VAL:HG22	2.09	0.53
1:C:1073:GLN:HB3	1:C:1089:VAL:O	2.08	0.53
1:A:917:LEU:HB2	1:A:944:VAL:HG21	1.90	0.53
1:C:717:LYS:NZ	1:C:956:HIS:O	2.36	0.53
1:C:865:GLU:HB2	1:C:906:LYS:NZ	2.23	0.53
1:A:766:LEU:HD12	1:A:767:PRO:HD2	1.90	0.53
1:A:907:VAL:HG12	1:A:908:THR:N	2.24	0.53
1:A:1066:SER:O	1:A:1068:LEU:N	2.35	0.53
1:B:1062:ALA:O	1:B:1063:LEU:HB2	2.08	0.53
1:B:1092:THR:O	1:B:1092:THR:HG22	2.08	0.53
1:C:678:ASP:OD1	1:C:682:TYR:HB3	2.08	0.53
1:C:832:PHE:CZ	1:D:860:ASP:HA	2.43	0.53
1:D:496:ARG:NH1	1:D:1056:LYS:HZ2	2.07	0.53
1:A:771:HIS:HB2	1:A:795:ASP:OD2	2.09	0.53
1:B:701:GLU:OE2	1:B:769:HIS:ND1	2.35	0.53
1:B:1027:PHE:HB3	1:B:1030:LEU:HD21	1.91	0.53
1:B:1063:LEU:O	1:B:1064:ALA:CB	2.56	0.53
1:D:569:THR:HA	1:D:573:ALA:CB	2.38	0.53
1:B:807:GLN:NE2	1:B:807:GLN:N	2.57	0.53
1:B:1015:ASP:HB3	1:B:1019:HIS:NE2	2.24	0.53
1:C:711:ALA:HA	1:C:754:MET:HE1	1.91	0.53
1:C:1049:GLU:HA	1:C:1058:LEU:O	2.09	0.53
1:D:919:GLN:HA	1:D:922:VAL:HG22	1.90	0.53
1:B:678:ASP:HB2	1:B:686:MET:CG	2.39	0.53
1:B:678:ASP:HB2	1:B:686:MET:HG3	1.91	0.53
1:C:732:ARG:HB2	1:C:732:ARG:NH1	2.24	0.53
1:D:906:LYS:C	1:D:911:SER:HB3	2.29	0.53
1:A:737:ILE:HG23	1:A:767:PRO:HB2	1.89	0.53
1:B:565:LEU:O	1:B:602:PHE:HB3	2.08	0.53
1:C:915:GLY:O	1:C:919:GLN:HG3	2.08	0.53
1:D:817:THR:HG21	1:D:824:THR:HG23	1.91	0.53
1:A:612:PHE:HB3	1:A:649:VAL:CG1	2.40	0.53
1:C:1005:GLU:H	1:C:1005:GLU:CD	2.12	0.53
1:C:1044:ILE:H	1:C:1044:ILE:CD1	2.11	0.53
1:A:907:VAL:O	1:A:908:THR:C	2.47	0.52
1:B:642:LEU:HD11	1:B:677:PHE:CD2	2.44	0.52
1:B:1088:LEU:HD23	1:B:1089:VAL:N	2.23	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:701:GLU:HG3	1:A:737:ILE:HB	1.92	0.52
1:A:1044:ILE:HD12	1:A:1044:ILE:N	2.15	0.52
1:C:829:GLU:O	1:C:832:PHE:HB2	2.08	0.52
1:C:738:LEU:HD12	1:C:739:CYS:H	1.74	0.52
1:D:899:GLN:HA	1:D:899:GLN:NE2	2.24	0.52
1:D:655:PRO:HB2	1:D:657:ASN:OD1	2.09	0.52
1:D:922:VAL:HG23	1:D:923:GLN:H	1.75	0.52
1:C:506:HIS:HD2	1:C:1090:LYS:HE2	1.73	0.52
1:C:887:PHE:O	1:C:890:VAL:HG22	2.09	0.52
1:A:820:THR:HB	1:A:821:PRO:HD2	1.92	0.52
1:B:879:HIS:CE1	1:B:884:GLY:HA3	2.45	0.52
1:B:977:ARG:NH1	1:B:977:ARG:HB3	2.25	0.52
1:C:641:MET:HB3	1:C:671:MET:HE1	1.90	0.52
1:C:766:LEU:HD12	1:C:767:PRO:CD	2.39	0.52
1:C:898:ASN:ND2	1:C:904:LEU:H	2.08	0.52
1:A:504:LEU:O	1:A:508:MET:HG3	2.10	0.52
1:B:736:HIS:O	1:B:737:ILE:HD13	2.09	0.52
1:C:601:LEU:CD2	1:C:603:SER:O	2.56	0.52
1:C:936:GLU:HB3	1:C:966:LYS:HZ1	1.75	0.52
1:D:793:VAL:HG12	1:D:794:VAL:N	2.24	0.52
1:C:644:ARG:NH1	1:C:644:ARG:CB	2.73	0.52
1:A:1073:GLN:HB3	1:A:1089:VAL:O	2.10	0.52
1:C:683:LEU:O	1:C:687:LEU:HG	2.10	0.52
1:C:1045:ALA:N	1:C:1063:LEU:HG	2.25	0.52
1:D:928:ARG:O	1:D:932:GLU:HG3	2.09	0.52
1:A:500:LEU:O	1:A:503:TYR:HB3	2.09	0.51
1:C:1066:SER:O	1:C:1068:LEU:N	2.34	0.51
1:D:648:ALA:HB3	1:D:1012:MET:CE	2.39	0.51
1:B:644:ARG:NH1	1:B:644:ARG:CB	2.73	0.51
1:B:704:ILE:HG23	1:B:726:LEU:HD23	1.91	0.51
1:D:898:ASN:HD21	1:D:904:LEU:H	1.56	0.51
1:D:1066:SER:O	1:D:1068:LEU:N	2.37	0.51
1:A:897:ALA:HB2	1:A:921:MET:HE2	1.91	0.51
1:B:810:MET:O	1:B:814:VAL:HG23	2.10	0.51
1:A:900:MET:HE2	1:A:928:ARG:CG	2.38	0.51
1:A:1008:LEU:O	1:A:1011:ALA:HB3	2.09	0.51
1:C:643:LEU:O	1:C:676:VAL:HA	2.10	0.51
1:D:641:MET:HB3	1:D:671:MET:HE1	1.92	0.51
1:A:923:GLN:O	1:A:923:GLN:HG2	2.10	0.51
1:B:756:VAL:O	1:B:759:LEU:HB2	2.11	0.51
1:C:644:ARG:HB3	1:C:644:ARG:NH1	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1089:VAL:CG1	1:C:1090:LYS:H	2.22	0.51
1:D:907:VAL:HG12	1:D:908:THR:H	1.76	0.51
1:D:1060:ILE:HG22	1:D:1061:LYS:N	2.26	0.51
1:A:1052:LEU:HD22	1:A:1056:LYS:HD2	1.92	0.51
1:A:1068:LEU:HD13	1:A:1074:ARG:HH22	1.72	0.51
1:C:553:PHE:O	1:C:557:VAL:HG23	2.10	0.51
1:C:1065:VAL:HG22	1:C:1076:VAL:CB	2.41	0.51
1:D:502:HIS:HA	1:D:1087:ILE:HG21	1.91	0.51
1:D:1017:PHE:CZ	1:D:1021:LYS:HD3	2.45	0.51
1:A:641:MET:HB3	1:A:671:MET:CE	2.41	0.51
1:A:887:PHE:HA	1:A:890:VAL:HG22	1.93	0.51
1:A:999:GLY:C	1:A:1001:GLU:H	2.14	0.51
1:A:1001:GLU:OE1	1:A:1001:GLU:HA	2.11	0.51
1:A:1001:GLU:O	1:A:1002:VAL:C	2.49	0.51
1:B:899:GLN:HA	1:B:899:GLN:HE21	1.75	0.51
1:B:1076:VAL:O	1:B:1086:SER:HB2	2.11	0.51
1:C:574:HIS:CD2	1:C:580:THR:HA	2.46	0.51
1:C:654:TYR:CE1	1:C:1012:MET:HE2	2.46	0.51
1:D:720:LEU:HD22	1:D:754:MET:SD	2.50	0.51
1:D:867:PRO:HG2	1:D:870:GLN:HB3	1.93	0.51
1:A:1062:ALA:O	1:A:1063:LEU:HB2	2.11	0.51
1:C:1054:ARG:O	1:C:1054:ARG:HD3	2.10	0.51
1:D:787:ALA:HB1	1:D:822:LEU:HD13	1.92	0.51
1:C:561:PRO:HG2	1:C:562:GLY:H	1.76	0.51
1:D:1073:GLN:O	1:D:1074:ARG:HB2	2.09	0.51
1:A:1080:LEU:HD23	1:A:1085:ARG:CZ	2.41	0.50
1:B:653:ASN:HB3	1:B:982:LEU:HD11	1.92	0.50
1:B:1069:ASN:O	1:B:1071:ALA:N	2.44	0.50
1:C:665:VAL:HG12	1:C:669:ASN:ND2	2.26	0.50
1:A:749:PRO:HD3	1:B:816:CYS:SG	2.51	0.50
1:A:1068:LEU:HA	1:A:1074:ARG:NE	2.26	0.50
1:B:506:HIS:CD2	1:B:1090:LYS:HE2	2.45	0.50
1:C:928:ARG:O	1:C:932:GLU:HG3	2.11	0.50
1:D:496:ARG:HH11	1:D:1056:LYS:HZ2	1.59	0.50
1:D:547:ARG:NH1	1:D:548:GLU:OE1	2.43	0.50
1:D:651:TYR:CD1	1:D:652:THR:HG23	2.46	0.50
1:D:686:MET:O	1:D:690:MET:HG3	2.11	0.50
1:D:881:MET:O	1:D:883:LEU:HG	2.11	0.50
1:D:900:MET:CE	1:D:928:ARG:HG3	2.41	0.50
1:A:648:ALA:HB3	1:A:1012:MET:CE	2.42	0.50
1:A:961:GLU:O	1:A:962:PRO:C	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1092:THR:O	1:A:1093:GLN:C	2.50	0.50
1:B:665:VAL:CG2	1:B:1008:LEU:HD11	2.30	0.50
1:C:678:ASP:HB2	1:C:686:MET:CG	2.41	0.50
1:C:887:PHE:CD2	1:C:891:LYS:HE3	2.46	0.50
1:C:949:GLN:HG3	1:C:968:LEU:CD2	2.41	0.50
1:A:1073:GLN:O	1:A:1074:ARG:HB2	2.10	0.50
1:B:502:HIS:CE1	1:B:1090:LYS:NZ	2.79	0.50
1:C:527:PRO:HB2	1:C:837:TYR:CE1	2.47	0.50
1:C:1015:ASP:HB3	1:C:1019:HIS:NE2	2.27	0.50
1:A:655:PRO:HB2	1:A:984:PRO:HA	1.92	0.50
1:B:833:ASP:O	1:B:836:GLU:HB3	2.11	0.50
1:B:898:ASN:HD21	1:B:904:LEU:N	2.06	0.50
1:B:965:SER:C	1:B:967:VAL:N	2.65	0.50
1:D:506:HIS:HD2	1:D:1090:LYS:HE2	1.77	0.50
1:D:1078:PHE:C	1:D:1079:GLU:OE1	2.50	0.50
1:A:1067:ASP:O	1:A:1069:ASN:N	2.45	0.50
1:B:683:LEU:O	1:B:687:LEU:HG	2.11	0.50
1:C:879:HIS:CE1	1:C:884:GLY:HA3	2.46	0.50
1:D:779:GLY:O	1:D:783:MET:HG2	2.11	0.50
1:D:894:TYR:CE2	1:D:906:LYS:HD2	2.46	0.50
1:B:807:GLN:H	1:B:807:GLN:HE21	1.59	0.50
1:C:505:GLY:O	1:C:508:MET:HB2	2.11	0.50
1:C:552:GLY:HA2	1:C:555:ARG:HD2	1.93	0.50
1:C:590:ILE:O	1:C:594:VAL:HG23	2.11	0.50
1:C:749:PRO:O	1:C:752:CYS:HB2	2.12	0.50
1:C:995:VAL:HA	1:C:999:GLY:O	2.12	0.50
1:D:641:MET:HB3	1:D:671:MET:HE3	1.93	0.50
1:D:936:GLU:HB3	1:D:966:LYS:HZ2	1.77	0.50
1:D:977:ARG:HB3	1:D:977:ARG:HH11	1.77	0.50
1:D:995:VAL:HG13	1:D:1000:GLU:HA	1.93	0.50
1:B:738:LEU:HD12	1:B:739:CYS:N	2.27	0.50
1:B:922:VAL:HG23	1:B:923:GLN:H	1.77	0.50
1:B:1090:LYS:H	1:B:1090:LYS:HD2	1.76	0.50
1:C:495:ASN:OD1	1:C:499:LYS:HE3	2.12	0.50
1:C:665:VAL:CG2	1:C:1008:LEU:HD11	2.36	0.50
1:C:1089:VAL:CG1	1:C:1090:LYS:N	2.74	0.50
1:A:655:PRO:HG3	1:A:985:LEU:HB2	1.93	0.49
1:A:1060:ILE:HG22	1:A:1061:LYS:N	2.28	0.49
1:A:1063:LEU:O	1:A:1064:ALA:HB3	2.11	0.49
1:D:865:GLU:HB2	1:D:906:LYS:NZ	2.27	0.49
1:B:598:PHE:O	1:B:601:LEU:HB2	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:664:GLU:O	1:B:668:GLU:HG3	2.11	0.49
1:B:802:SER:HB2	1:B:807:GLN:O	2.12	0.49
1:C:828:MET:O	1:C:831:VAL:HG22	2.11	0.49
1:D:874:LEU:N	1:D:874:LEU:CD1	2.75	0.49
1:D:1044:ILE:HA	1:D:1062:ALA:HB3	1.94	0.49
1:A:922:VAL:HG23	1:A:923:GLN:H	1.78	0.49
1:B:650:GLY:HA3	1:B:654:TYR:CE1	2.48	0.49
1:B:965:SER:C	1:B:967:VAL:H	2.15	0.49
1:C:762:ARG:HG3	1:C:763:PHE:CE1	2.47	0.49
1:C:934:GLN:O	1:C:938:LEU:HG	2.12	0.49
1:C:949:GLN:HG3	1:C:968:LEU:HD22	1.94	0.49
1:C:996:ASP:OD1	1:C:997:ARG:N	2.45	0.49
1:D:893:ALA:CB	1:D:922:VAL:HG13	2.42	0.49
1:A:590:ILE:O	1:A:594:VAL:HG23	2.12	0.49
1:A:919:GLN:HA	1:A:922:VAL:HG22	1.93	0.49
1:B:860:ASP:OD2	1:B:860:ASP:C	2.50	0.49
1:B:1010:ALA:HB2	1:B:1017:PHE:CD2	2.47	0.49
1:C:516:ILE:O	1:C:516:ILE:HG13	2.12	0.49
1:D:538:PRO:O	1:D:539:ALA:HB3	2.11	0.49
1:D:661:LYS:O	1:D:665:VAL:HG23	2.12	0.49
1:D:1066:SER:O	1:D:1068:LEU:HD23	2.12	0.49
1:A:650:GLY:HA3	1:A:654:TYR:CE1	2.47	0.49
1:C:656:ASP:CG	1:C:977:ARG:HH21	2.15	0.49
1:D:887:PHE:HA	1:D:890:VAL:HG22	1.95	0.49
1:C:779:GLY:O	1:C:783:MET:HG2	2.13	0.49
1:C:867:PRO:HD2	1:C:870:GLN:OE1	2.12	0.49
1:C:887:PHE:HA	1:C:890:VAL:HG22	1.95	0.49
1:C:893:ALA:HB2	1:C:922:VAL:CG1	2.41	0.49
1:D:496:ARG:NH1	1:D:1056:LYS:HZ1	2.11	0.49
1:A:617:ARG:HH21	1:A:1016:VAL:HG21	1.77	0.49
1:A:643:LEU:O	1:A:676:VAL:HA	2.12	0.49
1:C:591:ALA:HB3	1:C:633:LEU:HD13	1.94	0.49
1:D:807:GLN:H	1:D:807:GLN:NE2	2.11	0.49
1:D:945:VAL:HG23	1:D:946:GLU:N	2.28	0.49
1:D:997:ARG:HD2	1:D:998:HIS:CD2	2.47	0.49
1:D:1002:VAL:O	1:D:1002:VAL:HG23	2.12	0.49
1:A:1057:THR:HB	1:A:1059:HIS:CE1	2.48	0.49
1:B:539:ALA:HB1	1:B:543:ASP:OD2	2.12	0.49
1:C:650:GLY:HA3	1:C:654:TYR:CE1	2.48	0.49
1:C:942:ARG:O	1:C:945:VAL:CG2	2.55	0.49
1:C:995:VAL:CG2	1:C:1002:VAL:HG21	2.38	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:996:ASP:OD1	1:D:997:ARG:N	2.46	0.49
1:A:824:THR:O	1:A:825:GLU:HB2	2.12	0.49
1:A:860:ASP:OD2	1:A:860:ASP:C	2.51	0.49
1:A:1044:ILE:O	1:A:1045:ALA:CB	2.61	0.49
1:B:498:GLN:C	1:B:498:GLN:HE21	2.16	0.49
1:B:766:LEU:HD12	1:B:767:PRO:CD	2.43	0.49
1:C:1079:GLU:HA	1:C:1084:LEU:HB3	1.94	0.49
1:D:701:GLU:HG3	1:D:737:ILE:HB	1.94	0.49
1:D:736:HIS:O	1:D:737:ILE:HD13	2.13	0.49
1:D:828:MET:O	1:D:831:VAL:HG22	2.12	0.49
1:A:887:PHE:CE2	1:A:891:LYS:HE3	2.48	0.49
1:A:904:LEU:HD12	1:A:904:LEU:N	2.27	0.49
1:A:1044:ILE:HG22	1:A:1063:LEU:HA	1.95	0.49
1:A:1058:LEU:HD22	1:A:1080:LEU:HD11	1.95	0.49
1:A:1076:VAL:HG23	1:A:1078:PHE:CE1	2.48	0.49
1:B:780:VAL:HG13	1:B:813:LEU:HD22	1.94	0.49
1:B:903:ASP:C	1:B:904:LEU:HD12	2.32	0.49
1:B:1063:LEU:O	1:B:1064:ALA:HB3	2.13	0.49
1:C:961:GLU:HA	1:C:964:ARG:HB3	1.95	0.49
1:D:1044:ILE:O	1:D:1045:ALA:CB	2.61	0.49
1:A:673:VAL:HA	1:A:699:VAL:HB	1.94	0.48
1:A:701:GLU:HA	1:A:737:ILE:O	2.12	0.48
1:B:873:ASN:O	1:B:877:GLN:HG2	2.13	0.48
1:D:879:HIS:CE1	1:D:884:GLY:HA3	2.48	0.48
1:D:886:LYS:HD3	1:D:889:GLU:OE1	2.12	0.48
1:A:552:GLY:HA2	1:A:555:ARG:HD2	1.96	0.48
1:B:498:GLN:C	1:B:498:GLN:NE2	2.66	0.48
1:B:865:GLU:HB2	1:B:906:LYS:HZ2	1.78	0.48
1:D:1063:LEU:O	1:D:1064:ALA:HB3	2.12	0.48
1:D:771:HIS:HE1	1:D:807:GLN:OE1	1.97	0.48
1:D:952:ILE:HG13	1:D:953:GLY:H	1.77	0.48
1:C:965:SER:C	1:C:967:VAL:N	2.67	0.48
1:C:1065:VAL:HG22	1:C:1076:VAL:HG12	1.95	0.48
1:D:517:PRO:HG2	1:D:847:ALA:O	2.12	0.48
1:D:756:VAL:O	1:D:759:LEU:HB2	2.13	0.48
1:A:494:GLN:HG2	1:A:1056:LYS:HZ3	1.79	0.48
1:B:896:GLU:O	1:B:900:MET:HB2	2.13	0.48
1:B:1001:GLU:HA	1:B:1001:GLU:OE1	2.13	0.48
1:B:1089:VAL:CG1	1:B:1090:LYS:H	2.26	0.48
1:C:644:ARG:O	1:C:645:GLY:C	2.52	0.48
1:C:1088:LEU:HD23	1:C:1089:VAL:N	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:942:ARG:O	1:D:945:VAL:CG2	2.60	0.48
1:D:1074:ARG:O	1:D:1088:LEU:HD23	2.14	0.48
1:A:899:GLN:HE21	1:A:899:GLN:CA	2.24	0.48
1:B:829:GLU:O	1:B:832:PHE:HB2	2.13	0.48
1:C:566:MET:CE	1:C:605:GLU:HB2	2.42	0.48
1:C:900:MET:CE	1:C:928:ARG:HG3	2.41	0.48
1:C:1065:VAL:HG22	1:C:1076:VAL:CG1	2.44	0.48
1:D:711:ALA:HA	1:D:754:MET:CE	2.44	0.48
1:A:677:PHE:CE1	1:A:907:VAL:HG11	2.48	0.48
1:A:711:ALA:HA	1:A:754:MET:CE	2.43	0.48
1:A:743:MET:SD	1:A:907:VAL:HG22	2.54	0.48
1:A:793:VAL:HG12	1:A:794:VAL:N	2.28	0.48
1:A:870:GLN:O	1:A:874:LEU:HD13	2.14	0.48
1:C:883:LEU:HD22	1:C:886:LYS:HG3	1.95	0.48
1:C:1092:THR:HG22	1:C:1092:THR:O	2.13	0.48
1:A:959:PHE:HB2	1:A:964:ARG:HD2	1.96	0.48
1:C:502:HIS:HE1	1:C:1090:LYS:HZ3	1.61	0.48
1:C:860:ASP:OD2	1:C:860:ASP:C	2.52	0.48
1:B:1049:GLU:HA	1:B:1058:LEU:O	2.13	0.48
1:C:700:VAL:H	1:C:736:HIS:CD2	2.19	0.48
1:C:901:LEU:HA	1:C:960:PRO:HG3	1.94	0.48
1:D:581:ARG:HG3	1:D:848:PHE:CD2	2.49	0.48
1:D:756:VAL:CG1	1:D:789:ALA:HB3	2.43	0.48
1:D:887:PHE:O	1:D:890:VAL:HG22	2.13	0.48
1:D:1068:LEU:HA	1:D:1074:ARG:NE	2.29	0.48
1:D:1080:LEU:HD23	1:D:1085:ARG:CZ	2.44	0.48
1:A:865:GLU:HB2	1:A:906:LYS:NZ	2.29	0.48
1:B:665:VAL:HG12	1:B:669:ASN:HD22	1.79	0.48
1:B:893:ALA:HB2	1:B:922:VAL:CG1	2.43	0.48
1:C:517:PRO:HG2	1:C:847:ALA:O	2.13	0.48
1:B:643:LEU:CD1	1:B:648:ALA:HA	2.43	0.47
1:B:961:GLU:OE1	1:B:964:ARG:HD3	2.13	0.47
1:B:1079:GLU:HA	1:B:1084:LEU:HB3	1.95	0.47
1:C:936:GLU:HB3	1:C:966:LYS:HZ2	1.77	0.47
1:C:1001:GLU:OE1	1:C:1001:GLU:HA	2.14	0.47
1:D:679:SER:HB2	1:D:910:SER:OG	2.14	0.47
1:B:530:PRO:HB2	1:B:593:TYR:CD1	2.49	0.47
1:B:538:PRO:O	1:B:539:ALA:HB3	2.14	0.47
1:B:709:ASP:OD1	1:B:751:ALA:HB2	2.14	0.47
1:B:820:THR:HB	1:B:821:PRO:HD2	1.96	0.47
1:C:771:HIS:HB2	1:C:795:ASP:OD2	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:870:GLN:HA	1:D:873:ASN:HD22	1.79	0.47
1:D:1058:LEU:HB3	1:D:1060:ILE:HD11	1.96	0.47
1:B:922:VAL:CG2	1:B:923:GLN:N	2.76	0.47
1:A:738:LEU:HD12	1:A:739:CYS:H	1.78	0.47
1:B:712:ASP:OD1	1:B:714:SER:HB2	2.15	0.47
1:C:494:GLN:HG2	1:C:1056:LYS:HZ3	1.79	0.47
1:A:1079:GLU:N	1:A:1079:GLU:OE1	2.47	0.47
1:C:864:ASN:HA	1:C:895:VAL:HG22	1.96	0.47
1:D:947:PHE:O	1:D:959:PHE:HE2	1.98	0.47
1:A:571:ARG:HG3	1:A:607:TRP:O	2.15	0.47
1:C:876:PHE:O	1:C:880:SER:HB3	2.14	0.47
1:D:1054:ARG:O	1:D:1054:ARG:HD3	2.15	0.47
1:A:502:HIS:HA	1:A:1087:ILE:HG21	1.96	0.47
1:A:565:LEU:O	1:A:602:PHE:HB3	2.14	0.47
1:A:679:SER:HB2	1:A:910:SER:OG	2.14	0.47
1:A:779:GLY:O	1:A:783:MET:HG2	2.15	0.47
1:A:988:GLN:CD	1:A:988:GLN:H	2.17	0.47
1:B:680:LEU:HD11	1:B:952:ILE:HD12	1.96	0.47
1:B:904:LEU:N	1:B:904:LEU:CD1	2.77	0.47
1:C:682:TYR:CE1	1:C:684:PRO:HB2	2.50	0.47
1:C:965:SER:HA	1:C:973:ARG:NH2	2.29	0.47
1:D:503:TYR:O	1:D:507:VAL:HG23	2.14	0.47
1:D:890:VAL:HG23	1:D:891:LYS:N	2.30	0.47
1:D:923:GLN:HE21	1:D:924:ASN:ND2	2.13	0.47
1:A:624:TRP:CG	1:A:1005:GLU:HB3	2.49	0.47
1:B:641:MET:HB3	1:B:671:MET:HE3	1.96	0.47
1:B:679:SER:OG	1:B:680:LEU:HD12	2.13	0.47
1:B:1074:ARG:O	1:B:1088:LEU:HD23	2.14	0.47
1:C:641:MET:O	1:C:641:MET:HG3	2.15	0.47
1:C:1013:TYR:HB3	1:C:1016:VAL:HB	1.96	0.47
1:C:1063:LEU:O	1:C:1064:ALA:HB3	2.14	0.47
1:D:560:HIS:CD2	1:D:564:LEU:HD21	2.50	0.47
1:A:686:MET:O	1:A:690:MET:HG3	2.15	0.47
1:B:711:ALA:HA	1:B:754:MET:HE1	1.97	0.47
1:C:580:THR:O	1:C:614:VAL:HG11	2.14	0.47
1:C:1043:LYS:O	1:C:1046:GLU:HB2	2.15	0.47
1:C:1044:ILE:O	1:C:1045:ALA:CB	2.63	0.47
1:D:1089:VAL:HG12	1:D:1090:LYS:H	1.79	0.47
1:B:739:CYS:HA	1:B:769:HIS:O	2.15	0.47
1:D:648:ALA:HB3	1:D:1012:MET:HE1	1.96	0.47
1:D:1003:THR:HB	1:D:1004:PRO:HD2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:494:GLN:CG	1:A:1056:LYS:NZ	2.76	0.46
1:A:738:LEU:HD12	1:A:739:CYS:N	2.31	0.46
1:A:755:LEU:HD22	1:A:759:LEU:CD1	2.45	0.46
1:B:517:PRO:HG2	1:B:847:ALA:O	2.16	0.46
1:B:988:GLN:CD	1:B:988:GLN:H	2.16	0.46
1:C:904:LEU:N	1:C:904:LEU:HD12	2.30	0.46
1:D:824:THR:O	1:D:825:GLU:HB2	2.14	0.46
1:D:1079:GLU:OE1	1:D:1079:GLU:N	2.47	0.46
1:A:502:HIS:CE1	1:A:1090:LYS:HZ1	2.32	0.46
1:A:583:ARG:NH1	1:A:1033:LEU:O	2.48	0.46
1:A:704:ILE:HB	1:A:740:ILE:HD13	1.97	0.46
1:A:1078:PHE:C	1:A:1079:GLU:OE1	2.53	0.46
1:B:997:ARG:HD2	1:B:998:HIS:CD2	2.50	0.46
1:C:547:ARG:C	1:C:548:GLU:HG3	2.35	0.46
1:D:644:ARG:HD2	1:D:647:ASN:OD1	2.15	0.46
1:D:656:ASP:OD2	1:D:977:ARG:NH2	2.49	0.46
1:A:785:ALA:O	1:A:788:GLN:HB2	2.15	0.46
1:A:922:VAL:CG2	1:A:923:GLN:N	2.78	0.46
1:A:965:SER:C	1:A:967:VAL:H	2.19	0.46
1:C:664:GLU:O	1:C:668:GLU:HG3	2.14	0.46
1:A:900:MET:HE1	1:A:921:MET:SD	2.56	0.46
1:A:977:ARG:HB3	1:A:977:ARG:HH11	1.78	0.46
1:A:1066:SER:C	1:A:1068:LEU:N	2.67	0.46
1:C:997:ARG:HG2	1:C:998:HIS:N	2.31	0.46
1:D:961:GLU:OE1	1:D:964:ARG:HD3	2.15	0.46
1:D:1044:ILE:CD1	1:D:1044:ILE:N	2.71	0.46
1:D:1076:VAL:HG23	1:D:1078:PHE:CE1	2.50	0.46
1:A:779:GLY:O	1:A:782:ALA:HB3	2.15	0.46
1:B:507:VAL:O	1:B:511:GLY:N	2.48	0.46
1:B:743:MET:HE2	1:B:744:ALA:N	2.30	0.46
1:B:891:LYS:O	1:B:895:VAL:HG23	2.16	0.46
1:B:995:VAL:HG13	1:B:1000:GLU:HA	1.98	0.46
1:B:1029:PRO:C	1:B:1031:ASP:H	2.18	0.46
1:A:644:ARG:NH1	1:A:644:ARG:CB	2.78	0.46
1:A:701:GLU:OE2	1:A:769:HIS:ND1	2.36	0.46
1:A:704:ILE:HD11	1:A:730:LEU:HD12	1.97	0.46
1:C:656:ASP:OD2	1:C:977:ARG:NH2	2.48	0.46
1:C:965:SER:C	1:C:967:VAL:H	2.19	0.46
1:C:1020:PHE:O	1:C:1024:THR:HG23	2.15	0.46
1:D:640:GLN:HG3	1:D:673:VAL:HG12	1.96	0.46
1:D:656:ASP:CG	1:D:977:ARG:HH21	2.19	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:887:PHE:HD1	1:D:890:VAL:CG2	2.29	0.46
1:D:1049:GLU:HA	1:D:1058:LEU:O	2.16	0.46
1:A:862:TYR:CE1	1:B:815:ALA:HB1	2.51	0.46
1:A:1089:VAL:CG1	1:A:1090:LYS:N	2.77	0.46
1:B:631:ARG:NH2	1:B:639:PHE:CE1	2.84	0.46
1:B:899:GLN:HE21	1:B:899:GLN:CA	2.27	0.46
1:C:536:PRO:HA	1:C:537:PRO:HD3	1.75	0.46
1:C:894:TYR:HA	1:C:918:ALA:HB2	1.97	0.46
1:C:898:ASN:HD21	1:C:904:LEU:H	1.62	0.46
1:D:644:ARG:HB2	1:D:644:ARG:CZ	2.46	0.46
1:D:739:CYS:SG	1:D:740:ILE:N	2.88	0.46
1:A:625:ARG:HH21	1:A:629:GLU:CD	2.19	0.46
1:C:965:SER:HA	1:C:973:ARG:HH22	1.81	0.46
1:D:502:HIS:HE1	1:D:1090:LYS:NZ	2.14	0.46
1:D:650:GLY:HA3	1:D:654:TYR:CE1	2.51	0.46
1:B:1017:PHE:CZ	1:B:1021:LYS:HD3	2.50	0.46
1:B:1044:ILE:O	1:B:1045:ALA:CB	2.64	0.46
1:C:499:LYS:NZ	1:C:1025:ALA:O	2.32	0.46
1:C:667:LYS:HG2	1:C:696:ALA:O	2.16	0.46
1:C:780:VAL:HG22	1:C:808:PRO:HB2	1.98	0.46
1:C:807:GLN:HB3	1:C:808:PRO:HD2	1.98	0.46
1:D:1065:VAL:CG1	1:D:1076:VAL:HG12	2.44	0.46
1:A:538:PRO:O	1:A:539:ALA:HB3	2.16	0.45
1:B:894:TYR:HA	1:B:918:ALA:HB2	1.97	0.45
1:C:539:ALA:HA	1:C:636:ASN:CB	2.44	0.45
1:C:651:TYR:CD1	1:C:652:THR:HG23	2.51	0.45
1:B:502:HIS:HD2	1:B:1087:ILE:HD11	1.81	0.45
1:B:961:GLU:N	1:B:962:PRO:HD2	2.31	0.45
1:D:707:THR:OG1	1:D:905:ILE:HG12	2.15	0.45
1:B:644:ARG:O	1:B:645:GLY:C	2.53	0.45
1:C:502:HIS:CE1	1:C:1090:LYS:HZ3	2.35	0.45
1:C:814:VAL:O	1:C:817:THR:HG22	2.15	0.45
1:D:965:SER:C	1:D:967:VAL:N	2.69	0.45
1:A:498:GLN:C	1:A:498:GLN:NE2	2.70	0.45
1:A:571:ARG:NH2	1:A:642:LEU:HD22	2.32	0.45
1:A:707:THR:OG1	1:A:905:ILE:HG12	2.15	0.45
1:B:864:ASN:HA	1:B:895:VAL:HG22	1.99	0.45
1:C:899:GLN:HA	1:C:899:GLN:HE21	1.79	0.45
1:C:899:GLN:CA	1:C:899:GLN:HE21	2.30	0.45
1:C:1066:SER:C	1:C:1068:LEU:N	2.68	0.45
1:D:977:ARG:HH11	1:D:977:ARG:CB	2.30	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:717:LYS:NZ	1:B:956:HIS:O	2.36	0.45
1:B:814:VAL:O	1:B:817:THR:HG22	2.16	0.45
1:C:583:ARG:NH2	1:C:1033:LEU:O	2.49	0.45
1:D:500:LEU:O	1:D:503:TYR:HB3	2.16	0.45
1:D:937:GLU:O	1:D:938:LEU:HG	2.17	0.45
1:A:644:ARG:HB3	1:A:644:ARG:NH1	2.31	0.45
1:A:1054:ARG:HD3	1:A:1054:ARG:C	2.36	0.45
1:B:641:MET:HB3	1:B:671:MET:HE1	1.97	0.45
1:B:865:GLU:HB2	1:B:906:LYS:HZ1	1.79	0.45
1:B:936:GLU:OE2	1:B:937:GLU:N	2.50	0.45
1:B:1001:GLU:O	1:B:1002:VAL:C	2.53	0.45
1:B:1008:LEU:O	1:B:1011:ALA:HB3	2.17	0.45
1:B:1045:ALA:HB2	1:B:1063:LEU:HG	1.99	0.45
1:C:617:ARG:HH21	1:C:1016:VAL:CG2	2.28	0.45
1:D:654:TYR:CB	1:D:658:VAL:HG21	2.46	0.45
1:D:704:ILE:HD11	1:D:730:LEU:HD12	1.98	0.45
1:D:965:SER:HA	1:D:973:ARG:HH22	1.82	0.45
1:A:648:ALA:HB3	1:A:1012:MET:HE1	1.97	0.45
1:A:762:ARG:HG3	1:A:763:PHE:CE1	2.52	0.45
1:A:901:LEU:O	1:A:904:LEU:HD11	2.16	0.45
1:A:950:GLY:O	1:A:952:ILE:N	2.50	0.45
1:B:516:ILE:O	1:B:516:ILE:HG13	2.16	0.45
1:B:711:ALA:HA	1:B:754:MET:HE3	1.99	0.45
1:B:855:LYS:O	1:B:856:SER:HB3	2.15	0.45
1:C:534:ILE:CG2	1:C:535:GLY:N	2.80	0.45
1:C:1001:GLU:O	1:C:1002:VAL:C	2.54	0.45
1:C:1067:ASP:O	1:C:1069:ASN:N	2.50	0.45
1:D:545:LEU:O	1:D:549:GLY:N	2.49	0.45
1:D:907:VAL:HG12	1:D:908:THR:N	2.31	0.45
1:B:701:GLU:HG3	1:B:737:ILE:HB	1.99	0.45
1:C:815:ALA:HB1	1:D:862:TYR:CE1	2.52	0.45
1:C:967:VAL:O	1:C:969:LYS:HG3	2.16	0.45
1:D:536:PRO:HA	1:D:537:PRO:HD3	1.76	0.45
1:D:547:ARG:O	1:D:548:GLU:HG3	2.17	0.45
1:D:893:ALA:HB2	1:D:922:VAL:CG1	2.47	0.45
1:D:907:VAL:O	1:D:908:THR:C	2.54	0.45
1:D:1010:ALA:HB2	1:D:1017:PHE:CD2	2.51	0.45
1:A:678:ASP:HB2	1:A:686:MET:CG	2.47	0.45
1:A:894:TYR:CE2	1:A:906:LYS:HD2	2.52	0.45
1:A:965:SER:C	1:A:967:VAL:N	2.70	0.45
1:A:1003:THR:HB	1:A:1004:PRO:HD2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:894:TYR:CE2	1:B:906:LYS:HD2	2.52	0.45
1:B:1002:VAL:HG23	1:B:1002:VAL:O	2.17	0.45
1:B:1060:ILE:HG22	1:B:1061:LYS:N	2.31	0.45
1:B:1089:VAL:CG1	1:B:1090:LYS:N	2.77	0.45
1:B:1092:THR:O	1:B:1093:GLN:HG2	2.17	0.45
1:C:1010:ALA:HB2	1:C:1017:PHE:CD2	2.52	0.45
1:D:506:HIS:HA	1:D:1089:VAL:HG11	1.98	0.45
1:D:657:ASN:ND2	1:D:985:LEU:H	2.15	0.45
1:D:1001:GLU:O	1:D:1002:VAL:C	2.54	0.45
1:D:1066:SER:C	1:D:1068:LEU:N	2.69	0.45
1:A:597:ASN:HB3	1:A:830:ARG:HD3	1.99	0.45
1:A:599:SER:C	1:A:601:LEU:H	2.19	0.45
1:A:756:VAL:CG1	1:A:789:ALA:HB3	2.47	0.45
1:A:815:ALA:HB2	1:A:828:MET:CE	2.47	0.45
1:B:828:MET:O	1:B:831:VAL:HG22	2.17	0.45
1:C:549:GLY:C	1:C:551:GLU:H	2.20	0.45
1:C:769:HIS:NE2	1:C:795:ASP:OD1	2.50	0.45
1:C:1015:ASP:O	1:C:1016:VAL:C	2.54	0.45
1:C:1063:LEU:O	1:C:1064:ALA:CB	2.63	0.45
1:C:1068:LEU:HA	1:C:1074:ARG:NE	2.31	0.45
1:D:551:GLU:OE2	1:D:551:GLU:HA	2.17	0.45
1:D:650:GLY:HA3	1:D:654:TYR:OH	2.17	0.45
1:D:679:SER:OG	1:D:909:PRO:HB2	2.17	0.45
1:A:655:PRO:HB3	1:A:983:PRO:O	2.17	0.44
1:A:860:ASP:OD1	1:A:891:LYS:NZ	2.50	0.44
1:C:496:ARG:NH1	1:C:1056:LYS:NZ	2.64	0.44
1:C:807:GLN:H	1:C:807:GLN:HE21	1.64	0.44
1:D:711:ALA:HB2	1:D:751:ALA:HA	1.99	0.44
1:D:788:GLN:OE1	1:D:788:GLN:HA	2.17	0.44
1:D:893:ALA:HB2	1:D:922:VAL:HG13	1.99	0.44
1:D:1052:LEU:HD22	1:D:1056:LYS:HD2	1.99	0.44
1:A:987:LEU:O	1:A:991:GLU:N	2.45	0.44
1:B:552:GLY:HA2	1:B:555:ARG:HD2	1.99	0.44
1:C:947:PHE:HD1	1:C:952:ILE:HD11	1.83	0.44
1:C:1073:GLN:NE2	1:C:1088:LEU:HD22	2.32	0.44
1:D:948:LEU:HD22	1:D:964:ARG:HG3	2.00	0.44
1:D:1065:VAL:HG22	1:D:1076:VAL:CB	2.47	0.44
1:D:1079:GLU:HA	1:D:1084:LEU:HB3	1.99	0.44
1:A:643:LEU:HD12	1:A:648:ALA:HA	1.98	0.44
1:A:766:LEU:HD12	1:A:767:PRO:CD	2.46	0.44
1:B:534:ILE:CG2	1:B:535:GLY:N	2.79	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:964:ARG:HG2	1:B:968:LEU:HD12	1.99	0.44
1:D:908:THR:HG22	1:D:909:PRO:N	2.32	0.44
1:A:660:PHE:HA	1:A:692:ALA:HB1	1.98	0.44
1:B:591:ALA:HB3	1:B:633:LEU:HD13	2.00	0.44
1:B:1052:LEU:HD23	1:B:1053:GLU:HB2	1.98	0.44
1:C:959:PHE:CB	1:C:964:ARG:HD2	2.47	0.44
1:C:961:GLU:N	1:C:962:PRO:HD2	2.33	0.44
1:C:1073:GLN:O	1:C:1074:ARG:HB2	2.17	0.44
1:A:997:ARG:HD2	1:A:998:HIS:CD2	2.52	0.44
1:A:1089:VAL:CG1	1:A:1090:LYS:H	2.30	0.44
1:B:883:LEU:HD22	1:B:886:LYS:HG3	2.00	0.44
1:D:606:ASN:OD1	1:D:606:ASN:C	2.56	0.44
1:D:643:LEU:O	1:D:676:VAL:HA	2.18	0.44
1:D:891:LYS:O	1:D:895:VAL:HG23	2.17	0.44
1:D:1068:LEU:HD13	1:D:1074:ARG:CZ	2.47	0.44
1:A:539:ALA:HA	1:A:636:ASN:CB	2.42	0.44
1:B:645:GLY:HA2	1:B:689:GLY:HA3	2.00	0.44
1:B:657:ASN:ND2	1:B:985:LEU:H	2.16	0.44
1:B:743:MET:HE2	1:B:744:ALA:H	1.82	0.44
1:B:1045:ALA:CB	1:B:1063:LEU:HG	2.47	0.44
1:C:571:ARG:NH1	1:C:575:GLN:NE2	2.58	0.44
1:C:661:LYS:O	1:C:665:VAL:HG23	2.17	0.44
1:D:665:VAL:HG12	1:D:669:ASN:ND2	2.32	0.44
1:A:590:ILE:O	1:A:590:ILE:HG13	2.17	0.44
1:A:756:VAL:HG11	1:A:789:ALA:HB3	2.00	0.44
1:A:814:VAL:O	1:A:817:THR:HG22	2.18	0.44
1:B:859:SER:C	1:B:861:VAL:H	2.20	0.44
1:B:908:THR:CB	1:B:909:PRO:HD3	2.46	0.44
1:B:971:LEU:HA	1:B:972:PRO:HD3	1.71	0.44
1:D:708:GLY:HA2	1:D:715:ARG:NH1	2.32	0.44
1:A:656:ASP:OD2	1:A:977:ARG:NH2	2.51	0.44
1:A:961:GLU:N	1:A:962:PRO:HD2	2.33	0.44
1:A:995:VAL:CG1	1:A:1000:GLU:HA	2.48	0.44
1:B:949:GLN:HG3	1:B:968:LEU:HD22	1.99	0.44
1:C:1057:THR:HB	1:C:1059:HIS:CE1	2.53	0.44
1:D:1029:PRO:C	1:D:1031:ASP:H	2.21	0.44
1:A:1020:PHE:CE1	1:A:1024:THR:HG21	2.53	0.44
1:A:1052:LEU:HD23	1:A:1053:GLU:HB2	2.00	0.44
1:A:1074:ARG:O	1:A:1088:LEU:HD23	2.17	0.44
1:B:738:LEU:HD12	1:B:739:CYS:H	1.83	0.44
1:B:1050:VAL:O	1:B:1050:VAL:CG2	2.66	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:807:GLN:NE2	1:C:807:GLN:N	2.65	0.44
1:D:849:ASP:CB	1:D:851:THR:HG22	2.48	0.44
1:D:971:LEU:HA	1:D:972:PRO:HD3	1.85	0.44
1:A:876:PHE:O	1:A:880:SER:HB3	2.18	0.43
1:A:961:GLU:HA	1:A:964:ARG:HB3	2.00	0.43
1:B:987:LEU:O	1:B:991:GLU:N	2.49	0.43
1:D:785:ALA:O	1:D:788:GLN:HB2	2.18	0.43
1:B:502:HIS:HE1	1:B:1090:LYS:HZ3	1.66	0.43
1:C:824:THR:O	1:C:825:GLU:HB2	2.17	0.43
1:C:849:ASP:CB	1:C:851:THR:HG22	2.46	0.43
1:C:964:ARG:HE	1:C:968:LEU:HD11	1.83	0.43
1:B:532:VAL:HG23	1:B:532:VAL:O	2.18	0.43
1:B:827:PRO:HD2	1:B:830:ARG:HD2	2.00	0.43
1:C:658:VAL:HG23	1:C:659:VAL:N	2.32	0.43
1:C:743:MET:SD	1:C:907:VAL:HG22	2.58	0.43
1:D:829:GLU:O	1:D:832:PHE:HB2	2.19	0.43
1:D:883:LEU:HD22	1:D:886:LYS:HG3	2.00	0.43
1:A:593:TYR:CE1	1:A:597:ASN:ND2	2.86	0.43
1:A:624:TRP:CD1	1:A:1005:GLU:HB3	2.54	0.43
1:A:898:ASN:HD21	1:A:904:LEU:N	2.11	0.43
1:B:571:ARG:NH1	1:B:575:GLN:NE2	2.56	0.43
1:B:936:GLU:O	1:B:969:LYS:HE3	2.17	0.43
1:B:938:LEU:HB2	1:B:940:PHE:CE1	2.53	0.43
1:C:860:ASP:HA	1:D:832:PHE:CZ	2.54	0.43
1:C:907:VAL:HG12	1:C:908:THR:N	2.33	0.43
1:D:1067:ASP:OD1	1:D:1075:GLN:HB3	2.18	0.43
1:A:827:PRO:HD2	1:A:830:ARG:HD2	2.00	0.43
1:B:500:LEU:O	1:B:503:TYR:HB3	2.19	0.43
1:B:707:THR:CG2	1:B:708:GLY:N	2.81	0.43
1:C:756:VAL:O	1:C:759:LEU:HB2	2.18	0.43
1:A:948:LEU:HA	1:A:959:PHE:CE2	2.54	0.43
1:C:564:LEU:O	1:C:793:VAL:HA	2.19	0.43
1:C:679:SER:HB2	1:C:910:SER:OG	2.17	0.43
1:C:917:LEU:O	1:C:921:MET:HG3	2.18	0.43
1:A:899:GLN:NE2	1:A:899:GLN:CA	2.75	0.43
1:A:977:ARG:HH11	1:A:977:ARG:CB	2.31	0.43
1:A:1005:GLU:H	1:A:1005:GLU:CD	2.22	0.43
1:B:655:PRO:HB2	1:B:984:PRO:HA	2.01	0.43
1:C:743:MET:HE2	1:C:744:ALA:N	2.34	0.43
1:D:959:PHE:HB2	1:D:964:ARG:HD2	2.01	0.43
1:D:1015:ASP:HB3	1:D:1019:HIS:NE2	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:574:HIS:CD2	1:A:580:THR:HA	2.54	0.43
1:A:660:PHE:CD2	1:A:692:ALA:HA	2.54	0.43
1:A:849:ASP:CB	1:A:851:THR:HG22	2.43	0.43
1:A:893:ALA:HB2	1:A:922:VAL:CG1	2.48	0.43
1:B:677:PHE:CE1	1:B:907:VAL:HG11	2.53	0.43
1:B:901:LEU:HB2	1:B:904:LEU:HD11	2.00	0.43
1:B:952:ILE:HG13	1:B:953:GLY:H	1.84	0.43
1:C:528:VAL:O	1:C:530:PRO:HD3	2.19	0.43
1:C:562:GLY:HA3	1:C:823:ASP:O	2.19	0.43
1:C:793:VAL:HG12	1:C:794:VAL:N	2.33	0.43
1:D:494:GLN:HE21	1:D:494:GLN:HB2	1.69	0.43
1:D:865:GLU:HB2	1:D:906:LYS:HZ2	1.83	0.43
1:D:1065:VAL:HG22	1:D:1076:VAL:HB	2.00	0.43
1:A:860:ASP:HA	1:B:832:PHE:CE2	2.54	0.43
1:A:908:THR:HG22	1:A:909:PRO:N	2.33	0.43
1:B:680:LEU:HD12	1:B:680:LEU:N	2.34	0.43
1:B:977:ARG:NH1	1:B:980:ALA:HB2	2.33	0.43
1:C:948:LEU:HA	1:C:959:PHE:CE2	2.54	0.43
1:C:1063:LEU:HD23	1:C:1063:LEU:HA	1.89	0.43
1:D:624:TRP:CZ3	1:D:665:VAL:HG12	2.53	0.43
1:D:860:ASP:OD2	1:D:860:ASP:C	2.56	0.43
1:A:995:VAL:CG2	1:A:1002:VAL:HG21	2.45	0.43
1:A:1015:ASP:O	1:A:1018:ALA:N	2.51	0.43
1:C:997:ARG:HD2	1:C:998:HIS:CD2	2.54	0.43
1:D:544:ILE:O	1:D:545:LEU:C	2.57	0.43
1:D:961:GLU:OE2	1:D:965:SER:HB3	2.19	0.43
1:D:743:MET:HE2	1:D:744:ALA:N	2.34	0.42
1:A:547:ARG:C	1:A:548:GLU:HG3	2.39	0.42
1:A:919:GLN:O	1:A:922:VAL:HG22	2.19	0.42
1:A:988:GLN:N	1:A:988:GLN:OE1	2.51	0.42
1:B:564:LEU:O	1:B:793:VAL:HA	2.19	0.42
1:B:590:ILE:O	1:B:590:ILE:HG13	2.19	0.42
1:B:1068:LEU:HA	1:B:1074:ARG:NE	2.32	0.42
1:C:1074:ARG:O	1:C:1088:LEU:HD23	2.19	0.42
1:A:571:ARG:HD2	1:A:571:ARG:C	2.39	0.42
1:B:935:ALA:C	1:B:937:GLU:N	2.73	0.42
1:B:947:PHE:HD1	1:B:952:ILE:HD11	1.84	0.42
1:C:566:MET:HE1	1:C:605:GLU:HB2	2.01	0.42
1:C:907:VAL:O	1:C:908:THR:C	2.57	0.42
1:C:964:ARG:O	1:C:967:VAL:HB	2.19	0.42
1:D:897:ALA:HB2	1:D:921:MET:CE	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:523:SER:O	1:A:1036:ARG:NH2	2.48	0.42
1:A:967:VAL:O	1:A:969:LYS:HG3	2.19	0.42
1:B:762:ARG:CG	1:B:763:PHE:CE1	3.02	0.42
1:C:650:GLY:HA3	1:C:654:TYR:HE1	1.84	0.42
1:D:1003:THR:HB	1:D:1004:PRO:CD	2.48	0.42
1:A:901:LEU:HA	1:A:960:PRO:HG3	2.01	0.42
1:A:1017:PHE:CZ	1:A:1021:LYS:HD3	2.55	0.42
1:B:762:ARG:HG3	1:B:763:PHE:CZ	2.54	0.42
1:B:983:PRO:O	1:B:984:PRO:O	2.38	0.42
1:C:712:ASP:OD1	1:C:714:SER:HB2	2.19	0.42
1:C:881:MET:O	1:C:883:LEU:HG	2.20	0.42
1:C:947:PHE:CD1	1:C:952:ILE:HD11	2.55	0.42
1:D:502:HIS:CE1	1:D:1090:LYS:NZ	2.87	0.42
1:D:581:ARG:NH1	1:D:848:PHE:CE2	2.87	0.42
1:A:498:GLN:C	1:A:498:GLN:HE21	2.23	0.42
1:A:595:ALA:CB	1:A:634:ILE:HG23	2.48	0.42
1:B:502:HIS:CE1	1:B:1090:LYS:HZ3	2.38	0.42
1:B:601:LEU:CD2	1:B:603:SER:O	2.64	0.42
1:B:1045:ALA:N	1:B:1063:LEU:HG	2.35	0.42
1:C:990:LEU:O	1:C:994:LEU:HG	2.20	0.42
1:D:1001:GLU:HA	1:D:1001:GLU:OE1	2.20	0.42
1:A:656:ASP:CG	1:A:977:ARG:HH21	2.22	0.42
1:B:1057:THR:HB	1:B:1059:HIS:CE1	2.55	0.42
1:C:907:VAL:HG12	1:C:908:THR:H	1.85	0.42
1:A:494:GLN:HG2	1:A:1056:LYS:CE	2.49	0.42
1:A:1065:VAL:CG1	1:A:1076:VAL:HG12	2.44	0.42
1:B:900:MET:CE	1:B:921:MET:SD	3.08	0.42
1:B:954:VAL:HA	1:B:955:PRO:HD2	1.90	0.42
1:C:682:TYR:HD1	1:C:685:ASN:ND2	2.18	0.42
1:C:893:ALA:CB	1:C:922:VAL:HG13	2.50	0.42
1:C:968:LEU:HB2	1:C:973:ARG:HH21	1.85	0.42
1:A:551:GLU:OE2	1:A:551:GLU:HA	2.20	0.42
1:A:562:GLY:HA3	1:A:823:ASP:O	2.19	0.42
1:A:732:ARG:C	1:A:734:GLY:N	2.72	0.42
1:A:934:GLN:O	1:A:938:LEU:HG	2.20	0.42
1:A:945:VAL:HG23	1:A:946:GLU:N	2.35	0.42
1:A:1067:ASP:HB2	1:A:1074:ARG:HA	2.02	0.42
1:B:494:GLN:HB2	1:B:497:ALA:HB3	2.01	0.42
1:B:654:TYR:CB	1:B:658:VAL:HG21	2.49	0.42
1:B:785:ALA:O	1:B:788:GLN:HB2	2.19	0.42
1:B:1029:PRO:C	1:B:1031:ASP:N	2.73	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:603:SER:HA	1:C:638:PRO:HB2	2.00	0.42
1:C:901:LEU:HB2	1:C:904:LEU:CD1	2.48	0.42
1:C:918:ALA:O	1:C:922:VAL:HG13	2.20	0.42
1:C:959:PHE:HB2	1:C:964:ARG:HD2	2.02	0.42
1:D:597:ASN:O	1:D:830:ARG:NH1	2.53	0.42
1:D:658:VAL:HG23	1:D:659:VAL:N	2.34	0.42
1:D:987:LEU:O	1:D:991:GLU:N	2.45	0.42
1:A:614:VAL:HG13	1:A:618:PHE:HD1	1.84	0.42
1:A:893:ALA:CB	1:A:922:VAL:HG13	2.49	0.42
1:A:1065:VAL:HA	1:A:1075:GLN:O	2.19	0.42
1:C:570:PHE:HB3	1:C:606:ASN:CB	2.50	0.42
1:C:964:ARG:HG2	1:C:968:LEU:HD12	2.02	0.42
1:D:657:ASN:HD21	1:D:985:LEU:H	1.67	0.42
1:A:545:LEU:O	1:A:549:GLY:N	2.47	0.41
1:A:1092:THR:O	1:A:1093:GLN:HG2	2.20	0.41
1:B:502:HIS:HA	1:B:1087:ILE:HG12	2.01	0.41
1:C:763:PHE:HA	1:C:764:PRO:HD2	1.81	0.41
1:A:621:GLU:HG2	1:A:1031:ASP:CB	2.49	0.41
1:A:643:LEU:HD11	1:A:648:ALA:HA	2.01	0.41
1:A:1067:ASP:HA	1:D:1082:GLY:O	2.20	0.41
1:B:502:HIS:HA	1:B:1087:ILE:HG21	2.02	0.41
1:B:599:SER:C	1:B:601:LEU:H	2.22	0.41
1:C:737:ILE:HD12	1:C:767:PRO:CB	2.51	0.41
1:D:732:ARG:C	1:D:734:GLY:N	2.74	0.41
1:A:1002:VAL:O	1:A:1002:VAL:HG23	2.20	0.41
1:B:536:PRO:HA	1:B:537:PRO:HD3	1.84	0.41
1:B:742:ASP:HB2	1:B:747:LEU:CD1	2.50	0.41
1:C:560:HIS:CG	1:C:564:LEU:HD21	2.55	0.41
1:C:704:ILE:HB	1:C:740:ILE:HD13	2.02	0.41
1:C:737:ILE:HD12	1:C:767:PRO:HB2	2.02	0.41
1:C:739:CYS:SG	1:C:740:ILE:N	2.93	0.41
1:A:496:ARG:NH1	1:A:1056:LYS:NZ	2.69	0.41
1:A:749:PRO:O	1:A:752:CYS:HB2	2.20	0.41
1:A:788:GLN:HA	1:A:788:GLN:OE1	2.20	0.41
1:A:822:LEU:O	1:A:823:ASP:C	2.59	0.41
1:A:908:THR:CB	1:A:909:PRO:HD3	2.43	0.41
1:A:980:ALA:C	1:A:982:LEU:H	2.23	0.41
1:B:648:ALA:HB3	1:B:1012:MET:HE1	2.02	0.41
1:B:809:SER:O	1:B:813:LEU:HD23	2.20	0.41
1:B:897:ALA:O	1:B:901:LEU:HG	2.20	0.41
1:B:977:ARG:HB3	1:B:977:ARG:HH11	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1058:LEU:HD22	1:B:1080:LEU:HD11	2.01	0.41
1:B:1065:VAL:CG2	1:B:1076:VAL:HG12	2.48	0.41
1:C:502:HIS:CE1	1:C:1090:LYS:HZ1	2.37	0.41
1:C:506:HIS:CE1	1:C:510:ASN:HB2	2.56	0.41
1:C:590:ILE:O	1:C:590:ILE:HG13	2.21	0.41
1:C:612:PHE:HB3	1:C:649:VAL:HG12	2.02	0.41
1:D:571:ARG:NH1	1:D:575:GLN:NE2	2.62	0.41
1:D:965:SER:C	1:D:967:VAL:H	2.22	0.41
1:D:1005:GLU:H	1:D:1005:GLU:CD	2.23	0.41
1:D:1089:VAL:CG1	1:D:1090:LYS:N	2.83	0.41
1:A:749:PRO:CD	1:B:816:CYS:SG	3.08	0.41
1:B:625:ARG:HH21	1:B:629:GLU:CD	2.24	0.41
1:B:755:LEU:HD22	1:B:759:LEU:HD12	2.02	0.41
1:B:1067:ASP:O	1:B:1074:ARG:HA	2.21	0.41
1:D:624:TRP:CG	1:D:1005:GLU:HB3	2.55	0.41
1:D:950:GLY:O	1:D:952:ILE:N	2.53	0.41
1:A:879:HIS:CE1	1:A:884:GLY:HA3	2.56	0.41
1:A:1001:GLU:O	1:A:1002:VAL:O	2.39	0.41
1:A:1079:GLU:HA	1:A:1084:LEU:HB3	2.03	0.41
1:B:982:LEU:HA	1:B:983:PRO:HD3	1.91	0.41
1:C:545:LEU:O	1:C:549:GLY:N	2.52	0.41
1:C:579:ALA:O	1:C:581:ARG:HG2	2.20	0.41
1:C:586:ASP:OD2	1:C:1035:THR:OG1	2.27	0.41
1:C:680:LEU:HD11	1:C:952:ILE:HD12	2.02	0.41
1:C:707:THR:CG2	1:C:708:GLY:N	2.84	0.41
1:D:720:LEU:O	1:D:724:MET:HG2	2.21	0.41
1:D:923:GLN:HE21	1:D:924:ASN:HD21	1.67	0.41
1:A:565:LEU:O	1:A:601:LEU:HD23	2.20	0.41
1:A:580:THR:HG21	1:A:610:ALA:HB3	2.02	0.41
1:B:604:MET:HE1	1:B:634:ILE:HD13	2.02	0.41
1:B:769:HIS:CD2	1:B:793:VAL:HB	2.56	0.41
1:B:874:LEU:N	1:B:874:LEU:CD1	2.83	0.41
1:B:965:SER:O	1:B:967:VAL:N	2.54	0.41
1:C:498:GLN:NE2	1:C:498:GLN:C	2.74	0.41
1:C:787:ALA:HB1	1:C:822:LEU:HD13	2.02	0.41
1:C:883:LEU:HB3	1:C:886:LYS:HB2	2.02	0.41
1:C:945:VAL:CG2	1:C:946:GLU:N	2.84	0.41
1:D:949:GLN:HG3	1:D:968:LEU:HD22	2.02	0.41
1:A:815:ALA:HB2	1:A:828:MET:HE2	2.02	0.41
1:B:651:TYR:CD2	1:B:651:TYR:N	2.89	0.41
1:B:893:ALA:CB	1:B:922:VAL:HG13	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:603:SER:HA	1:D:638:PRO:HB2	2.01	0.41
1:D:961:GLU:O	1:D:962:PRO:C	2.58	0.41
1:A:502:HIS:HA	1:A:1087:ILE:HG12	2.03	0.41
1:A:506:HIS:HA	1:A:1089:VAL:HG11	2.02	0.41
1:A:906:LYS:HB3	1:A:911:SER:CB	2.51	0.41
1:B:654:TYR:HB3	1:B:658:VAL:HG21	2.02	0.41
1:B:1013:TYR:HB3	1:B:1016:VAL:HB	2.03	0.41
1:B:1013:TYR:O	1:B:1017:PHE:CB	2.69	0.41
1:C:650:GLY:HA3	1:C:654:TYR:OH	2.21	0.41
1:C:673:VAL:HA	1:C:699:VAL:HB	2.03	0.41
1:C:936:GLU:O	1:C:969:LYS:HE3	2.20	0.41
1:C:1043:LYS:HB2	1:C:1046:GLU:OE1	2.21	0.41
1:D:584:THR:HG22	1:D:588:LYS:HG3	2.02	0.41
1:D:738:LEU:HD12	1:D:739:CYS:N	2.36	0.41
1:D:963:PHE:O	1:D:964:ARG:C	2.59	0.41
1:A:542:ARG:HD3	1:A:542:ARG:O	2.21	0.41
1:A:654:TYR:CB	1:A:658:VAL:HG21	2.51	0.41
1:A:867:PRO:HD2	1:A:870:GLN:OE1	2.21	0.41
1:A:1067:ASP:CG	1:A:1075:GLN:HB3	2.42	0.41
1:B:686:MET:HE3	1:B:703:ALA:O	2.21	0.41
1:B:695:SER:C	1:B:697:GLY:N	2.74	0.41
1:B:793:VAL:HG12	1:B:794:VAL:N	2.35	0.41
1:C:832:PHE:CE2	1:D:860:ASP:HA	2.55	0.41
1:C:874:LEU:N	1:C:874:LEU:CD1	2.84	0.41
1:C:876:PHE:O	1:C:880:SER:CB	2.69	0.41
1:D:769:HIS:NE2	1:D:795:ASP:OD1	2.54	0.41
1:D:885:SER:OG	1:D:886:LYS:N	2.53	0.41
1:A:959:PHE:CB	1:A:964:ARG:HD2	2.51	0.40
1:A:1003:THR:HB	1:A:1004:PRO:CD	2.51	0.40
1:B:1088:LEU:HD23	1:B:1088:LEU:C	2.41	0.40
1:C:494:GLN:HE21	1:C:494:GLN:HB2	1.71	0.40
1:C:1060:ILE:CG2	1:C:1061:LYS:N	2.84	0.40
1:D:557:VAL:HG13	1:D:564:LEU:HD12	2.03	0.40
1:D:965:SER:HA	1:D:973:ARG:NH2	2.36	0.40
1:A:814:VAL:HG13	1:A:824:THR:OG1	2.21	0.40
1:A:849:ASP:C	1:A:851:THR:N	2.74	0.40
1:A:862:TYR:CE1	1:B:815:ALA:CB	3.04	0.40
1:A:896:GLU:O	1:A:900:MET:HB2	2.21	0.40
1:A:1075:GLN:OE1	1:D:1084:LEU:HD11	2.21	0.40
1:B:496:ARG:NH1	1:B:1056:LYS:NZ	2.69	0.40
1:B:643:LEU:HD12	1:B:648:ALA:HA	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:655:PRO:HB2	1:B:657:ASN:OD1	2.21	0.40
1:B:657:ASN:HD21	1:B:985:LEU:H	1.69	0.40
1:B:907:VAL:O	1:B:908:THR:C	2.58	0.40
1:B:945:VAL:CG2	1:B:946:GLU:N	2.85	0.40
1:C:654:TYR:HB3	1:C:658:VAL:HG21	2.03	0.40
1:C:756:VAL:CG1	1:C:789:ALA:HB3	2.51	0.40
1:C:815:ALA:CB	1:D:862:TYR:CE1	3.04	0.40
1:D:506:HIS:ND1	1:D:506:HIS:C	2.75	0.40
1:D:898:ASN:HD22	1:D:906:LYS:HD3	1.85	0.40
1:D:997:ARG:HG3	1:D:997:ARG:NH1	2.37	0.40
1:A:1045:ALA:HB2	1:A:1063:LEU:HG	2.02	0.40
1:B:496:ARG:NH1	1:B:1056:LYS:HZ2	2.19	0.40
1:B:707:THR:HG22	1:B:708:GLY:H	1.86	0.40
1:B:732:ARG:C	1:B:734:GLY:N	2.74	0.40
1:B:767:PRO:HA	1:B:792:ASP:OD2	2.20	0.40
1:B:787:ALA:O	1:B:788:GLN:C	2.60	0.40
1:B:964:ARG:HG2	1:B:968:LEU:CD1	2.52	0.40
1:C:507:VAL:O	1:C:511:GLY:N	2.52	0.40
1:C:649:VAL:N	1:C:1012:MET:HE1	2.32	0.40
1:C:1003:THR:HB	1:C:1004:PRO:HD2	2.02	0.40
1:D:867:PRO:HD2	1:D:870:GLN:OE1	2.21	0.40
1:D:1065:VAL:CG2	1:D:1076:VAL:HG12	2.50	0.40
1:A:961:GLU:OE2	1:A:965:SER:HB3	2.20	0.40
1:B:915:GLY:O	1:B:919:GLN:HG3	2.22	0.40
1:B:942:ARG:O	1:B:945:VAL:CG2	2.69	0.40
1:B:1043:LYS:HD3	1:B:1043:LYS:HA	1.93	0.40
1:C:495:ASN:H	1:C:496:ARG:HH21	1.70	0.40
1:C:922:VAL:CG2	1:C:923:GLN:N	2.85	0.40
1:D:494:GLN:HB2	1:D:497:ALA:CB	2.51	0.40
1:D:771:HIS:CE1	1:D:807:GLN:OE1	2.74	0.40
1:D:1045:ALA:HB2	1:D:1063:LEU:HG	2.03	0.40
1:A:712:ASP:OD1	1:A:714:SER:HB2	2.21	0.40
1:A:971:LEU:HA	1:A:972:PRO:HD3	1.79	0.40
1:B:547:ARG:C	1:B:548:GLU:HG3	2.42	0.40
1:B:807:GLN:HB3	1:B:808:PRO:HD2	2.03	0.40
1:C:923:GLN:HE21	1:C:924:ASN:ND2	2.19	0.40
1:C:1067:ASP:OD1	1:C:1075:GLN:HB3	2.21	0.40

All (1) 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:992:LYS:NZ	1:C:970:ASP:OD1[1_565]	2.18	0.02

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	599/718 (83%)	505 (84%)	72 (12%)	22 (4%)	3	19
1	B	599/718 (83%)	495 (83%)	83 (14%)	21 (4%)	3	20
1	C	599/718 (83%)	497 (83%)	80 (13%)	22 (4%)	3	19
1	D	599/718 (83%)	499 (83%)	76 (13%)	24 (4%)	3	17
All	All	2396/2872 (83%)	1996 (83%)	311 (13%)	89 (4%)	3	19

All (89) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	497	ALA
1	A	779	GLY
1	A	984	PRO
1	A	1002	VAL
1	A	1062	ALA
1	A	1064	ALA
1	A	1066	SER
1	A	1068	LEU
1	A	1070	ARG
1	B	779	GLY
1	B	984	PRO
1	B	1062	ALA
1	B	1064	ALA
1	B	1066	SER
1	B	1070	ARG
1	C	779	GLY
1	C	903	ASP

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Mol	Chain	Res	Type
1	C	984	PRO
1	C	1062	ALA
1	C	1066	SER
1	C	1068	LEU
1	C	1070	ARG
1	D	779	GLY
1	D	984	PRO
1	D	1062	ALA
1	D	1064	ALA
1	D	1066	SER
1	D	1068	LEU
1	D	1070	ARG
1	A	648	ALA
1	A	903	ASP
1	A	951	TYR
1	A	981	SER
1	A	1058	LEU
1	B	497	ALA
1	B	648	ALA
1	B	909	PRO
1	B	1002	VAL
1	B	1058	LEU
1	B	1068	LEU
1	C	539	ALA
1	C	648	ALA
1	C	1002	VAL
1	C	1058	LEU
1	C	1064	ALA
1	C	1067	ASP
1	D	497	ALA
1	D	903	ASP
1	D	909	PRO
1	D	1002	VAL
1	D	1058	LEU
1	A	908	THR
1	A	909	PRO
1	A	1067	ASP
1	B	903	ASP
1	B	908	THR
1	B	936	GLU
1	B	1074	ARG
1	C	497	ALA

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Mol	Chain	Res	Type
1	C	908	THR
1	C	909	PRO
1	C	1014	PRO
1	D	648	ALA
1	D	714	SER
1	D	951	TYR
1	D	1067	ASP
1	A	530	PRO
1	A	539	ALA
1	A	561	PRO
1	B	539	ALA
1	B	981	SER
1	D	908	THR
1	D	1074	ARG
1	B	1014	PRO
1	C	561	PRO
1	C	1074	ARG
1	D	981	SER
1	D	998	HIS
1	A	611	THR
1	B	530	PRO
1	B	561	PRO
1	C	964	ARG
1	C	998	HIS
1	D	539	ALA
1	D	561	PRO
1	D	1014	PRO
1	A	1014	PRO
1	D	530	PRO
1	C	530	PRO

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	493/593 (83%)	461 (94%)	32 (6%)	17 50

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	493/593 (83%)	465 (94%)	28 (6%)	20 56
1	C	493/593 (83%)	466 (94%)	27 (6%)	21 57
1	D	493/593 (83%)	467 (95%)	26 (5%)	22 58
All	All	1972/2372 (83%)	1859 (94%)	113 (6%)	20 56

All (113) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	494	GLN
1	A	496	ARG
1	A	498	GLN
1	A	542	ARG
1	A	601	LEU
1	A	607	TRP
1	A	632	GLU
1	A	712	ASP
1	A	729	GLU
1	A	732	ARG
1	A	739	CYS
1	A	743	MET
1	A	755	LEU
1	A	756	VAL
1	A	765	ASP
1	A	774	ASP
1	A	799	ASP
1	A	807	GLN
1	A	849	ASP
1	A	855	LYS
1	A	858	ASN
1	A	874	LEU
1	A	923	GLN
1	A	936	GLU
1	A	988	GLN
1	A	996	ASP
1	A	1044	ILE
1	A	1050	VAL
1	A	1067	ASP
1	A	1079	GLU
1	A	1084	LEU
1	A	1090	LYS
1	B	494	GLN

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Mol	Chain	Res	Type
1	B	496	ARG
1	B	498	GLN
1	B	542	ARG
1	B	601	LEU
1	B	607	TRP
1	B	680	LEU
1	B	712	ASP
1	B	729	GLU
1	B	732	ARG
1	B	743	MET
1	B	755	LEU
1	B	756	VAL
1	B	765	ASP
1	B	799	ASP
1	B	807	GLN
1	B	849	ASP
1	B	855	LYS
1	B	858	ASN
1	B	923	GLN
1	B	936	GLU
1	B	988	GLN
1	B	996	ASP
1	B	1044	ILE
1	B	1050	VAL
1	B	1067	ASP
1	B	1084	LEU
1	B	1090	LYS
1	C	494	GLN
1	C	496	ARG
1	C	498	GLN
1	C	542	ARG
1	C	601	LEU
1	C	607	TRP
1	C	632	GLU
1	C	729	GLU
1	C	743	MET
1	C	755	LEU
1	C	756	VAL
1	C	765	ASP
1	C	799	ASP
1	C	807	GLN
1	C	855	LYS

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Mol	Chain	Res	Type
1	C	858	ASN
1	C	923	GLN
1	C	936	GLU
1	C	988	GLN
1	C	996	ASP
1	C	1044	ILE
1	C	1050	VAL
1	C	1067	ASP
1	C	1068	LEU
1	C	1079	GLU
1	C	1084	LEU
1	C	1090	LYS
1	D	494	GLN
1	D	496	ARG
1	D	498	GLN
1	D	542	ARG
1	D	601	LEU
1	D	607	TRP
1	D	712	ASP
1	D	732	ARG
1	D	743	MET
1	D	755	LEU
1	D	756	VAL
1	D	765	ASP
1	D	799	ASP
1	D	807	GLN
1	D	855	LYS
1	D	858	ASN
1	D	923	GLN
1	D	936	GLU
1	D	988	GLN
1	D	996	ASP
1	D	1044	ILE
1	D	1050	VAL
1	D	1067	ASP
1	D	1079	GLU
1	D	1084	LEU
1	D	1090	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (73) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	494	GLN
1	A	498	GLN
1	A	502	HIS
1	A	560	HIS
1	A	574	HIS
1	A	575	GLN
1	A	721	GLN
1	A	736	HIS
1	A	807	GLN
1	A	858	ASN
1	A	873	ASN
1	A	879	HIS
1	A	898	ASN
1	A	899	GLN
1	A	924	ASN
1	A	949	GLN
1	A	998	HIS
1	B	494	GLN
1	B	498	GLN
1	B	502	HIS
1	B	506	HIS
1	B	560	HIS
1	B	574	HIS
1	B	575	GLN
1	B	721	GLN
1	B	736	HIS
1	B	771	HIS
1	B	807	GLN
1	B	858	ASN
1	B	873	ASN
1	B	879	HIS
1	B	898	ASN
1	B	899	GLN
1	B	924	ASN
1	B	934	GLN
1	B	949	GLN
1	B	998	HIS
1	C	494	GLN
1	C	498	GLN
1	C	502	HIS
1	C	506	HIS
1	C	560	HIS
1	C	574	HIS

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Mol	Chain	Res	Type
1	C	575	GLN
1	C	721	GLN
1	C	736	HIS
1	C	807	GLN
1	C	858	ASN
1	C	873	ASN
1	C	879	HIS
1	C	898	ASN
1	C	899	GLN
1	C	924	ASN
1	C	998	HIS
1	C	1075	GLN
1	D	494	GLN
1	D	498	GLN
1	D	502	HIS
1	D	506	HIS
1	D	560	HIS
1	D	574	HIS
1	D	575	GLN
1	D	721	GLN
1	D	736	HIS
1	D	771	HIS
1	D	807	GLN
1	D	858	ASN
1	D	873	ASN
1	D	879	HIS
1	D	898	ASN
1	D	899	GLN
1	D	924	ASN
1	D	998	HIS

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 4 ligands modelled in this entry, 4 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 (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	601/718 (83%)	-0.07	1 (0%)	95	87	47, 47, 47, 78	0
1	B	601/718 (83%)	-0.11	1 (0%)	95	87	47, 47, 47, 78	0
1	C	601/718 (83%)	-0.09	4 (0%)	87	69	1, 47, 47, 78	0
1	D	601/718 (83%)	-0.07	2 (0%)	94	84	47, 47, 47, 78	0
All	All	2404/2872 (83%)	-0.08	8 (0%)	94	84	1, 47, 47, 78	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	1094	ALA	3.4
1	A	494	GLN	2.6
1	D	1052	LEU	2.5
1	D	1055	GLY	2.2
1	C	960	PRO	2.1
1	C	1072	GLY	2.1
1	B	1052	LEU	2.1
1	C	935	ALA	2.0

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

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

6.3 Carbohydrates

There are no monosaccharides 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. The B-factors column lists the minimum, median, 95^{th} 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^2)	Q<0.9
2	MN	A	2001	1/1	0.93	0.21	87,87,87,87	0
2	MN	B	2001	1/1	0.95	0.24	87,87,87,87	0
2	MN	D	2001	1/1	0.97	0.23	87,87,87,87	0
2	MN	C	2001	1/1	0.99	0.21	87,87,87,87	0

6.5 Other polymers

There are no such residues in this entry.