



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 16, 2017 – 03:21 PM EDT

PDB ID : 5DO7
Title : Crystal Structure of the Human Sterol Transporter ABCG5/ABCG8
Authors : Lee, J.-Y.; Kinch, L.N.; Borek, D.M.; Urbatsch, I.L.; Xie, X.-S.; Grishin, N.V.;
Cohen, J.C.; Otwinowski, Z.; Hobbs, H.H.; Rosenbaum, D.M.
Deposited on : unknown
Resolution : 3.93 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20029824
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20029824

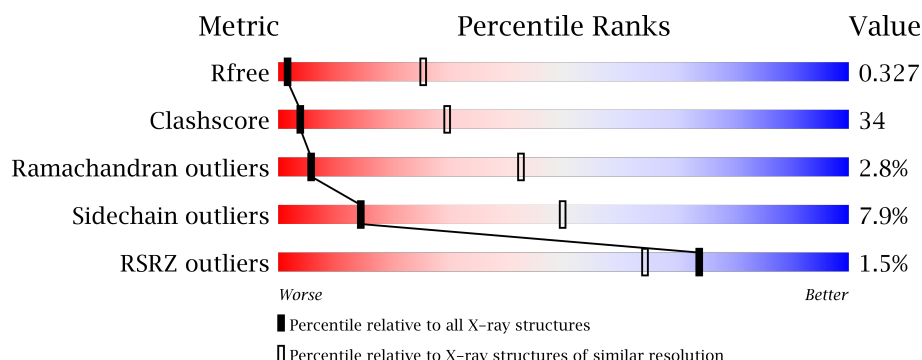
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.93 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}	100719	1021 (4.28-3.60)
Clashscore	112137	1117 (4.28-3.60)
Ramachandran outliers	110173	1076 (4.28-3.60)
Sidechain outliers	110143	1067 (4.28-3.60)
RSRZ outliers	101464	1034 (4.28-3.60)

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

Mol	Chain	Length	Quality of chain
1	A	666	<div> <div>0.1%</div> <div>39%</div> <div>44%</div> <div>5%</div> <div>12%</div> </div>
1	C	666	<div> <div>0.1%</div> <div>42%</div> <div>41%</div> <div>•</div> <div>13%</div> </div>
2	B	685	<div> <div>2%</div> <div>40%</div> <div>36%</div> <div>5%</div> <div>18%</div> </div>
2	D	685	<div> <div>0.1%</div> <div>38%</div> <div>39%</div> <div>6%</div> <div>17%</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 18150 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 ATP-binding cassette sub-family G member 5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	585	Total	C	N	O	S	0	0	0
			4606	2982	780	816	28			
1	C	579	Total	C	N	O	S	0	0	0
			4551	2945	770	807	29			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	GLU	GLY	engineered mutation	UNP Q9H222
A	652	GLY	-	expression tag	UNP Q9H222
A	653	SER	-	expression tag	UNP Q9H222
A	654	HIS	-	expression tag	UNP Q9H222
A	655	HIS	-	expression tag	UNP Q9H222
A	656	HIS	-	expression tag	UNP Q9H222
A	657	HIS	-	expression tag	UNP Q9H222
A	658	HIS	-	expression tag	UNP Q9H222
A	659	HIS	-	expression tag	UNP Q9H222
A	660	GLY	-	expression tag	UNP Q9H222
A	661	HIS	-	expression tag	UNP Q9H222
A	662	HIS	-	expression tag	UNP Q9H222
A	663	HIS	-	expression tag	UNP Q9H222
A	664	HIS	-	expression tag	UNP Q9H222
A	665	HIS	-	expression tag	UNP Q9H222
A	666	HIS	-	expression tag	UNP Q9H222
C	2	GLU	GLY	engineered mutation	UNP Q9H222
C	652	GLY	-	expression tag	UNP Q9H222
C	653	SER	-	expression tag	UNP Q9H222
C	654	HIS	-	expression tag	UNP Q9H222
C	655	HIS	-	expression tag	UNP Q9H222
C	656	HIS	-	expression tag	UNP Q9H222
C	657	HIS	-	expression tag	UNP Q9H222
C	658	HIS	-	expression tag	UNP Q9H222
C	659	HIS	-	expression tag	UNP Q9H222

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Chain	Residue	Modelled	Actual	Comment	Reference
C	660	GLY	-	expression tag	UNP Q9H222
C	661	HIS	-	expression tag	UNP Q9H222
C	662	HIS	-	expression tag	UNP Q9H222
C	663	HIS	-	expression tag	UNP Q9H222
C	664	HIS	-	expression tag	UNP Q9H222
C	665	HIS	-	expression tag	UNP Q9H222
C	666	HIS	-	expression tag	UNP Q9H222

- Molecule 2 is a protein called ATP-binding cassette sub-family G member 8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	562	Total	C	N	O	S	0	0	0
			4464	2905	756	775	28			
2	D	571	Total	C	N	O	S	0	0	0
			4529	2936	775	789	29			

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-1	MET	-	initiating methionine	UNP Q9H221
B	0	GLY	-	expression tag	UNP Q9H221
B	1	SER	-	expression tag	UNP Q9H221
B	674	ALA	-	expression tag	UNP Q9H221
B	675	SER	-	expression tag	UNP Q9H221
B	676	ASN	-	expression tag	UNP Q9H221
B	677	SER	-	expression tag	UNP Q9H221
B	678	LEU	-	expression tag	UNP Q9H221
B	679	GLU	-	expression tag	UNP Q9H221
B	680	VAL	-	expression tag	UNP Q9H221
B	681	LEU	-	expression tag	UNP Q9H221
B	682	PHE	-	expression tag	UNP Q9H221
B	683	GLN	-	expression tag	UNP Q9H221
D	-1	MET	-	initiating methionine	UNP Q9H221
D	0	GLY	-	expression tag	UNP Q9H221
D	1	SER	-	expression tag	UNP Q9H221
D	674	ALA	-	expression tag	UNP Q9H221
D	675	SER	-	expression tag	UNP Q9H221
D	676	ASN	-	expression tag	UNP Q9H221
D	677	SER	-	expression tag	UNP Q9H221
D	678	LEU	-	expression tag	UNP Q9H221
D	679	GLU	-	expression tag	UNP Q9H221
D	680	VAL	-	expression tag	UNP Q9H221

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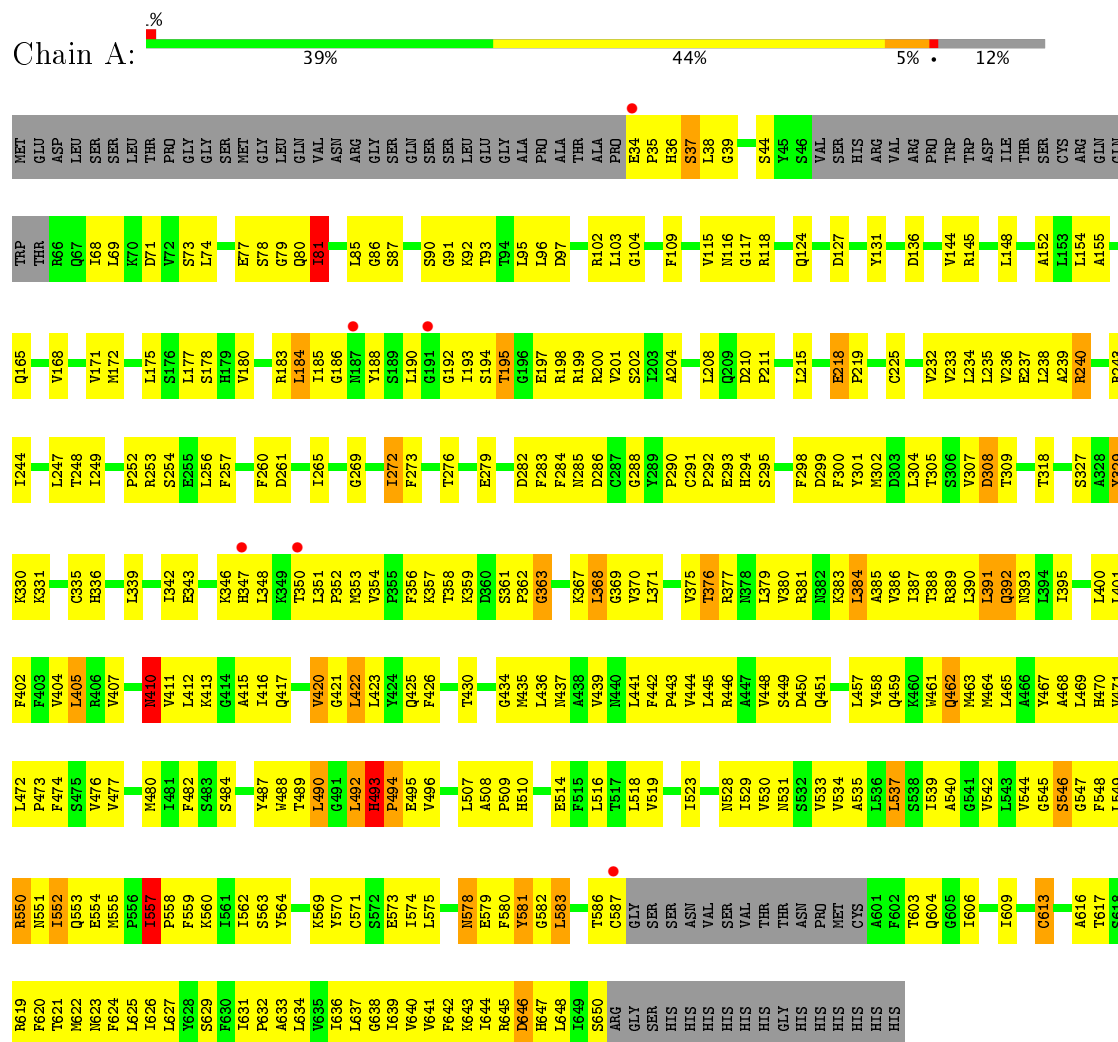
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Chain	Residue	Modelled	Actual	Comment	Reference
D	681	LEU	-	expression tag	UNP Q9H221
D	682	PHE	-	expression tag	UNP Q9H221
D	683	GLN	-	expression tag	UNP Q9H221

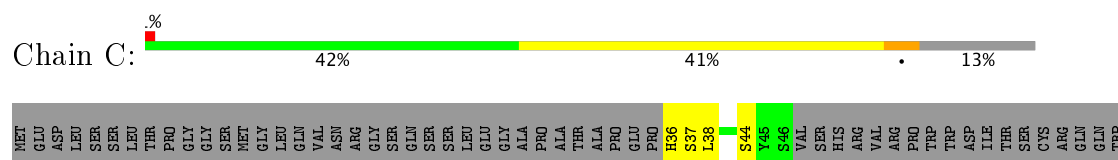
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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: ATP-binding cassette sub-family G member 5



- Molecule 1: ATP-binding cassette sub-family G member 5





4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	173.55Å 224.80Å 253.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 3.93 24.96 – 3.94	Depositor EDS
% Data completeness (in resolution range)	82.5 (25.00-3.93) 83.5 (24.96-3.94)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.79 (at 3.97Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.245 , 0.329 0.250 , 0.327	Depositor DCC
R_{free} test set	1845 reflections (5.29%)	DCC
Wilson B-factor (Å ²)	53.7	Xtriage
Anisotropy	0.196	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 59.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.84	EDS
Total number of atoms	18150	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.32% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.54	0/4697	0.82	4/6355 (0.1%)
1	C	0.52	0/4639	0.79	2/6272 (0.0%)
2	B	0.54	0/4572	0.84	4/6192 (0.1%)
2	D	0.55	0/4634	0.84	2/6273 (0.0%)
All	All	0.54	0/18542	0.82	12/25092 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	8
1	C	0	3
2	B	0	3
2	D	0	6
All	All	0	20

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	B	37	TYR	CA-CB-CG	8.16	128.91	113.40
2	B	571	TYR	CA-CB-CG	7.90	128.41	113.40
1	A	81	ILE	CB-CA-C	-6.54	98.52	111.60
2	D	486	LEU	CA-CB-CG	5.79	128.61	115.30
1	A	190	LEU	CA-CB-CG	5.56	128.09	115.30
1	A	546	SER	N-CA-C	-5.51	96.11	111.00
2	B	404	ARG	NE-CZ-NH1	5.36	122.98	120.30
1	C	603	THR	N-CA-C	5.21	125.06	111.00
1	C	384	LEU	CA-CB-CG	5.16	127.18	115.30
2	B	37	TYR	N-CA-CB	-5.16	101.31	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	552	LEU	CB-CG-CD2	5.14	119.75	111.00
1	A	384	LEU	CA-CB-CG	5.05	126.91	115.30

There are no chirality outliers.

All (20) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	104	GLY	Peptide
1	A	186	GLY	Peptide
1	A	192	GLY	Peptide
1	A	308	ASP	Peptide
1	A	34	GLU	Peptide
1	A	348	LEU	Peptide
1	A	492	LEU	Peptide
1	A	547	GLY	Peptide
2	B	31	GLU	Peptide
2	B	32	SER	Peptide
2	B	490	GLY	Peptide
1	C	414	GLY	Peptide
1	C	602	PHE	Peptide
1	C	89	GLY	Peptide
2	D	126	LYS	Peptide
2	D	24	GLN	Peptide
2	D	272	PRO	Peptide
2	D	324	LEU	Peptide
2	D	583	LEU	Peptide
2	D	607	GLN	Peptide

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	4606	0	4747	323	0
1	C	4551	0	4682	287	0
2	B	4464	0	4528	321	1
2	D	4529	0	4615	327	1
All	All	18150	0	18572	1233	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 34.

All (1233) 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:75:TYR:CZ	1:C:77:GLU:OE2	1.85	1.30
1:A:81:ILE:CD1	1:A:260:PHE:HA	1.60	1.29
2:B:36:LEU:CB	2:B:95:VAL:HG21	1.63	1.26
1:A:81:ILE:HD11	1:A:261:ASP:N	1.53	1.20
1:C:140:SER:HA	1:C:185:ILE:HD11	1.17	1.12
2:B:34:ASN:CG	2:B:135:ASN:HB3	1.69	1.11
2:B:36:LEU:HB3	2:B:95:VAL:HG21	1.14	1.11
1:C:81:ILE:HD11	1:C:236:VAL:HG13	1.32	1.11
1:C:75:TYR:CE2	1:C:77:GLU:OE2	2.04	1.10
2:B:488:THR:HA	2:B:491:PRO:HG2	1.17	1.09
2:D:94:LYS:HE3	2:D:353:VAL:HG21	1.29	1.09
2:D:293:TYR:CD1	2:D:343:GLN:HG3	1.89	1.08
2:B:36:LEU:HB3	2:B:95:VAL:CG2	1.83	1.07
2:D:293:TYR:OH	2:D:354:ARG:O	1.71	1.07
1:C:573:GLU:OE2	1:C:619:ARG:NH2	1.87	1.06
1:A:81:ILE:HD11	1:A:260:PHE:CA	1.84	1.06
2:B:34:ASN:OD1	2:B:135:ASN:HB3	1.57	1.04
2:B:488:THR:HA	2:B:491:PRO:CG	1.87	1.04
2:B:36:LEU:O	2:B:95:VAL:HG22	1.55	1.03
1:A:492:LEU:HD13	1:A:579:GLU:HG3	1.37	1.03
1:A:81:ILE:HD11	1:A:260:PHE:HA	1.29	1.03
1:A:603:THR:HB	1:A:604:GLN:OE1	1.57	1.02
1:A:81:ILE:CD1	1:A:260:PHE:CA	2.36	1.01
1:A:367:LYS:O	1:A:370:VAL:HG12	1.59	1.01
1:A:36:HIS:O	1:A:77:GLU:HA	1.59	1.00
2:B:445:PHE:HA	2:B:448:THR:HG22	1.44	1.00
2:B:423:GLU:OE1	2:B:462:ASN:ND2	1.93	0.99
2:D:414:LEU:O	2:D:418:LEU:HD12	1.61	0.99
2:D:492:TYR:HA	2:D:495:ALA:HB2	1.45	0.98
1:C:140:SER:CA	1:C:185:ILE:HD11	1.96	0.96
1:A:81:ILE:HD11	1:A:260:PHE:C	1.84	0.96
1:A:188:TYR:CD1	1:A:195:THR:HG23	2.01	0.95
1:C:140:SER:HA	1:C:185:ILE:CD1	1.95	0.95
2:B:36:LEU:O	2:B:95:VAL:CG2	2.15	0.95
2:B:104:ILE:HD11	2:B:272:PRO:HG2	1.49	0.94
1:A:36:HIS:HB2	1:A:78:SER:HB2	1.50	0.94
2:D:552:LEU:HD22	2:D:553:LEU:HD12	1.50	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:293:TYR:OH	2:D:355:ASP:C	2.07	0.93
1:A:81:ILE:HD11	1:A:261:ASP:H	1.22	0.93
2:D:402:LEU:HD21	2:D:486:LEU:HD11	1.51	0.93
2:D:487:TYR:O	2:D:491:PRO:HG2	1.68	0.92
2:B:36:LEU:H	2:B:95:VAL:HG23	1.34	0.92
2:D:335:GLU:O	2:D:338:THR:OG1	1.87	0.92
1:A:81:ILE:HD13	1:A:260:PHE:HA	1.50	0.91
1:A:545:GLY:O	1:A:569:LYS:HA	1.70	0.91
2:B:309:TYR:CZ	2:B:317:PRO:HG2	2.06	0.90
2:D:94:LYS:HE2	2:D:351:GLU:HB3	1.52	0.90
2:B:587:PRO:HA	2:B:590:ILE:HG22	1.54	0.90
1:A:252:PRO:HG2	1:A:298:PHE:CE2	2.06	0.90
2:D:287:THR:HG21	2:D:322:VAL:HA	1.53	0.90
2:D:293:TYR:HD1	2:D:343:GLN:HG3	1.33	0.90
2:D:309:TYR:OH	2:D:317:PRO:HG2	1.73	0.89
1:A:35:PRO:O	1:A:352:PRO:HG2	1.71	0.89
1:C:75:TYR:OH	1:C:77:GLU:OE2	1.90	0.89
2:B:488:THR:CA	2:B:491:PRO:CG	2.51	0.89
2:B:590:ILE:O	2:B:593:VAL:HG12	1.73	0.89
1:C:188:TYR:CG	1:C:195:THR:HB	2.09	0.88
2:B:309:TYR:CZ	2:B:317:PRO:CG	2.56	0.88
2:D:293:TYR:CE2	2:D:294:LEU:O	2.27	0.87
1:A:185:ILE:O	1:A:193:ILE:HB	1.74	0.87
2:D:590:ILE:O	2:D:593:VAL:HG12	1.73	0.87
2:B:443:LEU:HD13	2:B:448:THR:HB	1.56	0.86
2:D:492:TYR:HA	2:D:495:ALA:CB	2.05	0.86
2:B:36:LEU:CA	2:B:95:VAL:CG2	2.53	0.86
2:B:488:THR:CA	2:B:491:PRO:HG2	2.05	0.86
2:B:36:LEU:CA	2:B:95:VAL:HG21	2.06	0.85
2:B:36:LEU:CB	2:B:95:VAL:CG2	2.46	0.85
2:B:36:LEU:N	2:B:95:VAL:HG23	1.91	0.85
2:D:293:TYR:CZ	2:D:294:LEU:O	2.29	0.85
2:B:309:TYR:OH	2:B:317:PRO:HG2	1.75	0.85
2:B:272:PRO:O	2:B:273:ARG:HG2	1.78	0.84
1:A:545:GLY:O	1:A:569:LYS:CA	2.25	0.84
2:B:480:TYR:HB3	2:B:486:LEU:CD1	2.07	0.84
2:B:402:LEU:HD11	2:B:486:LEU:HD23	1.57	0.84
1:C:300:PHE:O	1:C:302:MET:N	2.11	0.84
2:D:583:LEU:HG	2:D:583:LEU:O	1.76	0.84
1:A:97:ASP:OD1	1:A:131:TYR:OH	1.95	0.82
2:B:134:ILE:O	2:B:136:GLY:N	2.11	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:329:TYR:O	1:A:335:CYS:SG	2.37	0.81
1:A:81:ILE:CD1	1:A:261:ASP:N	2.41	0.81
2:B:36:LEU:C	2:B:95:VAL:CG2	2.48	0.81
2:D:480:TYR:HB3	2:D:486:LEU:HD22	1.62	0.81
1:C:152:ALA:HB2	1:C:208:LEU:HD13	1.63	0.81
1:A:539:ILE:HG13	1:A:540:ALA:N	1.96	0.80
2:B:480:TYR:HB3	2:B:486:LEU:HD13	1.63	0.80
1:A:152:ALA:HB2	1:A:208:LEU:HD13	1.64	0.80
1:C:329:TYR:O	1:C:335:CYS:SG	2.39	0.80
1:A:430:THR:O	1:A:510:HIS:HA	1.81	0.80
2:D:321:TYR:HE1	2:D:339:ARG:HD3	1.47	0.80
2:D:97:SER:O	2:D:263:ARG:O	1.99	0.79
2:B:34:ASN:OD1	2:B:135:ASN:CB	2.30	0.79
2:B:35:SER:HB3	2:B:95:VAL:O	1.82	0.79
2:D:94:LYS:HD3	2:D:351:GLU:HA	1.63	0.79
2:B:444:SER:O	2:B:447:ASP:N	2.15	0.78
2:D:337:ALA:O	2:D:340:GLU:HB3	1.83	0.78
1:C:430:THR:O	1:C:510:HIS:HA	1.83	0.78
2:B:445:PHE:HA	2:B:448:THR:CG2	2.14	0.77
2:D:508:ILE:HD13	2:D:536:TRP:HA	1.66	0.77
1:C:296:ASN:O	1:C:299:ASP:N	2.17	0.77
2:B:104:ILE:CD1	2:B:272:PRO:HG2	2.15	0.77
2:D:285:LEU:HB2	2:D:314:TYR:OH	1.86	0.76
2:B:634:GLU:N	2:B:634:GLU:OE1	2.19	0.76
2:B:25:ASP:OD1	2:B:26:ARG:N	2.19	0.76
2:D:491:PRO:O	2:D:495:ALA:HB2	1.86	0.76
2:B:587:PRO:O	2:B:590:ILE:HG22	1.86	0.76
1:C:329:TYR:CD2	1:C:335:CYS:SG	2.79	0.76
2:B:508:ILE:HD13	2:B:536:TRP:HA	1.68	0.75
1:A:77:GLU:N	1:A:80:GLN:OE1	2.19	0.75
1:C:329:TYR:CE2	1:C:335:CYS:SG	2.79	0.75
2:B:95:VAL:O	2:B:95:VAL:HG23	1.84	0.75
1:C:307:VAL:HG11	1:C:319:SER:HA	1.66	0.75
1:A:465:LEU:O	1:A:469:LEU:HD12	1.86	0.75
2:D:94:LYS:CE	2:D:353:VAL:HG21	2.14	0.75
2:D:37:TYR:HB3	2:D:133:TRP:HB2	1.67	0.75
2:D:414:LEU:HG	2:D:418:LEU:HD11	1.67	0.75
2:D:321:TYR:HE1	2:D:339:ARG:CD	2.00	0.74
1:A:81:ILE:CD1	1:A:261:ASP:H	2.00	0.74
1:A:171:VAL:HG21	1:A:208:LEU:HD23	1.69	0.74
1:A:379:LEU:HD13	1:A:470:HIS:CE1	2.21	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:77:GLU:N	1:C:80:GLN:OE1	2.19	0.74
2:B:630:LEU:O	2:B:633:MET:O	2.05	0.74
1:C:545:GLY:O	1:C:569:LYS:HA	1.87	0.74
2:D:492:TYR:O	2:D:495:ALA:N	2.20	0.74
1:A:252:PRO:CG	1:A:298:PHE:CE2	2.71	0.74
1:A:423:LEU:HD22	1:A:575:LEU:HB3	1.70	0.73
1:C:171:VAL:HG21	1:C:208:LEU:HD23	1.70	0.73
1:C:87:SER:OG	1:C:306:SER:HB2	1.88	0.73
1:A:35:PRO:O	1:A:352:PRO:CG	2.35	0.73
2:D:32:SER:OG	2:D:33:ASP:N	2.21	0.73
2:B:213:LEU:HD13	2:B:214:SER:O	1.89	0.73
2:D:43:GLN:CG	2:D:126:LYS:O	2.37	0.73
2:B:584:TRP:HB2	2:B:587:PRO:CD	2.19	0.72
1:C:416:ILE:HD12	1:C:417:GLN:N	2.04	0.72
2:B:488:THR:CA	2:B:491:PRO:HG3	2.17	0.72
1:C:211:PRO:O	1:C:243:ARG:NH1	2.22	0.72
2:D:43:GLN:HG3	2:D:126:LYS:O	1.89	0.72
1:A:299:ASP:OD2	2:B:273:ARG:HD3	1.89	0.72
1:A:480:MET:O	1:A:484:SER:OG	2.08	0.72
1:C:423:LEU:HD22	1:C:575:LEU:HB3	1.72	0.72
1:A:273:PHE:HB2	1:A:329:TYR:CZ	2.24	0.72
2:B:35:SER:O	2:B:135:ASN:N	2.22	0.72
2:D:94:LYS:HE3	2:D:353:VAL:CG2	2.15	0.72
1:C:179:HIS:CD2	1:C:180:VAL:HG23	2.24	0.72
1:C:199:ARG:HH21	1:C:219:PRO:HA	1.53	0.72
2:D:246:PHE:CG	1:C:308:ASP:HB3	2.25	0.72
2:B:584:TRP:CB	2:B:587:PRO:HD2	2.20	0.71
1:A:492:LEU:HD13	1:A:579:GLU:CG	2.17	0.71
1:C:359:LYS:O	1:C:361:SER:N	2.22	0.71
2:D:587:PRO:O	2:D:589:TRP:N	2.23	0.71
1:A:582:GLY:C	1:A:583:LEU:HD12	2.10	0.71
2:B:309:TYR:OH	2:B:317:PRO:CG	2.38	0.71
1:A:487:TYR:CE1	1:A:492:LEU:HD12	2.25	0.71
1:A:211:PRO:O	1:A:243:ARG:NH1	2.23	0.71
1:C:379:LEU:HD13	1:C:470:HIS:CE1	2.25	0.71
1:A:81:ILE:HG12	1:A:261:ASP:OD1	1.90	0.71
2:B:583:LEU:HB3	2:B:587:PRO:HG2	1.72	0.71
2:D:313:ARG:NE	2:D:315:SER:HB2	2.05	0.71
1:A:272:ILE:HG22	1:A:329:TYR:HE1	1.56	0.70
2:B:628:LYS:O	2:B:632:VAL:HG23	1.91	0.70
1:C:480:MET:O	1:C:484:SER:OG	2.08	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:619:ARG:NH1	1:C:623:ASN:OD1	2.24	0.70
1:A:465:LEU:HG	1:A:469:LEU:HD11	1.73	0.70
2:B:540:PHE:CE2	2:B:544:ILE:HD11	2.26	0.70
2:D:293:TYR:HE1	2:D:343:GLN:HE21	1.40	0.70
1:A:302:MET:HA	1:A:305:THR:OG1	1.90	0.70
2:B:443:LEU:HD11	2:B:614:LYS:NZ	2.07	0.70
1:C:557:ILE:HB	1:C:558:PRO:HD3	1.74	0.69
1:A:416:ILE:HD12	1:A:417:GLN:N	2.07	0.69
1:A:379:LEU:CD1	1:A:470:HIS:CE1	2.75	0.69
2:B:587:PRO:CA	2:B:590:ILE:HG22	2.22	0.69
1:C:188:TYR:CD1	1:C:195:THR:HB	2.28	0.69
2:D:402:LEU:HD21	2:D:486:LEU:CD1	2.21	0.69
2:B:274:SER:O	2:B:277:PHE:HB3	1.93	0.69
1:C:90:SER:OG	1:C:93:THR:OG1	2.10	0.69
2:D:487:TYR:O	2:D:491:PRO:CG	2.39	0.69
1:A:632:PRO:O	1:A:636:ILE:HD12	1.93	0.69
2:B:402:LEU:CD1	2:B:486:LEU:HD23	2.23	0.69
2:D:347:ALA:O	2:D:349:PHE:N	2.26	0.69
1:A:225:CYS:SG	1:A:253:ARG:NH2	2.66	0.69
1:A:465:LEU:C	1:A:469:LEU:HD12	2.12	0.69
2:D:540:PHE:CE2	2:D:544:ILE:HD11	2.27	0.69
1:C:367:LYS:O	1:C:370:VAL:HG12	1.93	0.68
1:A:350:THR:HG23	1:A:352:PRO:HD2	1.75	0.68
1:C:465:LEU:HG	1:C:469:LEU:HD11	1.74	0.68
1:C:379:LEU:HD11	1:C:389:ARG:NH1	2.09	0.68
1:C:583:LEU:HD23	1:C:585:PHE:HE1	1.57	0.68
2:B:488:THR:C	2:B:491:PRO:HG3	2.13	0.68
2:B:31:GLU:OE2	2:B:32:SER:N	2.23	0.68
1:C:254:SER:HB3	1:C:296:ASN:CG	2.13	0.68
1:A:352:PRO:O	1:A:354:VAL:HG22	1.94	0.68
2:B:459:ILE:HD11	2:B:511:TYR:CE1	2.29	0.68
2:D:207:ASN:O	2:D:210:VAL:HG22	1.94	0.68
1:C:85:LEU:HD21	1:C:302:MET:SD	2.34	0.68
1:C:637:LEU:O	1:C:640:VAL:CG1	2.42	0.68
2:B:586:VAL:HG23	2:B:587:PRO:HD3	1.75	0.67
2:B:213:LEU:HD13	2:B:213:LEU:C	2.14	0.67
1:C:615:GLY:O	1:C:619:ARG:HG3	1.93	0.67
1:A:557:ILE:HB	1:A:558:PRO:HD3	1.76	0.67
1:A:637:LEU:O	1:A:640:VAL:CG1	2.42	0.67
1:A:622:MET:HE3	1:C:640:VAL:HG23	1.75	0.67
2:D:158:LEU:HB3	2:D:409:ASN:HD22	1.59	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:473:PRO:O	1:A:476:VAL:HG12	1.95	0.67
2:D:94:LYS:HB3	2:D:353:VAL:HG21	1.77	0.67
2:B:584:TRP:HB2	2:B:587:PRO:HD2	1.76	0.67
2:D:293:TYR:OH	2:D:354:ARG:C	2.33	0.67
1:C:389:ARG:HE	1:C:437:ASN:ND2	1.93	0.67
1:A:386:VAL:HG12	1:A:390:LEU:HD11	1.77	0.67
1:A:124:GLN:O	1:A:127:ASP:HB2	1.95	0.67
2:D:508:ILE:CD1	2:D:536:TRP:HA	2.24	0.67
1:A:469:LEU:O	1:A:472:LEU:HD12	1.95	0.66
2:B:587:PRO:HA	2:B:590:ILE:CG2	2.24	0.66
2:D:304:PHE:CB	2:D:309:TYR:CE1	2.78	0.66
1:A:185:ILE:O	1:A:193:ILE:CB	2.44	0.66
2:D:587:PRO:O	2:D:590:ILE:N	2.28	0.66
1:C:308:ASP:OD1	1:C:309:THR:N	2.29	0.66
1:A:307:VAL:HG23	1:A:318:THR:OG1	1.96	0.66
2:B:275:ASP:OD1	2:B:276:ILE:HD12	1.94	0.66
2:B:522:ARG:N	2:B:607:GLN:OE1	2.28	0.66
2:B:96:ARG:N	2:B:99:GLN:OE1	2.28	0.66
1:C:622:MET:O	1:C:625:LEU:N	2.28	0.66
2:B:304:PHE:HD2	2:B:309:TYR:HH	1.39	0.66
2:B:645:LEU:HA	2:B:648:ILE:HG22	1.78	0.66
1:A:407:VAL:HG12	1:A:490:LEU:O	1.96	0.66
1:A:622:MET:O	1:A:625:LEU:N	2.28	0.66
2:B:609:SER:HB3	2:B:630:LEU:HB2	1.78	0.66
1:A:102:ARG:O	1:A:103:LEU:HD12	1.95	0.65
1:A:302:MET:O	1:A:305:THR:OG1	2.14	0.65
2:D:645:LEU:HA	2:D:648:ILE:HG22	1.77	0.65
1:A:550:ARG:NH2	2:B:441:ILE:HD12	2.11	0.65
1:A:464:MET:HE1	1:A:639:ILE:N	2.11	0.65
2:B:42:GLY:O	2:B:128:LYS:N	2.25	0.65
2:B:420:HIS:NE2	2:B:466:ASP:OD1	2.29	0.65
1:C:469:LEU:O	1:C:472:LEU:HD12	1.96	0.65
1:C:379:LEU:CD1	1:C:470:HIS:CE1	2.78	0.65
2:D:267:ILE:HG22	2:D:269:LEU:HD13	1.77	0.65
2:D:293:TYR:CD1	2:D:343:GLN:CG	2.75	0.65
2:D:396:VAL:HG13	2:D:397:GLN:N	2.11	0.65
2:D:531:HIS:CD2	2:D:603:LEU:HD22	2.32	0.65
2:B:34:ASN:OD1	2:B:135:ASN:N	2.30	0.65
1:A:435:MET:O	1:A:439:VAL:HG12	1.97	0.65
2:B:345:LEU:C	2:B:345:LEU:HD12	2.16	0.65
2:D:643:ILE:HA	2:D:646:ILE:HD12	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:127:ASP:O	1:A:357:LYS:CG	2.44	0.65
2:B:551:ALA:HA	2:B:667:GLN:NE2	2.11	0.65
2:B:213:LEU:CD1	2:B:214:SER:O	2.44	0.65
1:A:253:ARG:HB2	1:A:256:LEU:CD1	2.27	0.65
1:A:492:LEU:HB2	1:A:579:GLU:OE2	1.97	0.65
1:A:604:GLN:N	1:A:604:GLN:OE1	2.30	0.65
2:B:492:TYR:HA	2:B:495:ALA:CB	2.27	0.65
2:D:323:ASP:N	2:D:323:ASP:OD1	2.30	0.64
2:B:488:THR:C	2:B:491:PRO:CG	2.66	0.64
1:A:389:ARG:HH21	1:A:471:VAL:HG23	1.62	0.64
1:C:606:ILE:HA	1:C:609:ILE:HD12	1.78	0.64
1:A:508:ALA:HB3	1:A:509:PRO:HD3	1.78	0.64
1:C:435:MET:O	1:C:439:VAL:HG12	1.97	0.64
1:A:573:GLU:OE1	1:A:619:ARG:NH2	2.31	0.64
1:C:187:ASN:OD1	1:C:190:LEU:N	2.29	0.64
1:C:127:ASP:O	1:C:357:LYS:CG	2.46	0.64
1:A:36:HIS:HB2	1:A:78:SER:CB	2.27	0.64
1:A:606:ILE:HA	1:A:609:ILE:HD12	1.79	0.64
1:C:379:LEU:O	1:C:379:LEU:HD23	1.98	0.64
1:C:473:PRO:O	1:C:476:VAL:HG12	1.98	0.64
2:D:33:ASP:OD1	2:D:34:ASN:N	2.30	0.64
2:B:508:ILE:CD1	2:B:536:TRP:HA	2.27	0.64
2:B:553:LEU:HD23	2:B:558:MET:HB3	1.79	0.64
2:D:321:TYR:CE1	2:D:339:ARG:CD	2.81	0.64
1:C:285:ASN:HD22	1:C:285:ASN:N	1.95	0.64
1:C:508:ALA:HB3	1:C:509:PRO:HD3	1.80	0.64
1:C:586:THR:O	1:C:587:CYS:HB3	1.97	0.64
2:D:293:TYR:CD2	2:D:300:MET:CE	2.81	0.64
2:D:313:ARG:NE	2:D:315:SER:CB	2.61	0.64
1:C:85:LEU:HG	1:C:302:MET:CE	2.28	0.63
1:A:545:GLY:O	1:A:569:LYS:N	2.31	0.63
1:C:197:GLU:O	1:C:200:ARG:HB2	1.98	0.63
2:D:660:VAL:O	2:D:662:LEU:O	2.16	0.63
2:D:343:GLN:O	2:D:344:SER:C	2.36	0.63
2:D:351:GLU:O	2:D:353:VAL:HG23	1.97	0.63
2:B:553:LEU:HD22	2:B:559:ALA:HA	1.79	0.63
1:C:300:PHE:O	1:C:303:ASP:N	2.30	0.63
2:D:293:TYR:CZ	2:D:355:ASP:C	2.71	0.63
1:A:603:THR:CB	1:A:604:GLN:OE1	2.41	0.63
1:C:188:TYR:CD2	1:C:195:THR:HB	2.34	0.63
2:D:304:PHE:HB3	2:D:309:TYR:CE1	2.33	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:36:LEU:HD23	2:B:95:VAL:HG11	1.80	0.63
2:D:94:LYS:HB3	2:D:353:VAL:CG2	2.28	0.63
1:A:235:LEU:HD13	1:A:247:LEU:HD21	1.81	0.62
1:A:35:PRO:HD2	1:A:352:PRO:HG3	1.81	0.62
1:A:127:ASP:O	1:A:357:LYS:HG2	1.99	0.62
2:D:158:LEU:HB3	2:D:409:ASN:ND2	2.14	0.62
1:A:79:GLY:HA2	1:A:239:ALA:O	1.99	0.62
2:B:33:ASP:OD1	2:B:34:ASN:N	2.31	0.62
2:B:492:TYR:HA	2:B:495:ALA:HB2	1.81	0.62
2:B:480:TYR:CB	2:B:486:LEU:HD13	2.30	0.62
1:C:235:LEU:HD13	1:C:247:LEU:HD21	1.81	0.62
1:A:379:LEU:O	1:A:379:LEU:HD23	1.99	0.62
2:B:273:ARG:HD2	2:B:275:ASP:OD1	1.99	0.62
2:B:36:LEU:CG	2:B:95:VAL:HG21	2.27	0.62
1:A:411:VAL:HG21	1:A:413:LYS:HB3	1.81	0.62
2:B:460:PRO:HA	2:B:463:VAL:HG12	1.82	0.62
1:A:402:PHE:CZ	2:B:586:VAL:HG21	2.33	0.62
2:B:149:ALA:HB3	2:B:234:LEU:HD12	1.81	0.62
2:D:149:ALA:HB3	2:D:234:LEU:HD12	1.81	0.62
1:A:73:SER:O	1:A:74:LEU:HD12	2.00	0.62
2:B:274:SER:OG	2:B:313:ARG:HG3	2.00	0.62
2:B:442:GLN:HB2	2:B:617:LEU:HD11	1.81	0.62
1:A:549:LEU:HD12	2:B:450:ALA:HB1	1.82	0.61
2:D:450:ALA:HB2	2:D:576:PHE:CZ	2.35	0.61
1:A:92:LYS:HG3	1:A:93:THR:N	2.15	0.61
2:B:643:ILE:HA	2:B:646:ILE:HD12	1.81	0.61
2:D:611:ARG:O	2:D:612:THR:HG23	2.00	0.61
1:C:386:VAL:HG12	1:C:390:LEU:HD11	1.81	0.61
1:C:315:GLU:HG3	1:C:316:ILE:N	2.14	0.61
2:D:293:TYR:HD1	2:D:343:GLN:CG	2.09	0.61
2:B:161:LEU:O	2:B:205:VAL:HG13	2.00	0.61
1:C:637:LEU:O	1:C:640:VAL:HG12	2.00	0.61
2:B:34:ASN:OD1	2:B:135:ASN:CA	2.49	0.61
1:C:435:MET:SD	1:C:531:ASN:ND2	2.74	0.61
1:A:185:ILE:O	1:A:193:ILE:CG2	2.49	0.60
1:A:136:ASP:OD2	1:A:199:ARG:HA	2.01	0.60
1:C:539:ILE:O	1:C:542:VAL:HG22	2.01	0.60
1:A:637:LEU:O	1:A:640:VAL:HG12	2.00	0.60
1:A:103:LEU:HD22	1:A:650:SER:OG	2.01	0.60
1:A:619:ARG:CG	1:A:622:MET:HE2	2.31	0.60
2:B:600:PHE:CE1	2:B:604:MET:CE	2.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:609:SER:CB	2:B:630:LEU:HB2	2.32	0.60
1:A:308:ASP:OD2	1:A:309:THR:N	2.33	0.60
2:B:34:ASN:CG	2:B:135:ASN:CB	2.59	0.60
2:D:600:PHE:CE1	2:D:604:MET:CE	2.85	0.60
1:C:79:GLY:HA2	1:C:239:ALA:O	2.01	0.60
2:D:553:LEU:HD22	2:D:559:ALA:HA	1.83	0.60
1:A:535:ALA:O	1:A:539:ILE:HG23	2.02	0.59
1:A:554:GLU:O	2:B:441:ILE:HG21	2.01	0.59
2:B:205:VAL:HG23	2:B:206:GLY:N	2.16	0.59
2:B:309:TYR:CZ	2:B:317:PRO:HG3	2.37	0.59
1:C:546:SER:HB3	1:C:548:PHE:CD2	2.37	0.59
2:D:492:TYR:O	2:D:494:PHE:N	2.35	0.59
1:C:364:VAL:O	1:C:367:LYS:HB3	2.02	0.59
2:D:293:TYR:CD2	2:D:300:MET:HE1	2.38	0.59
2:D:552:LEU:HD12	2:D:657:LEU:HD21	1.82	0.59
1:A:539:ILE:O	1:A:542:VAL:HG22	2.02	0.59
1:A:68:ILE:O	1:A:269:GLY:HA3	2.03	0.59
2:D:94:LYS:HD3	2:D:351:GLU:CA	2.33	0.59
2:D:480:TYR:CB	2:D:486:LEU:HD22	2.29	0.59
2:B:580:LEU:O	2:B:583:LEU:HG	2.02	0.59
2:D:335:GLU:O	2:D:338:THR:N	2.35	0.59
2:D:460:PRO:HA	2:D:463:VAL:HG12	1.84	0.59
1:A:401:LEU:HD13	1:A:490:LEU:CD1	2.32	0.59
2:B:127:ILE:HD12	2:B:127:ILE:O	2.03	0.59
2:D:522:ARG:H	2:D:607:GLN:NE2	2.01	0.59
2:D:552:LEU:CD1	2:D:657:LEU:HD21	2.33	0.59
1:A:445:LEU:HD23	1:A:463:MET:SD	2.43	0.59
1:C:149:HIS:O	1:C:153:LEU:HB2	2.02	0.59
1:A:197:GLU:O	1:A:200:ARG:HB3	2.03	0.59
1:A:487:TYR:CZ	1:A:492:LEU:O	2.55	0.59
2:B:584:TRP:HB3	2:B:586:VAL:HG22	1.84	0.59
2:D:409:ASN:OD1	2:D:410:ASP:N	2.35	0.59
1:A:442:PHE:CE2	1:A:446:ARG:HB2	2.38	0.58
1:C:136:ASP:OD2	1:C:199:ARG:HA	2.03	0.58
1:A:351:LEU:HG	1:A:352:PRO:HD3	1.84	0.58
2:D:293:TYR:CD2	2:D:294:LEU:O	2.57	0.58
1:A:272:ILE:HG22	1:A:329:TYR:CE1	2.37	0.58
1:A:284:PHE:O	1:A:288:GLY:O	2.20	0.58
1:C:461:TRP:O	1:C:462:GLN:C	2.40	0.58
2:B:35:SER:OG	2:B:96:ARG:HA	2.04	0.58
2:D:409:ASN:C	2:D:409:ASN:OD1	2.41	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:459:ILE:HG12	2:B:511:TYR:CZ	2.39	0.58
1:C:300:PHE:O	1:C:301:TYR:C	2.40	0.58
1:A:580:PHE:HA	1:A:583:LEU:HD13	1.84	0.58
1:C:408:ARG:NH1	1:C:410:ASN:HD21	2.02	0.58
1:C:534:VAL:HA	1:C:537:LEU:HD22	1.85	0.58
1:C:36:HIS:HB2	1:C:78:SER:HB2	1.86	0.58
2:D:552:LEU:CD2	2:D:553:LEU:HD12	2.30	0.58
2:B:109:CYS:SG	2:B:111:ARG:HB2	2.44	0.58
2:B:207:ASN:OD1	2:B:211:ARG:HA	2.03	0.58
2:B:213:LEU:HD13	2:B:214:SER:N	2.19	0.58
1:C:442:PHE:CE2	1:C:446:ARG:HB2	2.39	0.58
2:D:236:LEU:HD11	2:D:255:LEU:HD22	1.85	0.58
1:C:92:LYS:HG3	1:C:93:THR:N	2.19	0.58
2:D:553:LEU:HD23	2:D:558:MET:HB3	1.86	0.58
1:A:580:PHE:O	1:A:582:GLY:N	2.37	0.57
2:B:525:LEU:O	2:B:526:GLN:C	2.42	0.57
2:D:424:ALA:O	2:D:425:CYS:C	2.41	0.57
1:A:580:PHE:HA	1:A:583:LEU:CD1	2.34	0.57
2:D:304:PHE:HB2	2:D:309:TYR:CE1	2.38	0.57
2:B:350:LEU:O	2:B:353:VAL:HG12	2.04	0.57
1:C:314:ARG:O	1:C:318:THR:HG23	2.04	0.57
1:C:36:HIS:CE1	1:C:356:PHE:CD2	2.92	0.57
2:D:31:GLU:HB3	2:D:262:ASN:HB3	1.85	0.57
2:B:236:LEU:HD11	2:B:255:LEU:HD22	1.86	0.57
2:B:483:GLU:O	2:B:484:ASP:HB3	2.02	0.57
1:C:371:LEU:HD21	1:C:458:TYR:CD2	2.39	0.57
1:C:434:GLY:O	1:C:437:ASN:HB2	2.04	0.57
1:A:546:SER:HB2	1:A:548:PHE:CD2	2.40	0.57
2:D:273:ARG:HB2	2:D:276:ILE:HD13	1.87	0.57
2:D:321:TYR:CE1	2:D:339:ARG:HD2	2.40	0.57
1:C:542:VAL:O	1:C:546:SER:OG	2.18	0.57
1:C:557:ILE:HB	1:C:558:PRO:CD	2.35	0.57
2:D:229:TRP:O	2:D:230:ASN:OD1	2.23	0.57
2:B:585:THR:HA	2:B:588:ALA:HB3	1.87	0.57
2:D:461:PHE:CD2	2:D:461:PHE:O	2.57	0.57
1:A:459:GLN:O	1:A:462:GLN:HG2	2.05	0.57
1:A:464:MET:CE	1:A:638:GLY:C	2.73	0.57
2:B:277:PHE:HA	2:B:280:PHE:CE2	2.40	0.57
1:C:89:GLY:O	1:C:91:GLY:N	2.36	0.57
2:D:333:GLU:OE1	2:D:333:GLU:HA	2.04	0.57
2:D:611:ARG:O	2:D:612:THR:CG2	2.52	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:313:ARG:HG2	2:B:314:TYR:N	2.20	0.57
2:B:423:GLU:OE1	2:B:462:ASN:CG	2.43	0.57
1:C:392:GLN:O	1:C:393:ASN:C	2.41	0.57
2:B:424:ALA:O	2:B:425:CYS:C	2.44	0.56
2:B:36:LEU:CA	2:B:95:VAL:HG23	2.30	0.56
2:D:633:MET:O	2:D:634:GLU:HB2	2.04	0.56
1:C:459:GLN:O	1:C:462:GLN:HG2	2.05	0.56
1:C:85:LEU:HD21	1:C:302:MET:CG	2.35	0.56
2:D:492:TYR:C	2:D:495:ALA:H	2.08	0.56
2:B:316:ASN:HB3	2:B:317:PRO:HD3	1.87	0.56
1:C:218:GLU:HA	1:C:248:THR:O	2.05	0.56
1:C:466:ALA:HA	1:C:469:LEU:HD12	1.85	0.56
1:A:253:ARG:HB2	1:A:256:LEU:HD13	1.87	0.56
2:B:445:PHE:CA	2:B:448:THR:HG22	2.26	0.56
1:C:127:ASP:O	1:C:357:LYS:HG2	2.03	0.56
2:D:314:TYR:CD1	2:D:314:TYR:O	2.58	0.56
2:D:400:THR:O	2:D:403:ILE:HG22	2.06	0.56
2:D:459:ILE:HD11	2:D:507:TYR:HE1	1.70	0.56
1:C:637:LEU:O	1:C:640:VAL:HG13	2.05	0.56
2:D:109:CYS:SG	2:D:111:ARG:HB2	2.45	0.56
1:A:534:VAL:HA	1:A:537:LEU:HD22	1.87	0.56
2:D:316:ASN:HB3	2:D:317:PRO:HD3	1.87	0.56
2:B:600:PHE:CE1	2:B:604:MET:HE1	2.41	0.56
2:D:573:ALA:HB1	2:D:591:SER:HA	1.88	0.56
1:C:81:ILE:CD1	1:C:236:VAL:HG13	2.21	0.56
2:D:151:VAL:HB	2:D:236:LEU:HD23	1.88	0.56
2:D:659:TYR:HD1	2:D:659:TYR:O	1.89	0.56
1:A:218:GLU:HA	1:A:248:THR:O	2.06	0.56
1:A:301:TYR:O	1:A:305:THR:HG23	2.06	0.56
2:B:522:ARG:HD2	2:B:523:PRO:HD2	1.86	0.56
1:C:408:ARG:HH12	1:C:410:ASN:HD21	1.54	0.56
1:A:434:GLY:O	1:A:437:ASN:HB2	2.06	0.55
1:A:371:LEU:HD21	1:A:458:TYR:CD2	2.41	0.55
1:C:155:ALA:O	1:C:362:PRO:HG3	2.07	0.55
1:C:545:GLY:O	1:C:569:LYS:CA	2.53	0.55
1:C:569:LYS:HG3	1:C:573:GLU:OE1	2.06	0.55
1:A:495:GLU:OE1	1:A:496:VAL:N	2.39	0.55
1:A:273:PHE:HB2	1:A:329:TYR:CE1	2.41	0.55
1:A:85:LEU:C	1:A:85:LEU:HD23	2.27	0.55
2:D:583:LEU:CG	2:D:583:LEU:O	2.52	0.55
1:A:461:TRP:O	1:A:462:GLN:C	2.44	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:637:LEU:O	1:A:640:VAL:HG13	2.06	0.55
1:A:198:ARG:O	1:A:201:VAL:HG12	2.07	0.55
2:B:304:PHE:HD2	2:B:309:TYR:OH	1.89	0.55
2:D:605:LYS:HD2	2:D:630:LEU:HD21	1.87	0.55
2:B:160:ASN:HB2	2:B:409:ASN:HD22	1.72	0.55
2:B:40:TYR:O	2:B:130:GLY:HA2	2.06	0.55
1:C:445:LEU:HD23	1:C:463:MET:SD	2.46	0.55
1:C:580:PHE:O	1:C:582:GLY:N	2.39	0.55
1:C:638:GLY:O	1:C:639:ILE:C	2.43	0.55
2:D:170:ILE:HD13	2:D:225:VAL:HG13	1.89	0.55
2:B:36:LEU:C	2:B:95:VAL:HG21	2.23	0.55
1:C:254:SER:HB3	1:C:296:ASN:OD1	2.07	0.55
2:D:205:VAL:HA	2:D:213:LEU:HD23	1.89	0.55
2:B:259:ALA:HB2	2:B:265:VAL:HG21	1.88	0.55
2:B:614:LYS:HG3	2:B:616:PRO:HD3	1.89	0.55
1:C:152:ALA:CB	1:C:208:LEU:HD13	2.37	0.55
1:C:465:LEU:O	1:C:469:LEU:HG	2.07	0.55
1:A:285:ASN:N	1:A:285:ASN:HD22	2.04	0.55
1:A:81:ILE:HG13	1:A:81:ILE:O	2.06	0.55
2:D:600:PHE:CE1	2:D:604:MET:HE1	2.42	0.55
2:B:357:ASP:O	2:B:360:LEU:HB2	2.07	0.54
2:D:29:SER:OG	2:D:263:ARG:NH2	2.39	0.54
2:D:583:LEU:CD1	2:D:588:ALA:HB2	2.37	0.54
2:D:521:LEU:HD23	2:D:607:GLN:OE1	2.07	0.54
2:D:94:LYS:HE2	2:D:351:GLU:CB	2.33	0.54
1:A:247:LEU:HB3	1:A:249:ILE:HD11	1.88	0.54
1:A:407:VAL:HG13	1:A:407:VAL:O	2.06	0.54
2:B:540:PHE:CZ	2:B:544:ILE:HD11	2.41	0.54
2:D:324:LEU:HD13	2:D:329:ARG:NH1	2.21	0.54
2:D:522:ARG:N	2:D:607:GLN:NE2	2.55	0.54
2:B:489:THR:HA	2:B:663:ARG:HH21	1.73	0.54
1:C:437:ASN:HB3	1:C:514:GLU:OE2	2.07	0.54
2:D:309:TYR:CZ	2:D:317:PRO:HG2	2.42	0.54
1:A:69:LEU:HD21	1:A:95:LEU:HB2	1.88	0.54
2:B:443:LEU:HD11	2:B:614:LYS:HZ1	1.72	0.54
1:C:247:LEU:HB3	1:C:249:ILE:HD11	1.88	0.54
1:C:180:VAL:O	1:C:180:VAL:HG12	2.08	0.54
1:C:516:LEU:HD21	1:C:537:LEU:HD23	1.89	0.54
2:B:151:VAL:HB	2:B:236:LEU:HD23	1.88	0.54
2:B:442:GLN:CB	2:B:617:LEU:HD11	2.38	0.54
1:A:180:VAL:O	1:A:180:VAL:HG12	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:368:LEU:HD12	1:A:369:GLY:N	2.22	0.54
1:A:81:ILE:CD1	1:A:260:PHE:HD1	2.21	0.54
1:C:265:ILE:HG21	1:C:305:THR:HG21	1.90	0.54
2:D:38:PHE:CE2	2:D:132:ILE:HG12	2.42	0.54
2:D:94:LYS:CE	2:D:353:VAL:CG2	2.83	0.54
1:A:551:ASN:O	1:A:554:GLU:N	2.39	0.54
2:D:540:PHE:CZ	2:D:544:ILE:HD11	2.43	0.54
2:B:314:TYR:CG	2:B:314:TYR:O	2.61	0.54
2:B:352:LYS:O	2:B:355:ASP:HB3	2.07	0.54
2:B:580:LEU:HD23	2:B:581:SER:N	2.24	0.54
2:D:613:TYR:CD2	2:D:613:TYR:N	2.75	0.54
2:D:293:TYR:CE1	2:D:294:LEU:O	2.61	0.53
1:A:487:TYR:CE1	1:A:492:LEU:CD1	2.91	0.53
1:A:638:GLY:O	1:A:639:ILE:C	2.45	0.53
1:A:90:SER:OG	1:A:91:GLY:N	2.40	0.53
2:B:25:ASP:O	2:B:257:ARG:NH2	2.41	0.53
2:B:461:PHE:CG	2:B:461:PHE:O	2.61	0.53
1:C:408:ARG:NH2	1:C:410:ASN:OD1	2.42	0.53
2:D:35:SER:OG	2:D:135:ASN:HA	2.08	0.53
2:D:34:ASN:OD1	2:D:135:ASN:ND2	2.41	0.53
2:D:213:LEU:O	2:D:213:LEU:HD12	2.08	0.53
2:D:259:ALA:HB2	2:D:265:VAL:HG21	1.90	0.53
2:B:608:PHE:CZ	2:B:629:ILE:HD13	2.43	0.53
1:C:622:MET:HG3	1:C:623:ASN:N	2.24	0.53
2:D:311:CYS:SG	1:C:293:GLU:OE1	2.67	0.53
1:A:276:THR:HB	1:A:279:GLU:HB2	1.89	0.53
1:C:247:LEU:HD22	1:C:249:ILE:HD11	1.91	0.53
1:C:604:GLN:OE1	1:C:604:GLN:N	2.41	0.53
1:A:339:LEU:O	1:A:342:ILE:HG13	2.08	0.53
2:B:525:LEU:HD11	2:B:529:LEU:HD11	1.91	0.53
2:B:566:LEU:HD23	2:B:566:LEU:O	2.09	0.53
1:C:187:ASN:HD21	1:C:190:LEU:HB2	1.74	0.53
1:C:307:VAL:HG23	1:C:307:VAL:O	2.08	0.53
1:C:400:LEU:HD21	1:C:425:GLN:HG2	1.90	0.53
1:C:632:PRO:O	1:C:636:ILE:HG23	2.09	0.53
2:D:34:ASN:OD1	2:D:135:ASN:OD1	2.27	0.53
2:D:602:GLY:O	2:D:606:ILE:HG12	2.07	0.53
1:A:392:GLN:HG2	1:A:393:ASN:N	2.24	0.53
1:A:464:MET:CE	1:A:639:ILE:HD13	2.39	0.53
1:A:464:MET:HG3	1:A:642:PHE:CE1	2.44	0.53
1:A:622:MET:O	1:A:623:ASN:C	2.46	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:73:SER:C	1:A:74:LEU:HD12	2.29	0.53
2:B:23:LEU:HD22	2:B:253:LYS:NZ	2.24	0.53
2:D:194:GLU:O	2:D:257:ARG:NH1	2.38	0.53
2:D:267:ILE:CG2	2:D:269:LEU:HD13	2.39	0.53
2:B:208:MET:O	2:B:209:TYR:CD1	2.62	0.53
2:D:566:LEU:HD23	2:D:566:LEU:O	2.09	0.53
1:A:155:ALA:O	1:A:361:SER:HB3	2.09	0.53
1:A:392:GLN:O	1:A:393:ASN:C	2.43	0.53
1:A:343:GLU:HA	1:A:346:LYS:HE2	1.91	0.53
2:B:135:ASN:OD1	2:B:136:GLY:N	2.39	0.52
1:C:285:ASN:ND2	1:C:285:ASN:N	2.57	0.52
2:D:522:ARG:HG2	2:D:527:PRO:HG2	1.90	0.52
1:A:400:LEU:HD21	1:A:425:GLN:HG2	1.91	0.52
1:A:644:ILE:HG12	1:C:619:ARG:CD	2.39	0.52
2:D:493:PHE:CE1	2:D:494:PHE:HD2	2.27	0.52
1:A:86:GLY:N	1:A:92:LYS:HD3	2.24	0.52
2:B:309:TYR:OH	2:B:317:PRO:CB	2.56	0.52
2:B:34:ASN:OD1	2:B:35:SER:N	2.43	0.52
1:C:622:MET:O	1:C:623:ASN:C	2.47	0.52
2:D:506:ALA:HA	2:D:509:ILE:HG22	1.91	0.52
2:D:530:LEU:HD23	2:D:606:ILE:HG23	1.91	0.52
2:B:445:PHE:HB2	2:B:608:PHE:CZ	2.44	0.52
1:C:392:GLN:HG2	1:C:393:ASN:N	2.23	0.52
2:B:480:TYR:CB	2:B:486:LEU:CD1	2.85	0.52
2:D:660:VAL:HG13	2:D:661:SER:N	2.24	0.52
2:B:174:ARG:HD3	2:B:229:TRP:CE3	2.45	0.52
1:C:85:LEU:CD2	1:C:302:MET:CG	2.88	0.52
2:D:343:GLN:O	2:D:346:ALA:N	2.43	0.52
2:D:530:LEU:CD2	2:D:606:ILE:HD12	2.39	0.52
1:A:557:ILE:HB	1:A:558:PRO:CD	2.37	0.52
2:B:600:PHE:CZ	2:B:604:MET:CE	2.92	0.52
1:C:232:VAL:HG21	1:C:256:LEU:HD22	1.92	0.52
1:A:175:LEU:O	1:A:200:ARG:HD3	2.08	0.52
1:A:292:PRO:O	1:A:295:SER:OG	2.15	0.52
1:C:144:VAL:CG2	1:C:193:ILE:HD11	2.40	0.52
1:C:379:LEU:HD11	1:C:389:ARG:HH11	1.72	0.52
1:C:430:THR:O	1:C:510:HIS:CA	2.57	0.52
2:D:312:PRO:O	1:C:296:ASN:N	2.41	0.52
1:A:247:LEU:HD22	1:A:249:ILE:HD11	1.91	0.52
1:A:401:LEU:HD13	1:A:490:LEU:HD12	1.92	0.52
1:A:430:THR:O	1:A:510:HIS:CA	2.55	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:134:ILE:HD12	2:B:134:ILE:O	2.10	0.52
2:B:304:PHE:CB	2:B:309:TYR:CE1	2.92	0.52
2:B:36:LEU:N	2:B:95:VAL:CG2	2.66	0.52
2:B:403:ILE:O	2:B:407:ILE:HB	2.10	0.52
1:C:562:ILE:O	1:C:563:SER:C	2.49	0.52
2:D:309:TYR:OH	2:D:317:PRO:CG	2.53	0.52
2:D:414:LEU:C	2:D:418:LEU:HD12	2.28	0.52
2:D:445:PHE:CE1	2:D:629:ILE:HD11	2.44	0.52
1:C:472:LEU:HB2	1:C:473:PRO:CD	2.40	0.51
2:D:109:CYS:HB2	2:D:288:SER:O	2.10	0.51
1:A:36:HIS:O	1:A:77:GLU:CA	2.46	0.51
2:B:350:LEU:O	2:B:350:LEU:HD12	2.09	0.51
2:B:480:TYR:HB3	2:B:486:LEU:HD12	1.87	0.51
1:C:212:LYS:HD2	1:C:356:PHE:HD2	1.74	0.51
1:C:291:CYS:O	1:C:291:CYS:SG	2.68	0.51
1:C:339:LEU:O	1:C:342:ILE:HG13	2.11	0.51
1:C:530:VAL:O	1:C:533:VAL:HG12	2.10	0.51
2:D:238:GLU:OE2	2:D:270:HIS:N	2.42	0.51
2:D:454:MET:CE	2:D:458:LEU:HD12	2.40	0.51
1:A:127:ASP:O	1:A:357:LYS:HB3	2.11	0.51
1:A:516:LEU:HD21	1:A:537:LEU:HD23	1.91	0.51
2:B:552:LEU:HD12	2:B:552:LEU:C	2.30	0.51
2:B:580:LEU:HD23	2:B:581:SER:HA	1.92	0.51
2:B:583:LEU:HD13	2:B:587:PRO:HB2	1.91	0.51
1:C:551:ASN:O	1:C:554:GLU:N	2.38	0.51
2:D:299:HIS:CE1	2:D:354:ARG:CD	2.93	0.51
2:D:489:THR:O	2:D:493:PHE:CE2	2.64	0.51
2:D:319:ASP:OD1	2:D:319:ASP:C	2.48	0.51
1:A:363:GLY:O	1:A:367:LYS:N	2.43	0.51
2:B:444:SER:O	2:B:445:PHE:C	2.46	0.51
2:B:660:VAL:HG13	2:B:661:SER:N	2.25	0.51
1:C:313:GLU:HA	1:C:316:ILE:HD12	1.92	0.51
2:D:353:VAL:HG12	2:D:354:ARG:N	2.25	0.51
2:D:492:TYR:C	2:D:494:PHE:N	2.64	0.51
2:D:522:ARG:NE	2:D:612:THR:HG21	2.25	0.51
2:D:600:PHE:CZ	2:D:604:MET:CE	2.94	0.51
1:A:472:LEU:HB2	1:A:473:PRO:CD	2.41	0.51
2:B:609:SER:OG	2:B:610:ARG:N	2.42	0.51
2:B:618:GLY:N	2:B:621:THR:OG1	2.44	0.51
2:D:438:HIS:NE2	2:D:520:ASN:HB2	2.26	0.51
2:D:583:LEU:HD11	2:D:588:ALA:HB2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:475:ARG:O	2:D:476:ALA:C	2.49	0.51
2:D:490:GLY:N	2:D:491:PRO:CD	2.74	0.51
2:B:443:LEU:HD12	2:B:443:LEU:C	2.32	0.51
2:B:561:PHE:CD2	2:B:562:PHE:N	2.78	0.51
2:D:452:LEU:HD11	2:D:521:LEU:HD21	1.93	0.51
2:D:552:LEU:HD22	2:D:553:LEU:CD1	2.33	0.51
2:B:506:ALA:HA	2:B:509:ILE:HG22	1.93	0.51
2:B:584:TRP:CB	2:B:586:VAL:HG22	2.41	0.51
1:C:187:ASN:OD1	1:C:190:LEU:HG	2.11	0.51
2:B:205:VAL:CG2	2:B:206:GLY:N	2.74	0.51
2:B:555:THR:O	2:B:558:MET:N	2.44	0.51
1:A:188:TYR:CG	1:A:195:THR:HG23	2.45	0.50
1:A:35:PRO:CD	1:A:352:PRO:HG3	2.41	0.50
1:A:437:ASN:HB3	1:A:514:GLU:OE2	2.10	0.50
2:B:598:TRP:NE1	2:B:646:ILE:HG21	2.25	0.50
1:C:412:LEU:HD12	1:C:413:LYS:N	2.26	0.50
1:A:411:VAL:CG2	1:A:413:LYS:HB3	2.41	0.50
2:B:200:CYS:HG	2:B:217:GLU:CD	2.14	0.50
1:C:435:MET:CG	1:C:436:LEU:N	2.72	0.50
2:D:319:ASP:OD1	2:D:320:PHE:N	2.44	0.50
1:A:435:MET:CG	1:A:436:LEU:N	2.74	0.50
1:A:530:VAL:O	1:A:533:VAL:HG12	2.11	0.50
1:A:570:TYR:CD2	1:A:626:ILE:HG21	2.47	0.50
1:C:254:SER:HA	1:C:296:ASN:ND2	2.27	0.50
1:C:626:ILE:O	1:C:629:SER:HB2	2.11	0.50
2:D:114:LEU:O	2:D:117:VAL:HG22	2.12	0.50
2:D:200:CYS:HG	2:D:217:GLU:CD	2.15	0.50
1:A:387:ILE:O	1:A:391:LEU:HB2	2.11	0.50
2:B:614:LYS:HG3	2:B:615:MET:N	2.26	0.50
2:D:555:THR:O	2:D:558:MET:N	2.44	0.50
1:A:180:VAL:HG21	1:A:197:GLU:OE1	2.11	0.50
2:B:95:VAL:HA	2:B:99:GLN:OE1	2.11	0.50
2:D:598:TRP:NE1	2:D:646:ILE:HG21	2.26	0.50
2:D:159:PRO:HA	2:D:206:GLY:HA2	1.92	0.50
1:A:643:LYS:O	1:A:646:ASP:OD1	2.29	0.50
1:A:92:LYS:HG3	1:A:93:THR:H	1.75	0.50
2:B:551:ALA:HA	2:B:667:GLN:HE22	1.77	0.50
1:A:265:ILE:HG21	1:A:305:THR:HG21	1.93	0.50
2:B:227:LEU:HD21	2:B:258:LEU:HD21	1.92	0.50
1:A:626:ILE:O	1:A:629:SER:HB3	2.11	0.49
2:B:304:PHE:HB2	2:B:309:TYR:CE1	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:96:LEU:HD22	1:C:248:THR:HG23	1.94	0.49
1:C:252:PRO:HA	1:C:298:PHE:HE2	1.77	0.49
1:C:276:THR:HB	1:C:279:GLU:HB2	1.94	0.49
2:D:608:PHE:CZ	2:D:629:ILE:HD13	2.47	0.49
1:A:144:VAL:HG11	1:A:177:LEU:HD13	1.94	0.49
1:A:385:ALA:O	1:A:388:THR:OG1	2.28	0.49
1:A:426:PHE:CE1	1:A:482:PHE:HZ	2.30	0.49
1:A:103:LEU:CD2	1:A:650:SER:OG	2.59	0.49
2:B:587:PRO:C	2:B:590:ILE:HG22	2.32	0.49
2:D:277:PHE:HA	2:D:280:PHE:CE2	2.47	0.49
2:D:403:ILE:O	2:D:407:ILE:HB	2.12	0.49
2:D:522:ARG:H	2:D:607:GLN:HE21	1.60	0.49
2:D:525:LEU:HG	2:D:526:GLN:N	2.27	0.49
2:D:586:VAL:HB	2:D:587:PRO:HD3	1.94	0.49
2:D:478:LEU:HD22	2:D:668:LYS:HG2	1.94	0.49
1:A:550:ARG:HH22	2:B:441:ILE:HD12	1.76	0.49
1:C:301:TYR:O	1:C:305:THR:HG23	2.12	0.49
1:C:622:MET:O	1:C:625:LEU:HB3	2.12	0.49
2:D:561:PHE:CD2	2:D:562:PHE:N	2.80	0.49
2:B:38:PHE:CE2	2:B:132:ILE:HG12	2.47	0.49
2:B:454:MET:CE	2:B:458:LEU:HD12	2.42	0.49
1:C:435:MET:HG2	1:C:436:LEU:N	2.27	0.49
1:A:81:ILE:CG1	1:A:261:ASP:OD1	2.58	0.49
2:B:640:LEU:HD12	2:B:640:LEU:H	1.78	0.49
2:B:37:TYR:HD2	2:B:133:TRP:HB2	1.78	0.49
2:B:459:ILE:N	2:B:460:PRO:HD2	2.28	0.49
1:C:68:ILE:O	1:C:269:GLY:HA3	2.13	0.49
2:D:275:ASP:HB3	2:D:276:ILE:HD12	1.94	0.49
2:D:633:MET:O	2:D:634:GLU:CB	2.60	0.49
2:D:95:VAL:HG12	2:D:264:LEU:HD11	1.94	0.49
2:B:104:ILE:CD1	2:B:272:PRO:CG	2.89	0.49
2:B:452:LEU:HD11	2:B:521:LEU:HD21	1.94	0.49
2:B:626:GLY:O	2:B:629:ILE:HG22	2.12	0.49
1:C:412:LEU:HD12	1:C:412:LEU:C	2.33	0.49
2:D:104:ILE:HD13	2:D:314:TYR:CE1	2.48	0.49
2:D:614:LYS:HG3	2:D:615:MET:N	2.27	0.49
2:B:37:TYR:CD2	2:B:133:TRP:HB2	2.48	0.49
2:B:587:PRO:O	2:B:590:ILE:N	2.46	0.49
2:B:573:ALA:HB1	2:B:591:SER:HA	1.95	0.49
1:C:120:LEU:HD11	1:C:125:PHE:CD1	2.48	0.49
2:D:174:ARG:HD3	2:D:229:TRP:CE3	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:144:VAL:HG12	1:A:148:LEU:HD12	1.95	0.48
1:A:180:VAL:HG11	1:A:193:ILE:HD12	1.94	0.48
2:B:430:THR:O	2:B:431:ILE:C	2.52	0.48
2:D:197:LEU:HD11	2:D:220:ARG:HB3	1.95	0.48
2:D:392:MET:HB3	2:D:393:PRO:CD	2.43	0.48
2:D:551:ALA:HA	2:D:667:GLN:OE1	2.13	0.48
1:A:144:VAL:HG11	1:A:177:LEU:CD1	2.43	0.48
1:A:225:CYS:CB	1:A:253:ARG:HH22	2.25	0.48
1:A:552:ILE:HG23	1:A:553:GLN:N	2.28	0.48
1:A:583:LEU:N	1:A:583:LEU:HD12	2.28	0.48
1:A:464:MET:CE	1:A:639:ILE:N	2.76	0.48
2:B:586:VAL:HG23	2:B:587:PRO:CD	2.40	0.48
2:D:299:HIS:CE1	2:D:354:ARG:NE	2.81	0.48
1:A:165:GLN:O	1:A:168:VAL:HB	2.13	0.48
1:A:236:VAL:O	1:A:239:ALA:HB3	2.13	0.48
1:A:96:LEU:HD22	1:A:248:THR:HG23	1.94	0.48
1:A:476:VAL:HA	1:A:507:LEU:HD13	1.96	0.48
1:A:622:MET:O	1:A:625:LEU:HB3	2.12	0.48
2:D:95:VAL:CG1	2:D:264:LEU:HD11	2.44	0.48
1:A:461:TRP:CD1	1:A:462:GLN:N	2.82	0.48
2:B:493:PHE:HE1	2:B:658:TYR:HB3	1.78	0.48
1:C:386:VAL:O	1:C:387:ILE:C	2.51	0.48
2:B:447:ASP:O	2:B:450:ALA:HB3	2.14	0.48
2:D:445:PHE:CD2	2:D:616:PRO:HB3	2.48	0.48
1:A:404:VAL:C	1:A:405:LEU:HG	2.34	0.48
1:A:562:ILE:O	1:A:563:SER:C	2.51	0.48
1:A:81:ILE:HD12	1:A:260:PHE:HD1	1.79	0.48
2:B:492:TYR:O	2:B:495:ALA:N	2.47	0.48
2:B:443:LEU:HD11	2:B:614:LYS:HZ3	1.79	0.48
2:D:455:ILE:HD12	2:D:515:THR:HG21	1.95	0.48
1:A:560:LYS:O	1:A:563:SER:OG	2.26	0.48
2:B:584:TRP:HB2	2:B:587:PRO:HD3	1.94	0.48
1:C:615:GLY:O	1:C:619:ARG:CG	2.61	0.48
2:D:174:ARG:NE	2:D:229:TRP:CZ3	2.82	0.48
2:D:415:PRO:O	2:D:419:ILE:HG12	2.13	0.48
2:D:459:ILE:N	2:D:460:PRO:HD2	2.29	0.48
1:A:476:VAL:HG23	1:A:507:LEU:HD22	1.95	0.48
1:C:144:VAL:HG12	1:C:148:LEU:HD12	1.94	0.48
2:D:522:ARG:HG3	2:D:523:PRO:HD2	1.96	0.48
1:A:177:LEU:HD23	1:A:200:ARG:HG2	1.94	0.48
2:B:657:LEU:HA	2:B:660:VAL:HG12	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:410:ASN:O	1:C:586:THR:N	2.47	0.48
1:C:416:ILE:HD11	1:C:599:MET:HG2	1.95	0.48
1:A:412:LEU:HD12	1:A:415:ALA:HB3	1.96	0.47
2:D:26:ARG:C	2:D:27:LEU:HD12	2.35	0.47
1:A:422:LEU:HD21	1:A:490:LEU:HD23	1.96	0.47
1:C:419:ARG:HH12	1:C:583:LEU:HD21	1.79	0.47
1:C:476:VAL:HG23	1:C:507:LEU:HD22	1.95	0.47
2:D:333:GLU:O	2:D:336:LEU:HB2	2.14	0.47
1:A:38:LEU:HD23	1:A:244:ILE:HG21	1.97	0.47
2:B:360:LEU:HA	2:B:363:ALA:HB3	1.97	0.47
1:C:252:PRO:HA	1:C:298:PHE:CE2	2.49	0.47
1:C:408:ARG:CZ	1:C:410:ASN:OD1	2.62	0.47
2:D:566:LEU:O	2:D:569:SER:OG	2.32	0.47
1:A:368:LEU:C	1:A:368:LEU:HD12	2.34	0.47
1:A:552:ILE:HG23	1:A:553:GLN:H	1.79	0.47
2:B:30:SER:HB3	2:B:261:GLY:HA3	1.96	0.47
2:B:272:PRO:O	2:B:273:ARG:CG	2.57	0.47
1:C:85:LEU:CG	1:C:302:MET:SD	3.02	0.47
1:C:533:VAL:HG13	1:C:534:VAL:N	2.30	0.47
2:B:571:TYR:CE1	2:B:577:MET:HE1	2.50	0.47
1:C:201:VAL:O	1:C:204:ALA:HB3	2.15	0.47
1:C:426:PHE:CE1	1:C:482:PHE:HZ	2.32	0.47
1:C:493:HIS:CD2	1:C:498:ARG:HG3	2.49	0.47
1:C:518:LEU:O	1:C:519:VAL:C	2.53	0.47
2:D:447:ASP:O	2:D:450:ALA:HB3	2.14	0.47
2:D:640:LEU:HD12	2:D:640:LEU:H	1.79	0.47
1:A:620:PHE:O	1:A:621:THR:C	2.53	0.47
1:C:360:ASP:OD2	1:C:360:ASP:N	2.48	0.47
1:C:570:TYR:CE1	1:C:626:ILE:HD13	2.50	0.47
2:D:657:LEU:HA	2:D:660:VAL:HG12	1.95	0.47
1:A:237:GLU:O	1:A:240:ARG:HB3	2.15	0.47
1:A:350:THR:O	1:A:353:MET:HB2	2.14	0.47
1:A:356:PHE:O	1:A:357:LYS:HB2	2.14	0.47
1:A:464:MET:HE1	1:A:639:ILE:HD13	1.96	0.47
2:B:580:LEU:O	2:B:581:SER:C	2.53	0.47
2:B:174:ARG:NE	2:B:229:TRP:CZ3	2.83	0.47
2:B:423:GLU:OE1	2:B:462:ASN:OD1	2.33	0.47
2:B:455:ILE:HD12	2:B:515:THR:HG21	1.96	0.47
2:B:598:TRP:CE3	2:B:598:TRP:HA	2.49	0.47
1:A:404:VAL:O	1:A:405:LEU:HG	2.14	0.47
2:B:355:ASP:O	2:B:358:ASP:HB3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:85:LEU:CD2	1:C:302:MET:SD	3.02	0.47
2:D:293:TYR:HD2	2:D:300:MET:CE	2.26	0.47
2:D:492:TYR:O	2:D:493:PHE:C	2.52	0.47
1:A:435:MET:HG2	1:A:436:LEU:N	2.29	0.47
2:B:304:PHE:HB3	2:B:309:TYR:CE1	2.49	0.47
1:C:476:VAL:HA	1:C:507:LEU:HD13	1.96	0.47
2:D:43:GLN:CD	2:D:126:LYS:O	2.54	0.47
1:A:392:GLN:O	1:A:395:ILE:N	2.48	0.47
2:B:468:ILE:CD1	2:B:550:ALA:HB2	2.45	0.47
2:B:571:TYR:CE1	2:B:577:MET:CE	2.98	0.47
1:C:165:GLN:O	1:C:168:VAL:HB	2.14	0.47
1:C:237:GLU:O	1:C:240:ARG:HB3	2.14	0.47
1:C:312:LYS:O	1:C:315:GLU:HG2	2.15	0.47
2:D:396:VAL:CG1	2:D:397:GLN:N	2.78	0.47
2:D:627:ASP:OD1	2:D:627:ASP:O	2.33	0.47
1:A:109:PHE:CG	1:A:109:PHE:O	2.67	0.46
1:A:404:VAL:HG12	2:B:578:ILE:HD11	1.97	0.46
2:B:415:PRO:O	2:B:419:ILE:HG12	2.15	0.46
2:B:528:PHE:C	2:B:528:PHE:CD1	2.89	0.46
1:A:401:LEU:HD13	1:A:490:LEU:HD11	1.98	0.46
2:B:233:ILE:HG23	2:B:264:LEU:HD23	1.97	0.46
2:B:475:ARG:O	2:B:476:ALA:C	2.52	0.46
2:B:555:THR:O	2:B:556:PHE:C	2.54	0.46
1:C:236:VAL:O	1:C:239:ALA:HB3	2.13	0.46
2:B:472:TYR:OH	2:B:555:THR:N	2.49	0.46
1:C:38:LEU:HD23	1:C:244:ILE:HG21	1.97	0.46
1:C:69:LEU:HD21	1:C:95:LEU:CB	2.44	0.46
2:D:313:ARG:HG3	2:D:315:SER:H	1.80	0.46
1:A:644:ILE:HG12	1:C:619:ARG:HD3	1.97	0.46
1:A:648:LEU:HD23	1:A:648:LEU:C	2.35	0.46
2:D:344:SER:O	2:D:347:ALA:HB3	2.16	0.46
2:D:528:PHE:C	2:D:528:PHE:CD1	2.88	0.46
1:A:87:SER:O	1:A:90:SER:N	2.48	0.46
2:B:489:THR:N	2:B:491:PRO:HG3	2.30	0.46
1:C:296:ASN:HD22	1:C:296:ASN:C	2.18	0.46
1:C:552:ILE:HG23	1:C:553:GLN:N	2.31	0.46
2:D:233:ILE:HG23	2:D:264:LEU:HD23	1.98	0.46
2:D:402:LEU:O	2:D:406:GLN:HB3	2.16	0.46
1:A:285:ASN:ND2	1:A:290:PRO:HA	2.30	0.46
1:C:296:ASN:ND2	1:C:296:ASN:O	2.49	0.46
1:C:571:CYS:HA	1:C:627:LEU:HD22	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:521:LEU:HB3	2:D:607:GLN:NE2	2.29	0.46
1:A:539:ILE:CG1	1:A:540:ALA:N	2.75	0.46
2:D:414:LEU:HG	2:D:418:LEU:CD1	2.42	0.46
1:C:85:LEU:HG	1:C:302:MET:SD	2.56	0.46
2:D:273:ARG:HA	2:D:313:ARG:NH1	2.30	0.46
2:D:319:ASP:O	2:D:322:VAL:HG12	2.16	0.46
2:D:335:GLU:OE1	2:D:338:THR:OG1	2.33	0.46
2:D:459:ILE:HD11	2:D:507:TYR:CE1	2.51	0.46
2:D:555:THR:O	2:D:556:PHE:C	2.53	0.46
1:A:376:THR:HG23	1:A:470:HIS:HB2	1.97	0.46
2:B:93:PHE:CE1	2:B:284:LEU:HD22	2.51	0.46
1:C:356:PHE:O	1:C:357:LYS:HB2	2.16	0.46
1:C:92:LYS:HG3	1:C:93:THR:H	1.80	0.46
2:D:293:TYR:CD1	2:D:343:GLN:NE2	2.84	0.46
2:D:472:TYR:OH	2:D:555:THR:N	2.48	0.46
1:A:564:TYR:OH	1:C:648:LEU:HD11	2.16	0.46
1:A:81:ILE:CD1	1:A:260:PHE:CD1	2.99	0.46
2:B:609:SER:O	2:B:612:THR:HB	2.16	0.46
1:C:95:LEU:HD12	1:C:95:LEU:C	2.36	0.46
1:A:573:GLU:HG2	1:A:613:CYS:CB	2.46	0.45
2:B:501:LEU:HB3	2:B:502:PRO:HD3	1.98	0.45
1:C:358:THR:HG23	1:C:360:ASP:OD2	2.16	0.45
1:C:492:LEU:O	1:C:493:HIS:C	2.54	0.45
2:D:586:VAL:HB	2:D:587:PRO:CD	2.46	0.45
2:D:628:LYS:O	2:D:632:VAL:HG23	2.17	0.45
2:B:292:ILE:HG22	2:B:304:PHE:CZ	2.50	0.45
2:B:574:GLY:HA2	2:B:597:ARG:HB2	1.99	0.45
2:B:627:ASP:O	2:B:627:ASP:OD1	2.34	0.45
1:C:583:LEU:HD23	1:C:585:PHE:CE1	2.44	0.45
1:C:96:LEU:HD11	1:C:215:LEU:HB3	1.98	0.45
2:D:585:THR:HA	2:D:588:ALA:HB3	1.98	0.45
1:A:350:THR:OG1	1:A:351:LEU:N	2.48	0.45
2:B:134:ILE:HG12	2:B:143:LEU:CD2	2.46	0.45
2:B:459:ILE:CD1	2:B:511:TYR:CE1	2.99	0.45
1:C:387:ILE:O	1:C:391:LEU:HB2	2.16	0.45
1:C:411:VAL:CG1	1:C:413:LYS:HG2	2.47	0.45
2:D:34:ASN:HD22	2:D:232:GLY:HA3	1.80	0.45
2:D:459:ILE:HD13	2:D:511:TYR:CD2	2.51	0.45
2:D:574:GLY:HA2	2:D:597:ARG:HB2	1.99	0.45
1:A:115:VAL:O	1:A:115:VAL:HG13	2.16	0.45
1:A:96:LEU:HD11	1:A:215:LEU:HB3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:510:HIS:CD2	1:A:510:HIS:O	2.69	0.45
1:A:559:PHE:O	1:A:560:LYS:C	2.54	0.45
1:A:571:CYS:HA	1:A:627:LEU:HD22	1.98	0.45
2:B:492:TYR:HA	2:B:495:ALA:HB3	1.99	0.45
1:C:371:LEU:O	1:C:375:VAL:HG23	2.16	0.45
1:A:523:ILE:HD11	1:A:641:VAL:HG21	1.97	0.45
2:D:28:PHE:HD1	2:D:194:GLU:HA	1.81	0.45
2:D:598:TRP:HA	2:D:598:TRP:CE3	2.49	0.45
2:B:634:GLU:HG2	2:B:635:LEU:HD12	1.99	0.45
1:C:637:LEU:HD12	1:C:640:VAL:HG13	1.99	0.45
1:C:523:ILE:HD11	1:C:641:VAL:HG21	1.97	0.45
1:C:99:MET:O	1:C:125:PHE:CD1	2.70	0.45
1:A:225:CYS:CB	1:A:253:ARG:NH2	2.80	0.45
1:A:637:LEU:HD12	1:A:640:VAL:HG13	1.99	0.45
2:D:249:HIS:CE1	2:D:279:LEU:HD11	2.51	0.45
2:D:313:ARG:HE	2:D:315:SER:CB	2.29	0.45
2:D:468:ILE:CD1	2:D:550:ALA:HB2	2.46	0.45
1:A:285:ASN:ND2	1:A:285:ASN:N	2.64	0.45
2:B:459:ILE:HD12	2:B:539:VAL:CG2	2.46	0.45
2:B:580:LEU:HD23	2:B:581:SER:CA	2.47	0.45
2:B:625:SER:OG	2:B:626:GLY:N	2.50	0.45
1:A:293:GLU:HG2	2:B:311:CYS:O	2.17	0.45
1:A:371:LEU:O	1:A:375:VAL:HG23	2.17	0.45
1:A:619:ARG:HG2	1:A:622:MET:HE2	1.99	0.45
2:B:402:LEU:HD23	2:B:402:LEU:HA	1.78	0.45
2:B:584:TRP:C	2:B:587:PRO:HD2	2.37	0.45
2:B:584:TRP:CE3	2:B:586:VAL:HG22	2.52	0.45
2:D:312:PRO:HB3	1:C:254:SER:HB2	1.98	0.45
1:C:474:PHE:O	1:C:477:VAL:HG12	2.17	0.45
1:C:495:GLU:OE2	1:C:496:VAL:HG22	2.16	0.45
1:A:353:MET:O	1:A:353:MET:HG3	2.17	0.45
2:B:134:ILE:HG12	2:B:143:LEU:HD21	1.98	0.45
2:B:206:GLY:O	2:B:210:VAL:HG22	2.16	0.45
2:B:659:TYR:OH	2:B:663:ARG:NE	2.50	0.45
1:C:412:LEU:HD13	1:C:599:MET:HB2	1.98	0.45
1:C:559:PHE:O	1:C:560:LYS:C	2.56	0.45
2:D:117:VAL:HG12	2:D:122:GLY:HA2	1.98	0.45
2:D:430:THR:O	2:D:431:ILE:C	2.56	0.45
2:D:631:SER:HA	2:D:636:ASP:OD2	2.17	0.45
1:A:464:MET:CE	1:A:638:GLY:HA3	2.48	0.44
1:C:363:GLY:O	1:C:367:LYS:HB2	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:620:PHE:O	1:C:621:THR:C	2.55	0.44
2:D:28:PHE:CE1	2:D:193:ALA:O	2.70	0.44
1:A:571:CYS:O	1:A:574:ILE:HB	2.17	0.44
2:B:35:SER:OG	2:B:97:SER:N	2.51	0.44
1:C:127:ASP:O	1:C:357:LYS:HB3	2.18	0.44
2:D:321:TYR:CE1	2:D:339:ARG:HD3	2.37	0.44
2:D:501:LEU:HB3	2:D:502:PRO:HD3	1.99	0.44
2:D:605:LYS:HD2	2:D:630:LEU:CD2	2.47	0.44
1:A:81:ILE:HG13	1:A:261:ASP:HB2	1.98	0.44
1:A:533:VAL:HG13	1:A:534:VAL:N	2.32	0.44
2:B:566:LEU:O	2:B:569:SER:OG	2.35	0.44
1:C:179:HIS:NE2	1:C:197:GLU:OE1	2.45	0.44
1:C:539:ILE:O	1:C:540:ALA:C	2.56	0.44
2:D:249:HIS:HB2	2:D:275:ASP:OD2	2.17	0.44
2:D:309:TYR:CZ	2:D:317:PRO:CG	3.01	0.44
2:D:433:PHE:O	2:D:436:PHE:HB2	2.17	0.44
1:A:546:SER:HB2	1:A:548:PHE:CE2	2.53	0.44
2:B:522:ARG:CD	2:B:523:PRO:HD2	2.46	0.44
1:C:291:CYS:SG	1:C:297:PRO:HB3	2.57	0.44
1:C:383:LYS:O	1:C:384:LEU:C	2.56	0.44
2:D:208:MET:C	2:D:209:TYR:CD2	2.91	0.44
2:B:200:CYS:SG	2:B:217:GLU:CD	2.96	0.44
1:C:370:VAL:HG13	1:C:371:LEU:N	2.32	0.44
1:C:375:VAL:HG13	1:C:445:LEU:HD21	1.99	0.44
1:A:346:LYS:HG3	1:A:347:HIS:N	2.31	0.44
1:A:474:PHE:O	1:A:477:VAL:HG12	2.18	0.44
2:B:487:TYR:HB2	2:B:491:PRO:HB3	2.00	0.44
1:A:467:TYR:HD1	1:A:470:HIS:HE2	1.65	0.44
2:B:276:ILE:H	2:B:276:ILE:HD12	1.82	0.44
2:D:246:PHE:CD1	1:C:308:ASP:HB3	2.52	0.44
2:D:493:PHE:O	2:D:497:ILE:HD12	2.17	0.44
2:D:626:GLY:O	2:D:629:ILE:HG22	2.16	0.44
1:A:201:VAL:O	1:A:204:ALA:HB3	2.18	0.44
1:A:370:VAL:HG13	1:A:371:LEU:N	2.33	0.44
1:A:518:LEU:O	1:A:519:VAL:C	2.52	0.44
2:B:483:GLU:O	2:B:484:ASP:CB	2.66	0.44
2:B:424:ALA:HB1	2:B:511:TYR:HB2	2.00	0.44
1:C:411:VAL:HG12	1:C:413:LYS:HG2	1.98	0.44
2:D:313:ARG:HG3	2:D:315:SER:HB3	2.00	0.44
2:D:414:LEU:N	2:D:415:PRO:CD	2.80	0.44
2:D:590:ILE:HG23	2:D:591:SER:N	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:602:GLY:HA2	2:D:643:ILE:HD13	2.00	0.44
1:A:117:GLY:O	1:A:118:ARG:HB2	2.18	0.44
1:A:235:LEU:CD1	1:A:247:LEU:HD21	2.46	0.44
1:C:552:ILE:HG23	1:C:553:GLN:H	1.82	0.44
2:D:313:ARG:HD3	1:C:296:ASN:HB2	2.00	0.44
1:A:145:ARG:HG3	1:A:172:MET:HE2	2.00	0.43
1:A:467:TYR:CD2	1:A:518:LEU:HD13	2.53	0.43
1:A:616:ALA:O	1:A:617:THR:C	2.56	0.43
2:B:315:SER:O	2:B:318:ALA:HB3	2.18	0.43
2:B:35:SER:O	2:B:135:ASN:HA	2.18	0.43
1:C:93:THR:O	1:C:97:ASP:OD2	2.36	0.43
2:D:343:GLN:O	2:D:347:ALA:N	2.40	0.43
2:D:299:HIS:CE1	2:D:354:ARG:HD2	2.53	0.43
1:A:127:ASP:O	1:A:357:LYS:CB	2.66	0.43
1:A:410:ASN:O	1:A:586:THR:HB	2.19	0.43
2:B:530:LEU:HG	2:B:644:TYR:OH	2.17	0.43
1:C:296:ASN:O	1:C:297:PRO:C	2.57	0.43
2:D:313:ARG:CZ	1:C:296:ASN:OD1	2.66	0.43
2:D:254:THR:HA	2:D:257:ARG:HD3	2.00	0.43
1:A:426:PHE:CE1	1:A:482:PHE:CZ	3.06	0.43
1:A:550:ARG:O	1:A:551:ASN:C	2.56	0.43
2:B:420:HIS:CD2	2:B:466:ASP:OD2	2.71	0.43
2:B:586:VAL:CG2	2:B:587:PRO:HD3	2.45	0.43
1:C:235:LEU:CD1	1:C:247:LEU:HD21	2.46	0.43
1:C:302:MET:HA	1:C:305:THR:OG1	2.18	0.43
1:C:510:HIS:O	1:C:510:HIS:CD2	2.71	0.43
2:D:210:VAL:HG23	2:D:211:ARG:O	2.18	0.43
2:D:592:LYS:O	2:D:598:TRP:NE1	2.48	0.43
1:A:238:LEU:HB3	1:A:243:ARG:HD2	2.00	0.43
1:A:291:CYS:HB3	1:A:300:PHE:CD1	2.53	0.43
1:A:392:GLN:O	1:A:395:ILE:HB	2.18	0.43
2:B:104:ILE:HG23	2:B:285:LEU:HD12	2.01	0.43
2:D:316:ASN:CB	2:D:317:PRO:HD3	2.48	0.43
1:A:232:VAL:O	1:A:233:VAL:C	2.54	0.43
1:A:544:VAL:HG12	2:B:434:LEU:HD11	2.00	0.43
2:B:493:PHE:CE1	2:B:659:TYR:HB2	2.54	0.43
1:C:449:SER:OG	1:C:463:MET:HG2	2.19	0.43
2:D:294:LEU:HD23	2:D:352:LYS:O	2.17	0.43
2:D:299:HIS:NE2	2:D:354:ARG:NE	2.66	0.43
2:D:464:ILE:HD11	2:D:542:CYS:SG	2.59	0.43
1:A:210:ASP:N	1:A:211:PRO:CD	2.81	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:578:ASN:OD1	1:A:578:ASN:C	2.57	0.43
2:B:443:LEU:HD13	2:B:448:THR:CB	2.37	0.43
1:C:329:TYR:CG	1:C:335:CYS:SG	3.12	0.43
2:D:233:ILE:HG22	2:D:234:LEU:N	2.32	0.43
2:D:498:LEU:N	2:D:498:LEU:HD12	2.34	0.43
2:D:662:LEU:O	2:D:663:ARG:HB3	2.18	0.43
1:A:154:LEU:HD21	1:A:457:LEU:O	2.19	0.43
1:A:472:LEU:CB	1:A:473:PRO:CD	2.97	0.43
1:A:580:PHE:O	1:A:581:TYR:C	2.56	0.43
2:B:96:ARG:H	2:B:99:GLN:CD	2.20	0.43
2:D:256:SER:O	2:D:259:ALA:HB3	2.19	0.43
2:D:94:LYS:HB2	2:D:351:GLU:O	2.18	0.43
2:B:309:TYR:CE1	2:B:317:PRO:HG3	2.54	0.43
1:C:188:TYR:CD2	1:C:195:THR:CB	3.01	0.43
1:C:412:LEU:HA	1:C:415:ALA:HB3	1.99	0.43
2:D:230:ASN:HB2	2:D:263:ARG:HH22	1.84	0.43
2:D:483:GLU:O	2:D:484:ASP:CB	2.66	0.43
2:B:414:LEU:N	2:B:415:PRO:CD	2.82	0.43
2:B:483:GLU:OE1	2:B:483:GLU:HA	2.17	0.43
1:C:154:LEU:HD21	1:C:457:LEU:O	2.18	0.43
1:C:232:VAL:O	1:C:233:VAL:C	2.56	0.43
1:C:474:PHE:O	1:C:477:VAL:CG1	2.66	0.43
2:D:28:PHE:CD1	2:D:28:PHE:N	2.86	0.43
2:D:625:SER:OG	2:D:626:GLY:N	2.52	0.43
1:A:81:ILE:HD12	1:A:260:PHE:CD1	2.54	0.43
1:A:449:SER:OG	1:A:463:MET:HG2	2.19	0.43
1:A:648:LEU:HG	1:C:553:GLN:HE22	1.83	0.43
2:B:170:ILE:HG23	2:B:228:LEU:CD1	2.49	0.43
2:B:32:SER:OG	2:B:33:ASP:HB2	2.19	0.43
2:B:433:PHE:O	2:B:436:PHE:HB2	2.19	0.43
1:C:183:ARG:HG2	1:C:184:LEU:HD12	2.00	0.43
1:C:199:ARG:HH21	1:C:219:PRO:CA	2.24	0.43
1:C:238:LEU:HB3	1:C:243:ARG:HD2	2.00	0.43
1:C:296:ASN:O	1:C:298:PHE:N	2.52	0.43
1:C:571:CYS:O	1:C:574:ILE:HB	2.18	0.43
2:D:200:CYS:SG	2:D:217:GLU:CD	2.97	0.43
2:D:504:HIS:CD2	2:D:543:ARG:HD2	2.54	0.43
2:D:552:LEU:HD12	2:D:657:LEU:CD2	2.48	0.43
2:D:40:TYR:HA	2:D:90:ASN:HA	2.01	0.43
1:A:389:ARG:NH1	1:A:441:LEU:HD22	2.34	0.42
1:A:488:TRP:CZ3	1:A:494:PRO:HB2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:96:ARG:HH22	2:B:364:GLU:HG2	1.84	0.42
1:C:426:PHE:CE1	1:C:482:PHE:CZ	3.07	0.42
1:C:472:LEU:CB	1:C:473:PRO:CD	2.97	0.42
1:C:573:GLU:HG2	1:C:613:CYS:CB	2.48	0.42
2:D:303:TYR:CD1	2:D:303:TYR:C	2.92	0.42
2:D:457:ALA:HA	2:D:596:LEU:HD22	2.00	0.42
2:D:460:PRO:HB2	2:D:567:TYR:CE1	2.54	0.42
1:A:377:ARG:O	1:A:380:VAL:HG12	2.18	0.42
1:A:422:LEU:HD11	1:A:490:LEU:HD23	2.01	0.42
2:B:490:GLY:N	2:B:491:PRO:HD3	2.34	0.42
2:B:631:SER:HA	2:B:636:ASP:OD2	2.19	0.42
1:C:516:LEU:HA	1:C:634:LEU:HD22	2.00	0.42
1:C:461:TRP:HB2	1:C:639:ILE:HG23	2.00	0.42
2:D:313:ARG:CZ	2:D:315:SER:HB2	2.50	0.42
1:A:487:TYR:OH	1:A:492:LEU:O	2.38	0.42
2:B:526:GLN:N	2:B:527:PRO:CD	2.82	0.42
2:B:40:TYR:HA	2:B:90:ASN:HA	2.00	0.42
2:D:110:GLY:O	2:D:114:LEU:HB2	2.18	0.42
1:A:539:ILE:O	1:A:540:ALA:C	2.57	0.42
2:B:463:VAL:O	2:B:464:ILE:C	2.57	0.42
2:B:95:VAL:CA	2:B:99:GLN:OE1	2.68	0.42
1:C:253:ARG:HB2	1:C:256:LEU:HD11	2.00	0.42
1:C:304:LEU:CD1	1:C:321:ARG:HD3	2.50	0.42
1:C:392:GLN:O	1:C:395:ILE:N	2.51	0.42
2:D:303:TYR:HB2	2:D:355:ASP:O	2.18	0.42
2:D:498:LEU:CD1	2:D:498:LEU:N	2.83	0.42
2:D:571:TYR:HE2	2:D:577:MET:HE2	1.84	0.42
2:D:615:MET:HB3	2:D:622:ILE:HB	2.00	0.42
1:A:474:PHE:O	1:A:477:VAL:CG1	2.67	0.42
1:A:81:ILE:CG1	1:A:261:ASP:H	2.31	0.42
2:B:110:GLY:O	2:B:114:LEU:HB2	2.19	0.42
1:C:185:ILE:HD12	1:C:186:GLY:N	2.34	0.42
1:C:465:LEU:HD13	1:C:639:ILE:HD11	2.01	0.42
2:B:286:MET:HB3	2:B:291:PRO:HA	2.00	0.42
2:B:309:TYR:CE2	2:B:317:PRO:HG2	2.50	0.42
2:B:608:PHE:HE1	2:B:614:LYS:HG2	1.84	0.42
1:C:296:ASN:N	1:C:297:PRO:CD	2.83	0.42
2:D:276:ILE:H	2:D:276:ILE:HD12	1.84	0.42
2:D:343:GLN:O	2:D:345:LEU:N	2.52	0.42
1:A:529:ILE:O	1:A:530:VAL:C	2.58	0.42
1:A:539:ILE:HG13	1:A:540:ALA:H	1.78	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:149:HIS:O	1:C:153:LEU:CB	2.68	0.42
1:C:336:HIS:O	1:C:339:LEU:HB3	2.20	0.42
1:C:87:SER:HB3	1:C:306:SER:OG	2.20	0.42
2:D:323:ASP:HA	2:D:333:GLU:HG3	2.00	0.42
2:D:445:PHE:CE2	2:D:616:PRO:HB3	2.55	0.42
2:D:651:SER:O	2:D:652:GLY:C	2.57	0.42
1:A:219:PRO:HG3	1:A:247:LEU:CD2	2.49	0.42
1:A:358:THR:CG2	1:A:359:LYS:N	2.82	0.42
1:A:468:ALA:O	1:A:471:VAL:HG12	2.18	0.42
1:A:471:VAL:O	1:A:472:LEU:C	2.58	0.42
2:B:400:THR:O	2:B:403:ILE:HG13	2.19	0.42
2:B:402:LEU:O	2:B:406:GLN:HB3	2.19	0.42
2:B:154:HIS:HB3	2:B:475:ARG:NH2	2.35	0.42
2:B:600:PHE:CZ	2:B:604:MET:HE2	2.54	0.42
1:C:468:ALA:O	1:C:471:VAL:HG12	2.20	0.42
1:C:637:LEU:HA	1:C:640:VAL:HG12	2.02	0.42
1:A:81:ILE:CD1	1:A:260:PHE:C	2.70	0.42
1:A:283:PHE:O	1:A:286:ASP:HB3	2.20	0.42
1:A:293:GLU:HG2	2:B:311:CYS:HA	2.01	0.42
2:B:345:LEU:C	2:B:345:LEU:CD1	2.87	0.42
1:C:210:ASP:N	1:C:211:PRO:CD	2.82	0.42
1:C:329:TYR:CZ	1:C:335:CYS:SG	3.10	0.42
1:C:516:LEU:CA	1:C:634:LEU:HD22	2.50	0.42
1:C:633:ALA:HA	1:C:636:ILE:HG12	2.01	0.42
2:D:419:ILE:HG22	2:D:423:GLU:HG3	2.01	0.42
2:D:424:ALA:HB1	2:D:511:TYR:HB2	2.00	0.42
1:A:273:PHE:HB2	1:A:329:TYR:OH	2.18	0.42
1:A:293:GLU:OE1	1:A:294:HIS:CD2	2.73	0.42
1:A:420:VAL:CG1	1:A:421:GLY:N	2.83	0.42
1:A:389:ARG:HH11	1:A:441:LEU:HD22	1.84	0.42
2:B:260:LYS:C	2:B:261:GLY:O	2.56	0.42
2:B:429:MET:HE3	2:D:426:LEU:HD21	2.01	0.42
2:B:457:ALA:HA	2:B:596:LEU:HD22	2.02	0.42
1:C:185:ILE:HD12	1:C:186:GLY:O	2.20	0.42
1:C:273:PHE:CD1	1:C:283:PHE:CD2	3.08	0.42
1:C:364:VAL:O	1:C:367:LYS:CB	2.68	0.42
1:C:413:LYS:HA	1:C:413:LYS:HD3	1.90	0.42
2:D:530:LEU:HG	2:D:644:TYR:OH	2.20	0.42
2:D:521:LEU:HB3	2:D:607:GLN:CD	2.40	0.42
1:A:492:LEU:HB2	1:A:579:GLU:CD	2.40	0.41
2:B:256:SER:O	2:B:259:ALA:HB3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:254:SER:HB2	2:B:312:PRO:HB3	2.01	0.41
2:B:602:GLY:HA2	2:B:643:ILE:HD13	2.01	0.41
1:C:180:VAL:HG21	1:C:197:GLU:OE2	2.20	0.41
1:A:379:LEU:HD21	1:A:389:ARG:HD3	2.02	0.41
1:A:487:TYR:OH	1:A:493:HIS:O	2.36	0.41
1:A:465:LEU:HD13	1:A:639:ILE:HD11	2.02	0.41
2:B:174:ARG:NH2	2:B:483:GLU:O	2.53	0.41
2:B:600:PHE:CE2	2:B:635:LEU:HD21	2.55	0.41
1:C:392:GLN:O	1:C:395:ILE:HB	2.19	0.41
1:C:616:ALA:O	1:C:617:THR:C	2.58	0.41
2:D:509:ILE:CD1	2:D:513:MET:HB3	2.51	0.41
1:A:225:CYS:HB3	1:A:253:ARG:HH22	1.84	0.41
1:A:637:LEU:HA	1:A:640:VAL:HG12	2.02	0.41
2:B:460:PRO:HB2	2:B:567:TYR:CE1	2.55	0.41
1:C:251:GLN:CG	1:C:253:ARG:HG2	2.49	0.41
1:C:85:LEU:HD11	1:C:302:MET:SD	2.60	0.41
1:C:307:VAL:HG11	1:C:319:SER:CA	2.44	0.41
1:C:442:PHE:N	1:C:443:PRO:CD	2.83	0.41
2:D:37:TYR:CB	2:D:133:TRP:HB2	2.43	0.41
1:A:450:ASP:OD1	1:A:645:ARG:NH1	2.53	0.41
2:B:233:ILE:HG22	2:B:234:LEU:N	2.35	0.41
2:B:488:THR:C	2:B:491:PRO:CD	2.89	0.41
2:B:561:PHE:O	2:B:562:PHE:C	2.59	0.41
1:C:140:SER:C	1:C:185:ILE:HD11	2.38	0.41
2:D:396:VAL:HG13	2:D:397:GLN:H	1.85	0.41
2:D:441:ILE:HG13	2:D:442:GLN:H	1.84	0.41
2:D:538:VAL:HG21	2:D:599:CYS:HB2	2.01	0.41
2:B:419:ILE:O	2:B:420:HIS:C	2.59	0.41
2:B:461:PHE:C	2:B:461:PHE:CD2	2.91	0.41
2:B:618:GLY:H	2:B:621:THR:HG1	1.67	0.41
1:C:209:GLN:O	1:C:358:THR:HG22	2.19	0.41
1:C:377:ARG:O	1:C:380:VAL:HG12	2.20	0.41
2:D:286:MET:HB3	2:D:291:PRO:HA	2.02	0.41
2:D:94:LYS:HE2	2:D:353:VAL:HB	2.03	0.41
2:D:506:ALA:O	2:D:510:ILE:HG12	2.19	0.41
2:D:600:PHE:CE2	2:D:635:LEU:HD21	2.56	0.41
1:A:183:ARG:HG2	1:A:184:LEU:N	2.35	0.41
1:A:257:PHE:HB2	1:A:298:PHE:HB2	2.02	0.41
1:A:81:ILE:HD12	1:A:260:PHE:CA	2.44	0.41
1:A:458:TYR:HB2	1:A:462:GLN:HG3	2.01	0.41
1:A:461:TRP:CD1	1:A:461:TRP:C	2.93	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:478:LEU:HD11	2:B:668:LYS:HE2	2.02	0.41
2:B:521:LEU:HD23	2:B:607:GLN:NE2	2.35	0.41
1:C:315:GLU:O	1:C:318:THR:OG1	2.20	0.41
1:C:580:PHE:O	1:C:581:TYR:C	2.59	0.41
2:D:274:SER:O	2:D:275:ASP:C	2.59	0.41
2:D:493:PHE:CZ	2:D:494:PHE:CD2	3.08	0.41
2:B:33:ASP:O	2:B:34:ASN:HB2	2.21	0.41
2:B:498:LEU:N	2:B:498:LEU:HD12	2.35	0.41
2:B:651:SER:O	2:B:652:GLY:C	2.59	0.41
1:C:307:VAL:O	1:C:307:VAL:CG2	2.69	0.41
2:B:570:PHE:HE1	2:B:593:VAL:HG13	1.84	0.41
1:C:387:ILE:HG23	1:C:388:THR:N	2.36	0.41
2:D:240:THR:O	2:D:241:SER:C	2.59	0.41
2:D:298:GLN:OE1	2:D:299:HIS:N	2.54	0.41
2:D:303:TYR:OH	2:D:343:GLN:HB2	2.21	0.41
2:D:555:THR:HB	2:D:558:MET:HG3	2.03	0.41
2:D:570:PHE:HE1	2:D:593:VAL:HG13	1.86	0.41
1:A:37:SER:O	1:A:116:ASN:ND2	2.53	0.41
1:A:383:LYS:O	1:A:384:LEU:C	2.59	0.41
2:B:438:HIS:NE2	2:B:520:ASN:HB2	2.36	0.41
2:B:459:ILE:O	2:B:460:PRO:C	2.57	0.41
1:C:189:SER:O	1:C:190:LEU:HD23	2.21	0.41
1:C:283:PHE:O	1:C:286:ASP:HB3	2.21	0.41
1:C:450:ASP:OD1	1:C:645:ARG:NH1	2.53	0.41
1:C:526:ASN:O	1:C:528:ASN:N	2.53	0.41
1:A:201:VAL:O	1:A:202:SER:C	2.58	0.41
1:A:516:LEU:HA	1:A:634:LEU:HD22	2.03	0.41
1:A:624:PHE:O	1:A:625:LEU:C	2.59	0.41
1:A:631:ILE:N	1:A:632:PRO:HD2	2.36	0.41
1:A:632:PRO:C	1:A:636:ILE:HD12	2.40	0.41
2:B:362:LYS:O	2:B:365:THR:HB	2.20	0.41
2:B:576:PHE:CD1	2:B:576:PHE:C	2.95	0.41
2:B:584:TRP:O	2:B:587:PRO:HD2	2.21	0.41
2:B:589:TRP:CE3	2:B:589:TRP:HA	2.55	0.41
1:C:471:VAL:O	1:C:472:LEU:C	2.59	0.41
2:D:161:LEU:O	2:D:205:VAL:HG13	2.20	0.41
2:D:313:ARG:NE	2:D:315:SER:HB3	2.35	0.41
2:D:483:GLU:HA	2:D:483:GLU:OE1	2.20	0.41
1:A:327:SER:HA	1:A:330:LYS:HB3	2.04	0.41
1:A:439:VAL:HG21	1:A:531:ASN:HB2	2.03	0.41
1:A:647:HIS:CG	1:C:615:GLY:HA2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:93:PHE:HE1	2:B:284:LEU:HD22	1.84	0.41
1:C:95:LEU:HD23	1:C:266:LEU:HD21	2.02	0.41
1:C:337:LYS:HE2	1:C:341:ASN:OD1	2.20	0.41
1:C:410:ASN:O	1:C:586:THR:HB	2.20	0.41
2:D:205:VAL:HA	2:D:213:LEU:CD2	2.49	0.41
2:D:463:VAL:O	2:D:464:ILE:C	2.59	0.41
2:B:343:GLN:HB3	2:B:344:SER:H	1.73	0.40
2:B:426:LEU:O	2:B:427:MET:C	2.60	0.40
2:B:590:ILE:HG23	2:B:591:SER:N	2.35	0.40
1:C:285:ASN:ND2	1:C:289:TYR:O	2.53	0.40
1:C:75:TYR:CE2	1:C:341:ASN:HB3	2.56	0.40
1:C:619:ARG:O	1:C:622:MET:HG2	2.21	0.40
2:D:272:PRO:O	2:D:276:ILE:HD13	2.21	0.40
1:C:460:LYS:HG2	1:C:646:ASP:OD2	2.21	0.40
1:C:492:LEU:HD23	1:C:579:GLU:HG3	2.03	0.40
2:D:28:PHE:CD1	2:D:194:GLU:HA	2.56	0.40
2:D:314:TYR:O	2:D:314:TYR:CG	2.73	0.40
2:D:489:THR:O	2:D:493:PHE:CD2	2.74	0.40
1:A:293:GLU:OE2	1:A:294:HIS:CE1	2.73	0.40
1:A:336:HIS:O	1:A:339:LEU:HB3	2.21	0.40
1:A:39:GLY:HA2	1:A:74:LEU:O	2.21	0.40
2:B:196:ARG:HB3	2:B:198:ARG:HD3	2.03	0.40
2:B:292:ILE:O	2:B:293:TYR:HB2	2.21	0.40
2:B:498:LEU:CD1	2:B:498:LEU:N	2.85	0.40
2:B:506:ALA:O	2:B:510:ILE:HG12	2.22	0.40
2:B:629:ILE:HG23	2:B:630:LEU:N	2.37	0.40
1:C:219:PRO:HG3	1:C:247:LEU:CD2	2.51	0.40
1:C:212:LYS:CD	1:C:356:PHE:HD2	2.34	0.40
1:C:496:VAL:HG23	1:C:497:ALA:N	2.36	0.40
2:D:276:ILE:HD12	2:D:276:ILE:N	2.37	0.40
2:D:561:PHE:O	2:D:562:PHE:C	2.59	0.40
1:A:247:LEU:HB3	1:A:249:ILE:CD1	2.51	0.40
2:B:109:CYS:HB2	2:B:288:SER:HA	2.03	0.40
2:D:419:ILE:O	2:D:420:HIS:C	2.58	0.40
2:D:429:MET:HB2	2:D:429:MET:HE2	1.96	0.40
2:D:530:LEU:HD23	2:D:606:ILE:HD12	2.03	0.40
2:D:600:PHE:CZ	2:D:604:MET:HE2	2.56	0.40
2:D:611:ARG:C	2:D:612:THR:HG23	2.42	0.40
1:A:194:SER:HB2	1:A:197:GLU:CG	2.52	0.40
1:A:200:ARG:HE	1:A:234:LEU:CD1	2.35	0.40
1:A:442:PHE:N	1:A:443:PRO:CD	2.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:472:LEU:HB2	1:A:473:PRO:HD2	2.04	0.40
1:A:633:ALA:O	1:A:634:LEU:C	2.58	0.40
2:B:313:ARG:CG	2:B:314:TYR:N	2.85	0.40
2:B:592:LYS:O	2:B:598:TRP:NE1	2.48	0.40
2:D:31:GLU:CB	2:D:262:ASN:HB3	2.51	0.40
2:D:178:THR:HG21	2:D:391:LYS:HG3	2.04	0.40
2:D:459:ILE:O	2:D:460:PRO:C	2.59	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)
2:B:357:ASP:OD1	2:D:339:ARG:NH2[6_454]	2.09	0.11

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	579/666 (87%)	468 (81%)	101 (17%)	10 (2%)	11	52
1	C	571/666 (86%)	465 (81%)	92 (16%)	14 (2%)	6	44
2	B	554/685 (81%)	445 (80%)	91 (16%)	18 (3%)	5	39
2	D	565/685 (82%)	443 (78%)	101 (18%)	21 (4%)	4	36
All	All	2269/2702 (84%)	1821 (80%)	385 (17%)	63 (3%)	6	42

All (63) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	557	ILE
2	B	127	ILE
2	B	135	ASN

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Mol	Chain	Res	Type
2	B	484	ASP
2	B	491	PRO
2	D	25	ASP
2	D	348	LEU
2	D	484	ASP
2	D	489	THR
2	D	588	ALA
1	C	90	SER
1	C	301	TYR
1	C	357	LYS
1	C	360	ASP
1	C	551	ASN
1	C	557	ILE
1	A	363	GLY
2	B	30	SER
2	B	33	ASP
2	B	97	SER
2	B	201	ALA
2	B	310	PRO
2	B	640	LEU
2	D	97	SER
2	D	125	GLY
2	D	201	ALA
2	D	310	PRO
2	D	585	THR
2	D	587	PRO
2	D	640	LEU
1	A	362	PRO
1	A	410	ASN
1	A	552	ILE
2	B	27	LEU
2	B	312	PRO
2	B	554	PRO
2	B	619	ASN
2	B	634	GLU
2	D	312	PRO
2	D	493	PHE
2	D	554	PRO
2	D	666	LYS
1	C	89	GLY
1	C	581	TYR
1	A	272	ILE

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Mol	Chain	Res	Type
1	A	581	TYR
2	B	580	LEU
2	D	325	THR
2	D	579	ASN
1	C	272	ILE
1	A	493	HIS
2	D	439	GLY
1	C	552	ILE
2	B	610	ARG
1	C	587	CYS
1	A	494	PRO
2	D	441	ILE
1	C	493	HIS
2	D	392	MET
1	C	297	PRO
1	C	218	GLU
1	A	218	GLU
2	B	522	ARG

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	512/582 (88%)	474 (93%)	38 (7%)	16	52
1	C	505/582 (87%)	467 (92%)	38 (8%)	16	52
2	B	481/591 (81%)	441 (92%)	40 (8%)	13	47
2	D	490/591 (83%)	449 (92%)	41 (8%)	13	47
All	All	1988/2346 (85%)	1831 (92%)	157 (8%)	14	50

All (157) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	SER
1	A	44	SER
1	A	71	ASP

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Mol	Chain	Res	Type
1	A	81	ILE
1	A	178	SER
1	A	184	LEU
1	A	195	THR
1	A	240	ARG
1	A	282	ASP
1	A	304	LEU
1	A	329	TYR
1	A	331	LYS
1	A	368	LEU
1	A	376	THR
1	A	381	ARG
1	A	391	LEU
1	A	392	GLN
1	A	405	LEU
1	A	410	ASN
1	A	420	VAL
1	A	422	LEU
1	A	444	VAL
1	A	448	VAL
1	A	451	GLN
1	A	462	GLN
1	A	489	THR
1	A	490	LEU
1	A	493	HIS
1	A	528	ASN
1	A	537	LEU
1	A	550	ARG
1	A	555	MET
1	A	557	ILE
1	A	578	ASN
1	A	583	LEU
1	A	587	CYS
1	A	613	CYS
1	A	646	ASP
2	B	30	SER
2	B	31	GLU
2	B	97	SER
2	B	99	GLN
2	B	116	ASP
2	B	123	HIS
2	B	128	LYS

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Mol	Chain	Res	Type
2	B	131	GLN
2	B	177	ARG
2	B	202	ASP
2	B	285	LEU
2	B	305	THR
2	B	309	TYR
2	B	311	CYS
2	B	319	ASP
2	B	345	LEU
2	B	353	VAL
2	B	355	ASP
2	B	407	ILE
2	B	416	THR
2	B	444	SER
2	B	446	MET
2	B	458	LEU
2	B	459	ILE
2	B	465	LEU
2	B	475	ARG
2	B	488	THR
2	B	500	GLU
2	B	501	LEU
2	B	525	LEU
2	B	528	PHE
2	B	552	LEU
2	B	571	TYR
2	B	579	ASN
2	B	591	SER
2	B	597	ARG
2	B	610	ARG
2	B	640	LEU
2	B	671	GLN
2	B	673	TRP
2	D	25	ASP
2	D	28	PHE
2	D	32	SER
2	D	37	TYR
2	D	95	VAL
2	D	100	MET
2	D	116	ASP
2	D	137	GLN
2	D	146	LYS

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Mol	Chain	Res	Type
2	D	202	ASP
2	D	211	ARG
2	D	266	LEU
2	D	298	GLN
2	D	305	THR
2	D	309	TYR
2	D	311	CYS
2	D	319	ASP
2	D	323	ASP
2	D	335	GLU
2	D	338	THR
2	D	345	LEU
2	D	354	ARG
2	D	407	ILE
2	D	409	ASN
2	D	458	LEU
2	D	459	ILE
2	D	472	TYR
2	D	475	ARG
2	D	484	ASP
2	D	486	LEU
2	D	492	TYR
2	D	500	GLU
2	D	501	LEU
2	D	525	LEU
2	D	528	PHE
2	D	583	LEU
2	D	597	ARG
2	D	610	ARG
2	D	634	GLU
2	D	640	LEU
2	D	659	TYR
1	C	37	SER
1	C	44	SER
1	C	71	ASP
1	C	73	SER
1	C	77	GLU
1	C	87	SER
1	C	95	LEU
1	C	105	ARG
1	C	110	LEU
1	C	127	ASP

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Mol	Chain	Res	Type
1	C	176	SER
1	C	178	SER
1	C	184	LEU
1	C	282	ASP
1	C	285	ASN
1	C	296	ASN
1	C	319	SER
1	C	331	LYS
1	C	376	THR
1	C	391	LEU
1	C	392	GLN
1	C	405	LEU
1	C	411	VAL
1	C	412	LEU
1	C	420	VAL
1	C	422	LEU
1	C	444	VAL
1	C	489	THR
1	C	532	SER
1	C	536	LEU
1	C	537	LEU
1	C	550	ARG
1	C	555	MET
1	C	557	ILE
1	C	578	ASN
1	C	587	CYS
1	C	613	CYS
1	C	646	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	230	GLN
1	A	285	ASN
1	A	310	GLN
1	A	493	HIS
1	A	528	ASN
2	B	250	ASN
2	B	299	HIS
2	B	409	ASN
2	B	438	HIS
2	B	667	GLN

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Mol	Chain	Res	Type
2	D	334	GLN
2	D	420	HIS
2	D	607	GLN
1	C	36	HIS
1	C	149	HIS
1	C	230	GLN
1	C	285	ASN
1	C	470	HIS
1	C	528	ASN
1	C	531	ASN
1	C	553	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	585/666 (87%)	-0.53	6 (1%) 82 74	20, 64, 145, 252	0
1	C	579/666 (86%)	-0.48	6 (1%) 82 74	20, 65, 143, 220	0
2	B	562/685 (82%)	-0.39	12 (2%) 64 54	20, 77, 157, 247	0
2	D	571/685 (83%)	-0.52	10 (1%) 69 59	20, 49, 139, 234	0
All	All	2297/2702 (85%)	-0.48	34 (1%) 74 64	20, 63, 147, 252	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	621	THR	4.8
2	D	620	LEU	4.4
2	D	619	ASN	4.3
1	A	587	CYS	3.9
1	C	589	SER	3.7
2	B	619	ASN	3.4
2	D	112	ALA	3.4
1	C	588	GLY	3.2
1	C	286	ASP	3.1
2	B	39	THR	3.1
1	A	347	HIS	2.9
1	A	34	GLU	2.8
2	B	622	ILE	2.8
2	B	623	ALA	2.7
2	D	123	HIS	2.6
2	D	209	TYR	2.6
1	C	158	ARG	2.5
2	B	342	ALA	2.5
2	B	212	GLY	2.5
2	B	123	HIS	2.5
1	C	162	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
2	D	618	GLY	2.3
2	D	207	ASN	2.3
2	B	108	GLY	2.3
2	D	524	GLY	2.3
2	B	124	GLY	2.2
2	B	624	VAL	2.2
1	A	191	GLY	2.2
1	A	187	ASN	2.2
1	A	350	THR	2.2
2	B	620	LEU	2.1
1	C	102	ARG	2.0
2	B	32	SER	2.0
2	D	107	SER	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.