



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 06:58 PM GMT

PDB ID : 1DDX
Title : CRYSTAL STRUCTURE OF A MIXTURE OF ARACHIDONIC ACID AND PROSTAGLANDIN BOUND TO THE CYCLOOXYGENASE ACTIVE SITE OF COX-2: PROSTAGLANDIN STRUCTURE
Authors : Kiefer, J.R.; Pawlitz, J.L.; Moreland, K.T.; Stegeman, R.A.; Gierse, J.K.; Stevens, A.M.; Goodwin, D.C.; Rowlinson, S.W.; Marnett, L.J.; Stallings, W.C.; Kurumbail, R.G.
Deposited on : 1999-11-11
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
<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
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
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) : trunk26865

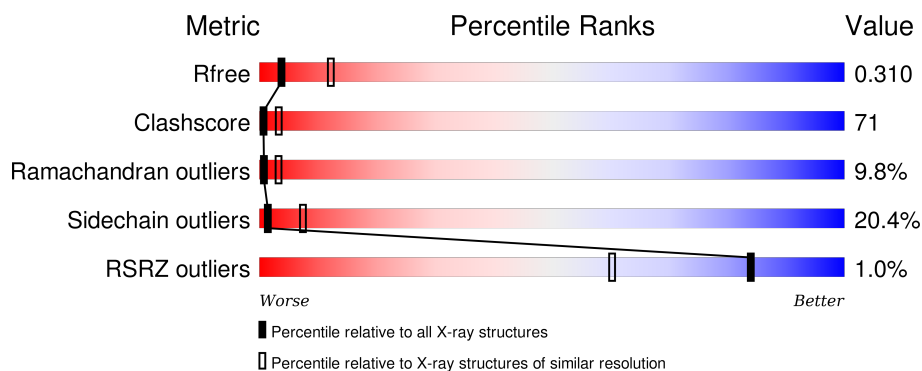
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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}	91344	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (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 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	552	<div> <div></div> <div> <div>19%</div> <div>59%</div> <div>21%</div> </div> <div>•</div> </div>
1	B	552	<div> <div></div> <div> <div>19%</div> <div>59%</div> <div>20%</div> </div> <div>•</div> </div>
1	C	552	<div> <div></div> <div> <div>20%</div> <div>57%</div> <div>22%</div> </div> <div>•</div> </div>
1	D	552	<div> <div></div> <div> <div>18%</div> <div>60%</div> <div>20%</div> </div> <div>•</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	A	661	-	-	-	X
2	NAG	C	2661	-	-	-	X
3	NAG	B	1681	-	-	-	X
3	NAG	C	2681	-	-	-	X
4	BOG	A	702	-	-	-	X
4	BOG	C	2702	-	-	-	X
4	BOG	D	3702	-	-	-	X
5	PGX	A	701	-	-	X	X
5	PGX	B	1701	-	-	X	X
5	PGX	C	2701	-	-	X	X
5	PGX	D	3701	-	-	X	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 18477 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 PROTEIN (PROSTAGLANDIN H2 SYNTHASE-2).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	552	Total	C	N	O	S	0	0	0
			4475	2885	750	815	25			
1	B	552	Total	C	N	O	S	0	0	0
			4475	2885	750	815	25			
1	C	552	Total	C	N	O	S	0	0	0
			4475	2885	750	815	25			
1	D	552	Total	C	N	O	S	0	0	0
			4475	2885	750	815	25			

- Molecule 2 is a polymer of unknown type called SUGAR (NAG-NAG).

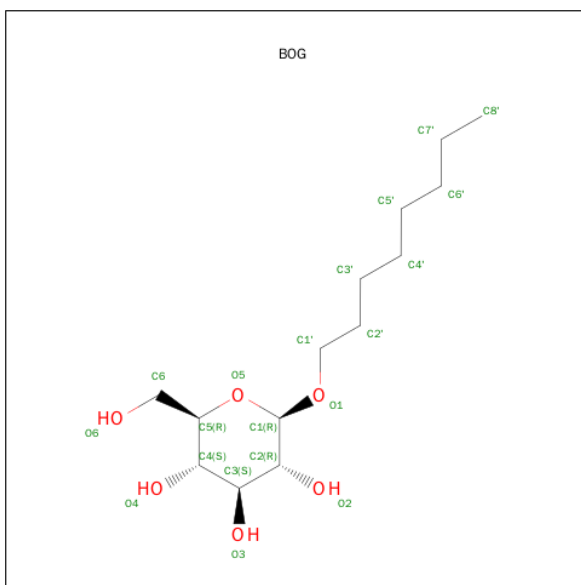
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	2	Total	C	N	O	0	0
			28	16	2	10		
2	B	2	Total	C	N	O	0	0
			28	16	2	10		
2	C	2	Total	C	N	O	0	0
			28	16	2	10		
2	D	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 3 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: C₈H₁₅NO₆).



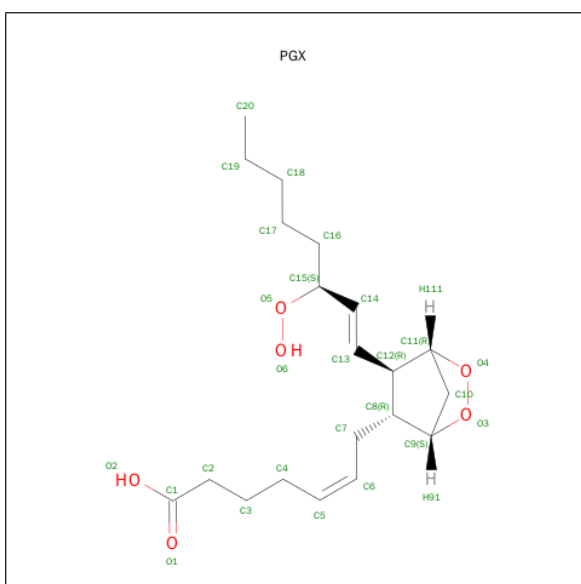
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	D	1	Total	C	N	O	0	0
			14	8	1	5		
3	D	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 4 is B-OCTYLGLUCOSIDE (three-letter code: BOG) (formula: $C_{14}H_{28}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			20	14	6		
4	B	1	Total	C	O	0	0
			20	14	6		
4	C	1	Total	C	O	0	0
			20	14	6		
4	D	1	Total	C	O	0	0
			20	14	6		

- Molecule 5 is 7-[6-(3-HYDROPEROXY-OCT-1-ENYL)-2,3-DIOXA-BICYCLO[2.2.1]HEPT-5-YL]-HEPT-5-ENOIC ACID (three-letter code: PGX) (formula: $C_{20}H_{32}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			25	20	5		
5	B	1	Total	C	O	0	0
			25	20	5		
5	C	1	Total	C	O	0	0
			25	20	5		
5	D	1	Total	C	O	0	0
			25	20	5		

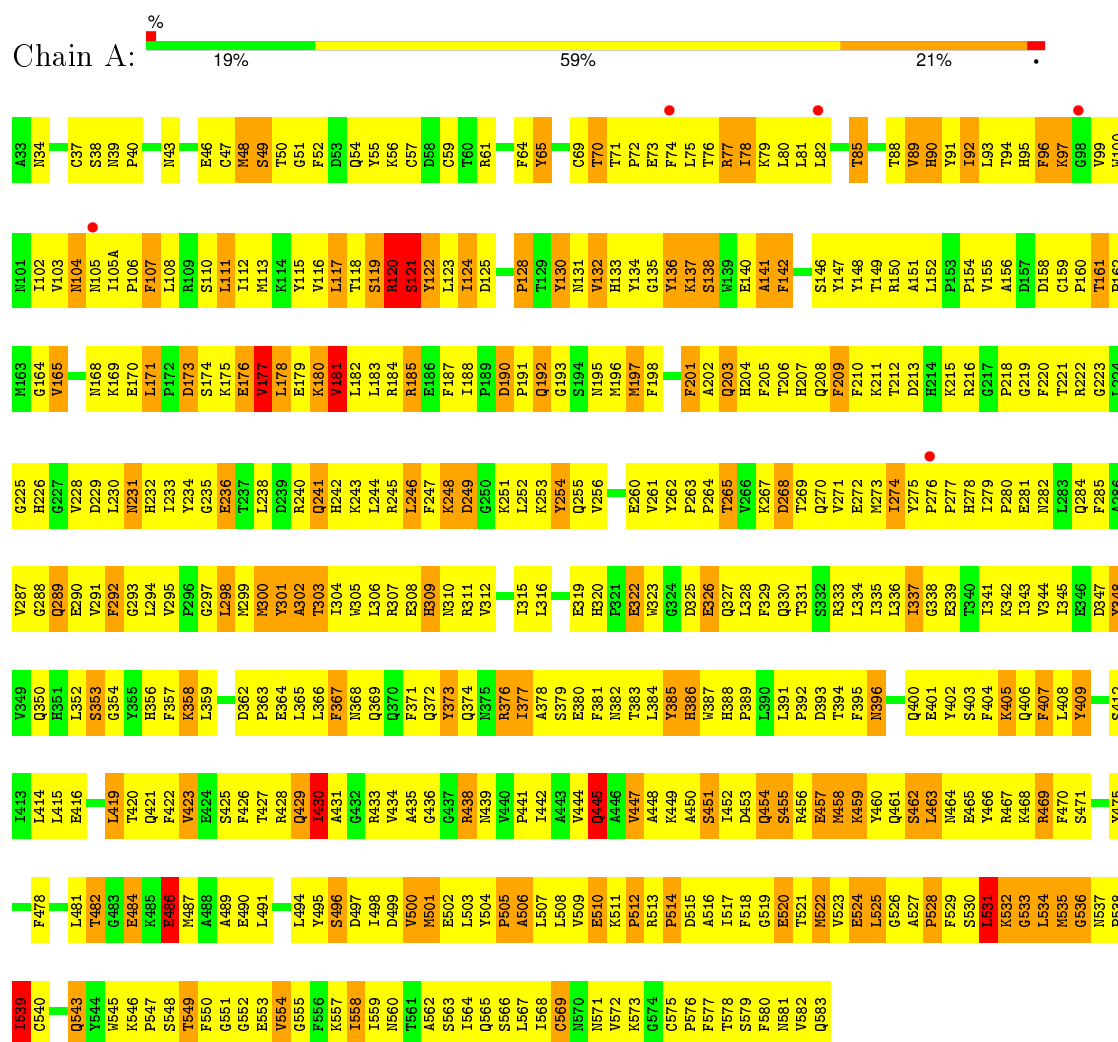
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	45	Total	O	0	0
			45	45		
6	B	39	Total	O	0	0
			39	39		
6	C	46	Total	O	0	0
			46	46		
6	D	43	Total	O	0	0
			43	43		

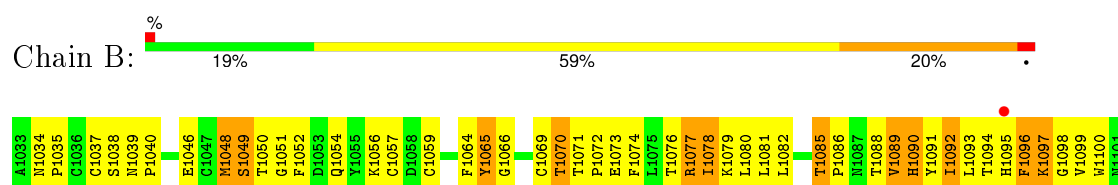
3 Residue-property plots

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

• Molecule 1: PROTEIN (PROSTAGLANDIN H2 SYNTHASE-2)



• Molecule 1: PROTEIN (PROSTAGLANDIN H2 SYNTHASE-2)







4 Data and refinement statistics

Property	Value	Source
Space group	P 2 ₁ 2 ₁ 2	Depositor
Cell constants a, b, c, α , β , γ	180.24Å 134.80Å 122.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.00 36.19 – 3.00	Depositor EDS
% Data completeness (in resolution range)	76.1 (20.00-3.00) 75.8 (36.19-3.00)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.34 (at 3.00Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.267 , 0.324 0.256 , 0.310	Depositor DCC
R_{free} test set	4324 reflections (10.43%)	DCC
Wilson B-factor (Å ²)	34.0	Xtriage
Anisotropy	0.915	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 60.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	3 of 45890 reflections (0.007%)	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	18477	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 48.65 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 8.3521e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, PGX, BOG

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	0.45	0/4602	0.65	0/6239
1	B	0.45	0/4602	0.65	0/6239
1	C	0.45	0/4602	0.65	0/6239
1	D	0.46	0/4602	0.64	0/6239
All	All	0.45	0/18408	0.64	0/24956

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	4475	0	4373	650	0
1	B	4475	0	4373	653	0
1	C	4475	0	4373	663	0
1	D	4475	0	4373	668	0
2	A	28	0	25	0	0
2	B	28	0	25	0	0
2	C	28	0	25	0	0
2	D	28	0	25	0	0
3	A	28	0	26	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	28	0	26	0	0
3	C	28	0	26	0	0
3	D	28	0	26	0	0
4	A	20	0	28	0	0
4	B	20	0	28	0	0
4	C	20	0	28	0	0
4	D	20	0	28	1	0
5	A	25	0	30	9	0
5	B	25	0	30	13	0
5	C	25	0	30	14	0
5	D	25	0	30	11	0
6	A	45	0	0	14	0
6	B	39	0	0	12	0
6	C	46	0	0	20	0
6	D	43	0	0	15	0
All	All	18477	0	17928	2579	0

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 71.

All (2579) 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:D:3312:VAL:HA	1:D:3315:ILE:HD12	1.33	1.09
1:A:312:VAL:HA	1:A:315:ILE:HD12	1.33	1.08
1:B:1312:VAL:HA	1:B:1315:ILE:HD12	1.36	1.07
1:B:1301:TYR:HA	1:B:1304:ILE:HD12	1.37	1.07
1:A:99:VAL:HA	1:A:102:ILE:HD12	1.37	1.06
1:C:2301:TYR:HA	1:C:2304:ILE:HD12	1.35	1.05
1:C:2273:MET:HE1	1:C:2287:VAL:HG22	1.36	1.05
1:B:1099:VAL:HA	1:B:1102:ILE:HD12	1.38	1.05
1:D:3230:LEU:HB3	1:D:3233:ILE:HD12	1.39	1.04
1:D:3099:VAL:HA	1:D:3102:ILE:HD12	1.38	1.04
1:D:3301:TYR:HA	1:D:3304:ILE:HD12	1.35	1.03
1:C:2312:VAL:HA	1:C:2315:ILE:HD12	1.34	1.03
1:A:301:TYR:HA	1:A:304:ILE:HD12	1.37	1.02
1:B:1230:LEU:HB3	1:B:1233:ILE:HD12	1.39	1.01
1:C:2099:VAL:HA	1:C:2102:ILE:HD12	1.39	1.01
1:A:389:PRO:HG2	1:A:434:VAL:HG13	1.42	1.01
1:A:230:LEU:HB3	1:A:233:ILE:HD12	1.43	1.00
1:D:3273:MET:HE1	1:D:3287:VAL:HG22	1.45	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2208:GLN:HB3	1:C:2232:HIS:HD2	1.28	0.99
1:B:1208:GLN:HB3	1:B:1232:HIS:HD2	1.26	0.98
1:A:273:MET:HE1	1:A:287:VAL:HG22	1.46	0.98
1:D:3389:PRO:HG2	1:D:3434:VAL:HG13	1.44	0.97
1:A:208:GLN:HB3	1:A:232:HIS:HD2	1.29	0.96
1:B:1389:PRO:HG2	1:B:1434:VAL:HG13	1.48	0.96
1:B:1273:MET:HE1	1:B:1287:VAL:HG22	1.49	0.95
1:A:507:LEU:HD22	1:A:522:MET:HE3	1.49	0.94
1:C:2526:GLY:HA3	5:C:2701:PGX:H61	1.46	0.94
1:C:2385:TYR:HA	5:C:2701:PGX:O3	1.68	0.94
1:C:2308:GLU:HB2	1:C:2571:ASN:HD21	1.31	0.94
1:C:2507:LEU:HD22	1:C:2522:MET:HE3	1.50	0.94
1:D:3208:GLN:HB3	1:D:3232:HIS:HD2	1.32	0.94
1:D:3191:PRO:HD2	1:D:3433:ARG:HG3	1.50	0.94
1:A:308:GLU:HG3	1:A:336:LEU:HD11	1.49	0.93
1:B:1203:GLN:HG2	1:B:1298:LEU:HD11	1.49	0.93
1:A:191:PRO:HD2	1:A:433:ARG:HG3	1.50	0.93
1:B:1385:TYR:HA	5:B:1701:PGX:O3	1.68	0.93
1:A:308:GLU:HB2	1:A:571:ASN:HD21	1.31	0.93
1:B:1463:LEU:HD13	1:B:1506:ALA:HB3	1.48	0.92
1:B:1191:PRO:HD2	1:B:1433:ARG:HG3	1.51	0.92
1:C:2389:PRO:HG2	1:C:2434:VAL:HG13	1.50	0.92
1:C:2463:LEU:HD13	1:C:2506:ALA:HB3	1.49	0.92
1:A:463:LEU:HD13	1:A:506:ALA:HB3	1.50	0.92
1:B:1184:ARG:HD3	1:B:1187:PHE:HA	1.51	0.92
1:B:1245:ARG:HH22	1:B:1326:GLU:HG2	1.33	0.92
1:C:2191:PRO:HD2	1:C:2433:ARG:HG3	1.50	0.92
1:D:3463:LEU:HD13	1:D:3506:ALA:HB3	1.51	0.92
1:C:2230:LEU:HB3	1:C:2233:ILE:HD12	1.51	0.92
1:A:414:LEU:HA	1:A:422:PHE:CE1	2.05	0.91
1:B:1308:GLU:HB2	1:B:1571:ASN:HD21	1.35	0.91
1:D:3308:GLU:HB2	1:D:3571:ASN:HD21	1.35	0.90
1:A:203:GLN:HG2	1:A:298:LEU:HD11	1.54	0.90
1:C:2308:GLU:HG3	1:C:2336:LEU:HD11	1.52	0.90
1:A:275:TYR:HE1	1:A:293:GLY:HA3	1.37	0.89
1:B:1308:GLU:HG3	1:B:1336:LEU:HD11	1.52	0.89
1:D:3308:GLU:HG3	1:D:3336:LEU:HD11	1.54	0.89
1:C:2184:ARG:HD3	1:C:2187:PHE:HA	1.55	0.89
1:C:2414:LEU:HA	1:C:2422:PHE:CE1	2.08	0.88
1:D:3203:GLN:HG2	1:D:3298:LEU:HD11	1.56	0.88
1:C:2203:GLN:HG2	1:C:2298:LEU:HD11	1.56	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3507:LEU:HD22	1:D:3522:MET:CE	2.03	0.87
1:C:2507:LEU:HD22	1:C:2522:MET:CE	2.04	0.87
1:D:3396:ASN:ND2	1:D:3401:GLU:HG2	1.89	0.87
1:B:1526:GLY:HA3	5:B:1701:PGX:H61	1.55	0.87
1:C:2391:LEU:HD23	1:C:2392:PRO:HD2	1.57	0.87
1:C:2502:GLU:HB2	1:C:2505:PRO:HG2	1.57	0.87
1:D:3414:LEU:HA	1:D:3422:PHE:CE1	2.10	0.87
1:A:502:GLU:HB2	1:A:505:PRO:HG2	1.57	0.86
1:B:1502:GLU:HB2	1:B:1505:PRO:HG2	1.56	0.86
1:A:245:ARG:HH22	1:A:326:GLU:HG2	1.39	0.86
1:A:526:GLY:HA3	5:A:701:PGX:H61	1.57	0.86
1:B:1507:LEU:HD22	1:B:1522:MET:CE	2.05	0.86
1:C:2275:TYR:HE1	1:C:2293:GLY:HA3	1.39	0.86
1:C:2350:GLN:HE22	1:C:2358:LYS:HA	1.39	0.86
1:A:350:GLN:HE22	1:A:358:LYS:HA	1.41	0.86
1:A:88:THR:HG22	1:A:92:ILE:HD11	1.58	0.86
1:C:2245:ARG:HH22	1:C:2326:GLU:HG2	1.36	0.86
1:D:3391:LEU:HD23	1:D:3392:PRO:HD2	1.58	0.86
1:D:3275:TYR:HE1	1:D:3293:GLY:HA3	1.41	0.86
1:D:3245:ARG:HH22	1:D:3326:GLU:HG2	1.40	0.86
1:D:3184:ARG:HD3	1:D:3187:PHE:HA	1.58	0.85
1:D:3088:THR:HG22	1:D:3092:ILE:HD11	1.58	0.85
1:B:1275:TYR:HE1	1:B:1293:GLY:HA3	1.39	0.85
1:C:2088:THR:HG22	1:C:2092:ILE:HD11	1.56	0.85
1:D:3507:LEU:HD22	1:D:3522:MET:HE3	1.56	0.85
1:B:1088:THR:HG22	1:B:1092:ILE:HD11	1.59	0.84
1:C:2103:VAL:HG22	1:C:2108:LEU:HB3	1.59	0.84
1:A:507:LEU:HD22	1:A:522:MET:CE	2.05	0.84
1:A:103:VAL:HG22	1:A:108:LEU:HB3	1.60	0.84
1:C:2419:LEU:O	1:C:2423:VAL:HG23	1.78	0.84
1:B:1350:GLN:HE22	1:B:1358:LYS:HA	1.42	0.84
1:A:184:ARG:HD3	1:A:187:PHE:HA	1.58	0.83
1:B:1414:LEU:HA	1:B:1422:PHE:CE1	2.13	0.83
1:C:2322:GLU:HG2	1:D:3052:PHE:N	1.94	0.83
1:B:1396:ASN:ND2	1:B:1401:GLU:HG2	1.92	0.83
1:D:3338:GLY:HA3	1:D:3559:ILE:HD13	1.60	0.83
1:D:3350:GLN:HE22	1:D:3358:LYS:HA	1.42	0.82
1:C:2051:GLY:C	1:D:3322:GLU:HG2	1.98	0.82
1:C:2396:ASN:ND2	1:C:2401:GLU:HG2	1.94	0.82
1:D:3502:GLU:HB2	1:D:3505:PRO:HG2	1.59	0.82
1:A:391:LEU:HD23	1:A:392:PRO:HD2	1.60	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1507:LEU:HD22	1:B:1522:MET:HE3	1.61	0.82
1:D:3103:VAL:HG22	1:D:3108:LEU:HB3	1.62	0.82
1:B:1391:LEU:HD23	1:B:1392:PRO:HD2	1.61	0.82
1:D:3230:LEU:HG	1:D:3337:ILE:HG13	1.63	0.81
1:B:1208:GLN:HB3	1:B:1232:HIS:CD2	2.14	0.81
1:C:2387:TRP:CZ2	5:C:2701:PGX:H71	2.16	0.81
1:D:3526:GLY:HA3	5:D:3701:PGX:H61	1.62	0.81
1:A:396:ASN:ND2	1:A:401:GLU:HG2	1.95	0.81
1:A:197:MET:HE1	1:A:423:VAL:HA	1.63	0.80
1:D:3273:MET:SD	1:D:3290:GLU:HA	2.20	0.80
1:A:216:ARG:HB3	1:A:220:PHE:CD1	2.17	0.80
1:C:2534:LEU:HD22	5:C:2701:PGX:H182	1.62	0.80
1:A:537:ASN:OD1	1:A:539:ILE:HG23	1.81	0.80
1:A:275:TYR:CE1	1:A:293:GLY:HA3	2.16	0.80
1:B:1103:VAL:HG22	1:B:1108:LEU:HB3	1.64	0.80
1:C:2208:GLN:HB3	1:C:2232:HIS:CD2	2.14	0.80
1:C:2456:ARG:HA	6:C:4117:HOH:O	1.80	0.80
1:A:338:GLY:HA3	1:A:559:ILE:HD13	1.62	0.80
1:B:1338:GLY:HA3	1:B:1559:ILE:HD13	1.63	0.80
1:C:2578:THR:HG22	1:C:2579:SER:N	1.98	0.79
1:B:1178:LEU:HA	1:B:1182:LEU:HD12	1.65	0.79
1:D:3208:GLN:HB3	1:D:3232:HIS:CD2	2.18	0.79
1:D:3578:THR:HG22	1:D:3579:SER:N	1.96	0.79
1:A:322:GLU:HG2	1:B:1052:PHE:N	1.96	0.79
1:D:3182:LEU:O	1:D:3438:ARG:HA	1.82	0.79
1:A:51:GLY:C	1:B:1322:GLU:HG2	2.03	0.79
1:A:419:LEU:O	1:A:423:VAL:HG23	1.82	0.79
1:A:88:THR:O	1:A:91:TYR:HB3	1.83	0.79
1:C:2275:TYR:CE1	1:C:2293:GLY:HA3	2.18	0.78
1:D:3275:TYR:CE1	1:D:3293:GLY:HA3	2.18	0.78
1:A:161:THR:HG21	1:A:165:VAL:O	1.83	0.78
1:A:208:GLN:HB3	1:A:232:HIS:CD2	2.15	0.78
1:D:3312:VAL:HA	1:D:3315:ILE:CD1	2.14	0.78
1:C:2273:MET:SD	1:C:2290:GLU:HA	2.24	0.78
1:A:578:THR:HG22	1:A:579:SER:N	1.98	0.78
1:C:2387:TRP:HZ2	5:C:2701:PGX:H71	1.48	0.78
1:B:1275:TYR:CE1	1:B:1293:GLY:HA3	2.17	0.78
1:A:276:PRO:HD2	1:A:279:ILE:HG13	1.66	0.78
1:B:1088:THR:O	1:B:1091:TYR:HB3	1.84	0.78
1:A:414:LEU:HD11	1:A:419:LEU:HD22	1.66	0.77
1:C:2322:GLU:HG2	1:D:3051:GLY:C	2.03	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1216:ARG:HB3	1:B:1220:PHE:CD1	2.18	0.77
1:B:1182:LEU:O	1:B:1438:ARG:HA	1.84	0.77
1:D:3449:LYS:HA	1:D:3452:ILE:HD12	1.66	0.77
1:D:3161:THR:HG21	1:D:3165:VAL:O	1.83	0.77
1:C:2449:LYS:HA	1:C:2452:ILE:HD12	1.65	0.77
1:D:3149:THR:O	1:D:3378:ALA:HA	1.84	0.77
1:A:185:ARG:HH21	1:A:438:ARG:NE	1.83	0.77
1:B:1553:GLU:OE1	1:B:1553:GLU:HA	1.83	0.77
1:D:3188:ILE:HD12	1:D:3439:ASN:HB2	1.66	0.77
1:D:3414:LEU:HD11	1:D:3419:LEU:HD22	1.67	0.77
1:D:3216:ARG:HB3	1:D:3220:PHE:CD1	2.20	0.77
1:C:2230:LEU:HG	1:C:2337:ILE:HG13	1.67	0.77
1:B:1197:MET:HE1	1:B:1423:VAL:HA	1.65	0.77
1:D:3273:MET:HG3	1:D:3285:PHE:O	1.85	0.77
1:D:3419:LEU:O	1:D:3423:VAL:HG23	1.85	0.77
1:A:525:LEU:O	1:A:528:PRO:HD2	1.85	0.77
1:C:2273:MET:HG3	1:C:2285:PHE:O	1.85	0.77
1:B:1273:MET:SD	1:B:1290:GLU:HA	2.25	0.77
1:B:1504:TYR:HB3	1:B:1505:PRO:HD3	1.67	0.77
1:C:2052:PHE:N	1:D:3322:GLU:HG2	1.99	0.77
1:C:2276:PRO:HD2	1:C:2279:ILE:HG13	1.65	0.77
1:B:1414:LEU:HD11	1:B:1419:LEU:HD22	1.66	0.76
1:D:3525:LEU:O	1:D:3528:PRO:HD2	1.84	0.76
1:C:2216:ARG:HB3	1:C:2220:PHE:CD1	2.19	0.76
1:C:2088:THR:O	1:C:2091:TYR:HB3	1.84	0.76
1:C:2174:SER:OG	1:C:2449:LYS:HE2	1.85	0.76
1:B:1463:LEU:HD12	1:B:1503:LEU:HD12	1.67	0.76
1:A:273:MET:HG3	1:A:285:PHE:O	1.84	0.76
1:D:3276:PRO:HD2	1:D:3279:ILE:HG13	1.67	0.76
1:D:3573:LYS:O	1:D:3576:PRO:HD3	1.85	0.76
1:B:1578:THR:HG22	1:B:1579:SER:N	2.01	0.76
1:C:2197:MET:HE1	1:C:2423:VAL:HA	1.67	0.76
1:D:3389:PRO:HB2	1:D:3434:VAL:HG22	1.68	0.76
1:A:403:SER:OG	1:A:406:GLN:HG3	1.86	0.76
1:C:2308:GLU:CB	1:C:2571:ASN:HD21	1.98	0.76
1:B:1276:PRO:HD2	1:B:1279:ILE:HG13	1.68	0.76
1:C:2389:PRO:HB2	1:C:2434:VAL:HG22	1.68	0.76
1:A:308:GLU:CB	1:A:571:ASN:HD21	1.99	0.76
1:B:1105(B):ILE:HG21	1:B:1108:LEU:HD12	1.68	0.76
1:B:1573:LYS:O	1:B:1576:PRO:HD3	1.86	0.76
1:D:3088:THR:O	1:D:3091:TYR:HB3	1.87	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3537:ASN:OD1	1:D:3539:ILE:HG23	1.87	0.75
1:A:497:ASP:HB3	1:A:500:VAL:HG23	1.68	0.75
1:A:430:ILE:HG13	1:A:431:ALA:N	2.00	0.75
1:B:1449:LYS:HA	1:B:1452:ILE:HD12	1.67	0.75
1:A:322:GLU:HG2	1:B:1051:GLY:C	2.06	0.75
1:C:2178:LEU:HA	1:C:2182:LEU:HD12	1.66	0.75
1:C:2244:LEU:O	1:C:2252:LEU:HD23	1.87	0.75
1:C:2497:ASP:HB3	1:C:2500:VAL:HG23	1.69	0.75
1:C:2504:TYR:HB3	1:C:2505:PRO:HD3	1.67	0.75
1:A:534:LEU:HD22	5:A:701:PGX:H182	1.68	0.75
1:B:1510:GLU:O	1:B:1512:PRO:HD3	1.85	0.75
1:C:2553:GLU:OE1	1:C:2553:GLU:HA	1.87	0.75
1:C:2281:GLU:HA	1:C:2284:GLN:HG3	1.69	0.75
1:C:2338:GLY:HA3	1:C:2559:ILE:HD13	1.67	0.75
1:C:2573:LYS:O	1:C:2576:PRO:HD3	1.86	0.75
1:B:1230:LEU:HG	1:B:1337:ILE:HG13	1.68	0.74
1:B:1430:ILE:HG13	1:B:1431:ALA:N	2.02	0.74
1:C:2182:LEU:O	1:C:2438:ARG:HA	1.87	0.74
1:C:2312:VAL:HA	1:C:2315:ILE:CD1	2.16	0.74
1:D:3430:ILE:HG13	1:D:3431:ALA:N	2.02	0.74
1:D:3185:ARG:HH21	1:D:3438:ARG:NE	1.86	0.74
1:D:3463:LEU:HD12	1:D:3503:LEU:HD12	1.69	0.74
1:C:2161:THR:HG21	1:C:2165:VAL:O	1.87	0.74
1:A:553:GLU:HA	1:A:553:GLU:OE1	1.86	0.74
1:D:3497:ASP:HB3	1:D:3500:VAL:HG23	1.68	0.74
1:A:273:MET:SD	1:A:290:GLU:HA	2.27	0.74
1:C:2442:ILE:O	1:C:2445:GLN:HB2	1.87	0.74
1:C:2463:LEU:HD12	1:C:2503:LEU:HD12	1.70	0.74
1:D:3402:TYR:HA	1:D:3406:GLN:OE1	1.87	0.74
1:C:2210:PHE:CE1	1:C:2382:ASN:HA	2.23	0.74
1:B:1161:THR:HG21	1:B:1165:VAL:O	1.88	0.74
1:A:573:LYS:O	1:A:576:PRO:HD3	1.88	0.74
1:A:402:TYR:HA	1:A:406:GLN:OE1	1.87	0.73
1:B:1402:TYR:HA	1:B:1406:GLN:OE1	1.88	0.73
1:D:3197:MET:HE1	1:D:3423:VAL:HA	1.70	0.73
1:A:510:GLU:O	1:A:512:PRO:HD3	1.87	0.73
1:C:2537:ASN:OD1	1:C:2539:ILE:HG23	1.87	0.73
1:C:2185:ARG:HH21	1:C:2438:ARG:NE	1.85	0.73
1:A:178:LEU:HA	1:A:182:LEU:HD12	1.70	0.73
1:B:1185:ARG:HH21	1:B:1438:ARG:NE	1.87	0.73
1:B:1273:MET:HG3	1:B:1285:PHE:O	1.89	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2510:GLU:O	1:C:2512:PRO:HD3	1.86	0.73
1:D:3190:ASP:OD1	1:D:3517:ILE:HB	1.88	0.73
1:A:188:ILE:HD12	1:A:439:ASN:HB2	1.70	0.73
1:B:1442:ILE:O	1:B:1445:GLN:HB2	1.89	0.73
1:A:52:PHE:N	1:B:1322:GLU:HG2	2.03	0.73
1:A:182:LEU:O	1:A:438:ARG:HA	1.89	0.72
1:A:174:SER:OG	1:A:449:LYS:HE2	1.88	0.72
1:D:3504:TYR:HB3	1:D:3505:PRO:HD3	1.70	0.72
1:B:1389:PRO:HB2	1:B:1434:VAL:HG22	1.71	0.72
1:B:1525:LEU:O	1:B:1528:PRO:HD2	1.89	0.72
1:B:1537:ASN:OD1	1:B:1539:ILE:HG23	1.89	0.72
1:D:3178:LEU:HA	1:D:3182:LEU:HD12	1.71	0.72
1:B:1387:TRP:CZ2	5:B:1701:PGX:H71	2.25	0.72
1:D:3510:GLU:O	1:D:3512:PRO:HD3	1.88	0.72
1:A:244:LEU:O	1:A:252:LEU:HD23	1.88	0.72
1:B:1312:VAL:HA	1:B:1315:ILE:CD1	2.16	0.72
1:A:389:PRO:HB2	1:A:434:VAL:HG22	1.70	0.72
1:D:3442:ILE:O	1:D:3445:GLN:HB2	1.88	0.72
1:C:2178:LEU:O	1:C:2182:LEU:HB2	1.90	0.72
1:C:2402:TYR:HA	1:C:2406:GLN:OE1	1.89	0.72
1:A:312:VAL:HA	1:A:315:ILE:CD1	2.15	0.72
1:C:2188:ILE:HD12	1:C:2439:ASN:HB2	1.72	0.72
1:B:1210:PHE:CE1	1:B:1382:ASN:HA	2.25	0.72
1:A:527:ALA:HB3	1:A:528:PRO:HD3	1.72	0.72
1:C:2525:LEU:O	1:C:2528:PRO:HD2	1.89	0.72
1:C:2414:LEU:HD11	1:C:2419:LEU:HD22	1.69	0.72
1:B:1178:LEU:O	1:B:1182:LEU:HB2	1.90	0.72
1:C:2430:ILE:HG13	1:C:2431:ALA:N	2.04	0.72
1:C:2184:ARG:HB2	1:C:2439:ASN:C	2.10	0.72
1:B:1534:LEU:HD22	5:B:1701:PGX:H182	1.71	0.72
1:D:3385:TYR:HA	5:D:3701:PGX:O4	1.89	0.72
1:B:1149:THR:O	1:B:1378:ALA:HA	1.90	0.72
1:A:449:LYS:HA	1:A:452:ILE:HD12	1.69	0.71
1:D:3311:ARG:HB2	6:D:4149:HOH:O	1.90	0.71
1:B:1308:GLU:CB	1:B:1571:ASN:HD21	2.02	0.71
1:A:442:ILE:O	1:A:445:GLN:HB2	1.90	0.71
1:B:1382:ASN:O	1:B:1385:TYR:HB3	1.91	0.71
1:C:2218:PRO:HD2	6:C:4099:HOH:O	1.91	0.71
1:B:1497:ASP:HB3	1:B:1500:VAL:HG23	1.72	0.71
1:D:3553:GLU:OE1	1:D:3553:GLU:HA	1.89	0.71
1:C:2527:ALA:HB3	1:C:2528:PRO:HD3	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1244:LEU:HD23	1:B:1271:VAL:HG21	1.71	0.70
1:A:232:HIS:O	1:A:288:GLY:HA3	1.90	0.70
1:A:454:GLN:HA	1:A:457:GLU:OE2	1.91	0.70
1:D:3527:ALA:HB3	1:D:3528:PRO:HD3	1.73	0.70
1:C:2335:ILE:HA	1:C:2559:ILE:HD11	1.72	0.70
1:A:190:ASP:OD1	1:A:517:ILE:HB	1.91	0.70
1:B:1403:SER:OG	1:B:1406:GLN:HG3	1.91	0.70
1:D:3387:TRP:CZ2	5:D:3701:PGX:H121	2.27	0.70
1:D:3501:MET:HE3	1:D:3505:PRO:HB2	1.73	0.70
1:D:3308:GLU:CB	1:D:3571:ASN:HD21	2.03	0.70
1:A:404:PHE:HB2	1:A:405:LYS:HE3	1.74	0.70
1:B:1188:ILE:HD12	1:B:1439:ASN:HB2	1.72	0.70
1:B:1293:GLY:HA2	1:B:1299:MET:CE	2.22	0.70
1:D:3563:SER:OG	1:D:3565:GLN:HB3	1.90	0.70
1:B:1385:TYR:HB2	5:B:1701:PGX:H101	1.73	0.70
1:A:230:LEU:HG	1:A:337:ILE:HG13	1.73	0.70
1:D:3138:SER:O	1:D:3141:ALA:HB3	1.92	0.70
1:C:2377:ILE:HA	6:C:4133:HOH:O	1.92	0.70
1:D:3454:GLN:HA	1:D:3457:GLU:OE2	1.92	0.70
1:C:2274:ILE:HG13	1:C:2290:GLU:O	1.92	0.69
1:A:385:TYR:O	1:A:387:TRP:N	2.25	0.69
1:B:1184:ARG:HB2	1:B:1439:ASN:C	2.12	0.69
1:D:3178:LEU:O	1:D:3182:LEU:HB2	1.90	0.69
1:C:2190:ASP:OD1	1:C:2517:ILE:HB	1.92	0.69
1:B:1513:ARG:CZ	1:B:1520:GLU:HA	2.22	0.69
1:D:3513:ARG:CZ	1:D:3520:GLU:HA	2.22	0.69
1:B:1281:GLU:HA	1:B:1284:GLN:HG3	1.74	0.69
1:C:2404:PHE:HB2	1:C:2405:LYS:HE3	1.74	0.69
1:B:1404:PHE:HB2	1:B:1405:LYS:HE3	1.72	0.69
1:D:3350:GLN:NE2	1:D:3358:LYS:HA	2.08	0.69
1:A:335:ILE:HA	1:A:559:ILE:HD11	1.74	0.69
1:C:2350:GLN:NE2	1:C:2358:LYS:HA	2.06	0.69
1:A:350:GLN:NE2	1:A:358:LYS:HA	2.08	0.69
1:A:281:GLU:HA	1:A:284:GLN:HG3	1.74	0.69
1:B:1275:TYR:CE2	1:B:1284:GLN:HA	2.28	0.69
1:C:2149:THR:O	1:C:2378:ALA:HA	1.92	0.69
1:A:524:GLU:HA	1:A:524:GLU:OE2	1.92	0.69
1:A:132:VAL:HG12	1:A:133:HIS:N	2.06	0.69
1:A:210:PHE:CE1	1:A:382:ASN:HA	2.27	0.69
1:B:1206:THR:HG21	5:B:1701:PGX:H111	1.74	0.69
1:B:1244:LEU:O	1:B:1252:LEU:HD23	1.93	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2226:HIS:ND1	1:C:2376:ARG:HD2	2.07	0.69
1:A:184:ARG:HB2	1:A:439:ASN:C	2.12	0.69
1:A:513:ARG:CZ	1:A:520:GLU:HA	2.23	0.69
1:B:1414:LEU:HD11	1:B:1419:LEU:CD2	2.22	0.69
1:C:2148:TYR:HD1	1:C:2377:ILE:HG22	1.58	0.69
1:D:3210:PHE:CE1	1:D:3382:ASN:HA	2.28	0.69
1:C:2322:GLU:OE1	1:D:3049:SER:HB2	1.93	0.69
1:D:3382:ASN:O	1:D:3385:TYR:HB3	1.93	0.68
1:D:3281:GLU:HA	1:D:3284:GLN:HG3	1.75	0.68
1:B:1132:VAL:HG12	1:B:1133:HIS:N	2.07	0.68
1:D:3404:PHE:HB2	1:D:3405:LYS:HE3	1.73	0.68
1:A:184:ARG:HB2	1:A:439:ASN:HA	1.76	0.68
1:B:1274:ILE:HG13	1:B:1290:GLU:O	1.94	0.68
1:C:2180:LYS:O	1:C:2181:VAL:HG13	1.93	0.68
1:A:504:TYR:HB3	1:A:505:PRO:HD3	1.74	0.68
1:B:1203:GLN:CG	1:B:1298:LEU:HD11	2.22	0.68
1:B:1138:SER:O	1:B:1141:ALA:HB3	1.93	0.68
1:C:2385:TYR:O	1:C:2387:TRP:N	2.27	0.68
1:A:463:LEU:HD12	1:A:503:LEU:HD12	1.75	0.68
1:C:2308:GLU:HB2	1:C:2571:ASN:ND2	2.07	0.68
1:A:293:GLY:HA2	1:A:299:MET:CE	2.24	0.68
1:A:178:LEU:O	1:A:182:LEU:HB2	1.94	0.68
1:A:149:THR:O	1:A:378:ALA:HA	1.94	0.68
1:D:3385:TYR:O	1:D:3387:TRP:N	2.26	0.68
1:C:2537:ASN:HB2	6:C:4123:HOH:O	1.93	0.68
1:B:1385:TYR:O	1:B:1387:TRP:N	2.26	0.68
1:D:3534:LEU:HD22	5:D:3701:PGX:H182	1.76	0.68
1:A:501:MET:HE3	1:A:505:PRO:HB2	1.75	0.67
1:B:1179:GLU:HA	1:B:1183:LEU:HD12	1.75	0.67
1:C:2403:SER:OG	1:C:2406:GLN:HG3	1.93	0.67
1:C:2513:ARG:CZ	1:C:2520:GLU:HA	2.24	0.67
1:C:2293:GLY:HA2	1:C:2299:MET:CE	2.24	0.67
1:D:3134:TYR:HD2	1:D:3136:TYR:CE1	2.12	0.67
1:C:2563:SER:OG	1:C:2565:GLN:HB3	1.94	0.67
1:C:2275:TYR:CE2	1:C:2284:GLN:HA	2.30	0.67
1:C:2463:LEU:HD13	1:C:2506:ALA:CB	2.23	0.67
1:A:148:TYR:HD1	1:A:377:ILE:HG22	1.59	0.67
1:B:1190:ASP:OD1	1:B:1517:ILE:HB	1.95	0.67
1:B:1563:SER:OG	1:B:1565:GLN:HB3	1.94	0.67
1:A:89:VAL:HA	1:A:92:ILE:HG13	1.75	0.67
1:B:1419:LEU:O	1:B:1423:VAL:HG23	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2244:LEU:HD23	1:C:2271:VAL:HG21	1.77	0.67
1:A:226:HIS:ND1	1:A:376:ARG:HD2	2.09	0.67
1:C:2382:ASN:O	1:C:2385:TYR:HB3	1.94	0.67
1:A:148:TYR:CD1	1:A:377:ILE:HG22	2.30	0.67
1:D:3179:GLU:HA	1:D:3183:LEU:HD12	1.75	0.67
1:D:3184:ARG:HB2	1:D:3439:ASN:C	2.15	0.66
1:A:381:PHE:CD1	1:A:529:PHE:HB3	2.30	0.66
1:C:2148:TYR:CD1	1:C:2377:ILE:HG22	2.30	0.66
1:C:2150:ARG:HD3	6:C:4134:HOH:O	1.95	0.66
1:A:308:GLU:HB2	1:A:571:ASN:ND2	2.08	0.66
1:B:1425:SER:O	1:B:1428:ARG:HG2	1.95	0.66
1:D:3567:LEU:HD12	1:D:3567:LEU:O	1.96	0.66
1:A:132:VAL:O	1:A:154:PRO:HG3	1.93	0.66
1:B:1463:LEU:HD13	1:B:1506:ALA:CB	2.23	0.66
1:D:3293:GLY:HA2	1:D:3299:MET:CE	2.24	0.66
1:B:1381:PHE:CD1	1:B:1529:PHE:HB3	2.31	0.66
1:D:3148:TYR:HD1	1:D:3377:ILE:HG22	1.60	0.66
1:B:1350:GLN:NE2	1:B:1358:LYS:HA	2.09	0.66
1:A:563:SER:OG	1:A:565:GLN:HB3	1.96	0.66
1:B:1454:GLN:HA	1:B:1457:GLU:OE2	1.95	0.66
1:D:3453:ASP:O	1:D:3456:ARG:HB2	1.96	0.66
1:B:1148:TYR:HD1	1:B:1377:ILE:HG22	1.60	0.66
1:A:263:PRO:HD3	1:A:303:THR:HG23	1.77	0.66
1:A:482:THR:HG22	6:A:4032:HOH:O	1.96	0.66
1:D:3428:ARG:HA	1:D:3582:VAL:HG23	1.78	0.66
1:D:3501:MET:CE	1:D:3505:PRO:HB2	2.26	0.66
1:C:2132:VAL:HG12	1:C:2133:HIS:N	2.10	0.66
1:C:2184:ARG:HB2	1:C:2439:ASN:HA	1.76	0.66
1:B:1174:SER:OG	1:B:1449:LYS:HE2	1.94	0.66
1:D:3176:GLU:OE1	1:D:3180:LYS:HE2	1.96	0.66
1:D:3403:SER:OG	1:D:3406:GLN:HG3	1.95	0.66
1:C:2425:SER:O	1:C:2428:ARG:HG2	1.94	0.66
1:B:1132:VAL:O	1:B:1154:PRO:HG3	1.95	0.66
1:D:3132:VAL:O	1:D:3154:PRO:HG3	1.95	0.66
1:D:3241:GLN:HG3	1:D:3242:HIS:N	2.11	0.66
1:C:2076:THR:O	1:C:2080:LEU:HG	1.96	0.66
1:A:179:GLU:HA	1:A:183:LEU:HD12	1.78	0.66
1:A:453:ASP:O	1:A:456:ARG:HB2	1.96	0.66
1:B:1205:PHE:O	1:B:1208:GLN:HG2	1.96	0.66
1:B:1148:TYR:CD1	1:B:1377:ILE:HG22	2.31	0.66
1:D:3274:ILE:HG13	1:D:3290:GLU:O	1.94	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3180:LYS:O	1:D:3181:VAL:HG13	1.96	0.66
1:C:2280:PRO:HB2	1:C:2282:ASN:OD1	1.95	0.66
1:C:2089:VAL:HA	1:C:2092:ILE:HG13	1.76	0.65
1:D:3174:SER:OG	1:D:3449:LYS:HE2	1.95	0.65
1:B:1527:ALA:HB3	1:B:1528:PRO:HD3	1.77	0.65
1:C:2381:PHE:CD1	1:C:2529:PHE:HB3	2.31	0.65
1:C:2179:GLU:HA	1:C:2183:LEU:HD12	1.78	0.65
1:C:2453:ASP:O	1:C:2456:ARG:HB2	1.96	0.65
1:D:3148:TYR:CD1	1:D:3377:ILE:HG22	2.30	0.65
1:D:3335:ILE:HA	1:D:3559:ILE:HD11	1.78	0.65
1:B:1335:ILE:HA	1:B:1559:ILE:HD11	1.78	0.65
1:C:2524:GLU:OE2	1:C:2524:GLU:HA	1.95	0.65
1:B:1524:GLU:HA	1:B:1524:GLU:OE2	1.97	0.65
1:C:2454:GLN:HA	1:C:2457:GLU:OE2	1.96	0.65
1:A:456:ARG:HA	6:A:4021:HOH:O	1.96	0.65
1:B:1507:LEU:HD22	1:B:1522:MET:HE2	1.77	0.65
1:D:3089:VAL:HA	1:D:3092:ILE:HG13	1.78	0.65
1:D:3226:HIS:ND1	1:D:3376:ARG:HD2	2.12	0.65
1:C:2203:GLN:CG	1:C:2298:LEU:HD11	2.26	0.65
1:C:2238:LEU:HD22	1:C:2242:HIS:NE2	2.11	0.65
1:C:2176:GLU:OE1	1:C:2180:LYS:HE2	1.96	0.65
1:C:2138:SER:O	1:C:2141:ALA:HB3	1.97	0.65
1:B:1206:THR:HA	1:B:1209:PHE:CZ	2.32	0.65
1:B:1532:LYS:O	1:B:1534:LEU:N	2.30	0.65
1:D:3381:PHE:CD1	1:D:3529:PHE:HB3	2.32	0.65
1:D:3306:LEU:HD23	1:D:3306:LEU:C	2.17	0.65
1:A:205:PHE:O	1:A:208:GLN:HG2	1.96	0.65
1:B:1232:HIS:O	1:B:1288:GLY:HA3	1.97	0.65
1:D:3208:GLN:HG3	1:D:3209:PHE:CD1	2.32	0.65
1:D:3414:LEU:HD11	1:D:3419:LEU:CD2	2.26	0.65
1:D:3578:THR:CG2	1:D:3579:SER:N	2.60	0.65
1:A:134:TYR:HD2	1:A:136:TYR:CE1	2.14	0.65
1:C:2567:LEU:O	1:C:2567:LEU:HD12	1.97	0.65
1:C:2232:HIS:O	1:C:2288:GLY:HA3	1.97	0.65
1:C:2388:HIS:HB3	1:C:2444:VAL:HG11	1.79	0.65
1:D:3085:THR:O	1:D:3089:VAL:HG23	1.97	0.65
1:A:428:ARG:HA	1:A:582:VAL:HG23	1.79	0.65
1:C:2428:ARG:HA	1:C:2582:VAL:HG23	1.77	0.65
1:D:3563:SER:HB2	6:D:4157:HOH:O	1.96	0.65
1:A:218:PRO:HD2	6:A:4003:HOH:O	1.97	0.64
1:B:1391:LEU:HD22	1:B:1404:PHE:CZ	2.32	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:388:HIS:HB3	1:A:444:VAL:HG11	1.79	0.64
1:D:3238:LEU:HD22	1:D:3242:HIS:NE2	2.12	0.64
1:A:238:LEU:HD22	1:A:242:HIS:NE2	2.12	0.64
1:D:3388:HIS:HB3	1:D:3444:VAL:HG11	1.80	0.64
1:A:97:LYS:HB2	1:A:356:HIS:CE1	2.32	0.64
1:D:3206:THR:HA	1:D:3209:PHE:CZ	2.32	0.64
1:A:203:GLN:CG	1:A:298:LEU:HD11	2.27	0.64
1:C:2385:TYR:HA	5:C:2701:PGX:O4	1.97	0.64
1:A:389:PRO:CG	1:A:434:VAL:HG13	2.21	0.64
1:A:85:THR:O	1:A:89:VAL:HG23	1.98	0.64
1:B:1176:GLU:OE1	1:B:1180:LYS:HE2	1.97	0.64
1:B:1295:VAL:HB	1:B:1298:LEU:HD22	1.79	0.64
1:B:1229:ASP:OD2	1:B:1231:ASN:HB3	1.98	0.64
1:A:414:LEU:HD11	1:A:419:LEU:CD2	2.27	0.64
1:D:3280:PRO:HB2	1:D:3282:ASN:OD1	1.98	0.64
1:C:2134:TYR:HD2	1:C:2136:TYR:CE1	2.15	0.64
1:A:425:SER:O	1:A:428:ARG:HG2	1.97	0.64
1:C:2532:LYS:O	1:C:2534:LEU:N	2.31	0.64
1:D:3205:PHE:O	1:D:3208:GLN:HG2	1.98	0.64
1:D:3463:LEU:HD13	1:D:3506:ALA:CB	2.24	0.64
1:A:275:TYR:CE2	1:A:284:GLN:HA	2.33	0.64
1:D:3244:LEU:O	1:D:3252:LEU:HD23	1.97	0.64
1:D:3524:GLU:OE2	1:D:3524:GLU:HA	1.96	0.64
1:D:3191:PRO:CD	1:D:3433:ARG:HG3	2.27	0.63
1:D:3130:TYR:HB3	1:D:3134:TYR:O	1.97	0.63
1:A:138:SER:O	1:A:141:ALA:HB3	1.97	0.63
1:B:1238:LEU:HD22	1:B:1242:HIS:NE2	2.13	0.63
1:C:2396:ASN:ND2	1:C:2396:ASN:N	2.45	0.63
1:C:2130:TYR:HB3	1:C:2134:TYR:O	1.98	0.63
1:B:1089:VAL:HA	1:B:1092:ILE:HG13	1.79	0.63
1:D:3244:LEU:HD23	1:D:3271:VAL:HG21	1.79	0.63
1:D:3057:CYS:HB3	1:D:3069:CYS:SG	2.38	0.63
1:A:274:ILE:HG13	1:A:290:GLU:O	1.97	0.63
1:D:3132:VAL:HG12	1:D:3133:HIS:N	2.13	0.63
1:A:245:ARG:NH2	1:A:326:GLU:HG2	2.12	0.63
1:D:3578:THR:HG22	1:D:3579:SER:H	1.61	0.63
1:B:1057:CYS:HB3	1:B:1069:CYS:SG	2.38	0.63
1:B:1184:ARG:HB2	1:B:1439:ASN:HA	1.80	0.63
1:C:2272:GLU:HA	6:C:4108:HOH:O	1.97	0.63
1:B:1203:GLN:HG2	1:B:1298:LEU:CD1	2.27	0.63
1:A:280:PRO:HB2	1:A:282:ASN:OD1	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1567:LEU:HD12	1:B:1567:LEU:O	1.99	0.63
1:C:2226:HIS:CE1	1:C:2376:ARG:HD2	2.34	0.63
1:A:226:HIS:CE1	1:A:376:ARG:HD2	2.33	0.63
1:A:463:LEU:HD13	1:A:506:ALA:CB	2.25	0.63
1:A:241:GLN:HG3	1:A:242:HIS:N	2.14	0.63
1:C:2132:VAL:O	1:C:2154:PRO:HG3	1.97	0.63
1:C:2502:GLU:HB3	6:C:4124:HOH:O	1.99	0.63
1:A:306:LEU:HD23	1:A:306:LEU:C	2.18	0.63
1:A:532:LYS:O	1:A:534:LEU:N	2.31	0.63
1:D:3203:GLN:CG	1:D:3298:LEU:HD11	2.27	0.63
1:B:1465:GLU:OE2	1:B:1465:GLU:HA	1.98	0.63
1:A:208:GLN:HG3	1:A:209:PHE:CD1	2.34	0.63
1:A:391:LEU:HD22	1:A:404:PHE:CZ	2.34	0.63
1:D:3308:GLU:O	1:D:3311:ARG:HB3	1.99	0.62
1:A:465:GLU:HA	1:A:465:GLU:OE2	1.98	0.62
1:C:2578:THR:CG2	1:C:2579:SER:N	2.61	0.62
1:A:180:LYS:O	1:A:181:VAL:HG13	1.99	0.62
1:A:382:ASN:O	1:A:385:TYR:HB3	1.99	0.62
1:A:578:THR:CG2	1:A:579:SER:N	2.61	0.62
1:D:3507:LEU:HD22	1:D:3522:MET:HE2	1.80	0.62
1:B:1245:ARG:NH2	1:B:1326:GLU:HG2	2.09	0.62
1:B:1308:GLU:HB2	1:B:1571:ASN:ND2	2.11	0.62
1:D:3229:ASP:OD2	1:D:3231:ASN:HB3	1.99	0.62
1:B:1447:VAL:HG12	1:B:1448:ALA:N	2.13	0.62
1:D:3275:TYR:CE2	1:D:3284:GLN:HA	2.34	0.62
1:A:118:THR:HA	1:A:121:SER:OG	2.00	0.62
1:C:2391:LEU:HD22	1:C:2404:PHE:CZ	2.34	0.62
1:A:385:TYR:HA	5:A:701:PGX:O4	1.98	0.62
1:B:1510:GLU:OE1	1:B:1519:GLY:HA3	1.98	0.62
1:C:2085:THR:O	1:C:2089:VAL:HG23	2.00	0.62
1:B:1428:ARG:HA	1:B:1582:VAL:HG23	1.80	0.62
1:B:1442:ILE:N	1:B:1442:ILE:HD12	2.15	0.62
1:D:3578:THR:CG2	1:D:3579:SER:H	2.13	0.62
1:A:353:SER:HA	6:A:4023:HOH:O	2.00	0.62
1:C:2205:PHE:O	1:C:2208:GLN:HG2	1.99	0.62
1:D:3184:ARG:NH1	1:D:3441:PRO:HG3	2.13	0.62
1:B:1208:GLN:HG3	1:B:1209:PHE:CD1	2.35	0.62
1:D:3532:LYS:O	1:D:3534:LEU:N	2.33	0.62
1:C:2208:GLN:HG3	1:C:2209:PHE:CD1	2.34	0.62
1:A:327:GLN:NE2	1:B:1136:TYR:CD2	2.68	0.62
1:D:3197:MET:CE	1:D:3423:VAL:HG13	2.29	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3425:SER:O	1:D:3428:ARG:HG2	1.99	0.62
1:C:2245:ARG:NH2	1:C:2326:GLU:HG2	2.11	0.62
1:C:2229:ASP:OD2	1:C:2231:ASN:HB3	2.00	0.62
1:D:3078:ILE:O	1:D:3082:LEU:HD12	2.00	0.62
1:D:3184:ARG:HB2	1:D:3439:ASN:HA	1.82	0.62
1:C:2193:GLY:O	1:C:2582:VAL:HG12	2.00	0.62
1:B:1134:TYR:HD2	1:B:1136:TYR:CE1	2.17	0.62
1:A:76:THR:O	1:A:80:LEU:HG	1.99	0.62
1:C:2131:ASN:ND2	1:C:2147:TYR:CD2	2.68	0.62
1:D:3308:GLU:HB2	1:D:3571:ASN:ND2	2.12	0.61
1:A:136:TYR:HD2	1:B:1327:GLN:NE2	1.98	0.61
1:C:2465:GLU:HA	1:C:2465:GLU:OE2	2.00	0.61
1:A:113:MET:HE3	1:A:117:LEU:HD22	1.82	0.61
1:A:386:HIS:HB3	1:A:388:HIS:CE1	2.36	0.61
1:B:1072:PRO:HG2	1:B:1077:ARG:HE	1.64	0.61
1:C:2198:PHE:CE1	1:C:2352:LEU:HD13	2.35	0.61
1:A:206:THR:HA	1:A:209:PHE:CZ	2.35	0.61
1:A:229:ASP:OD2	1:A:231:ASN:HB3	2.00	0.61
1:D:3232:HIS:O	1:D:3288:GLY:HA3	2.01	0.61
1:D:3454:GLN:O	1:D:3457:GLU:HG3	2.00	0.61
1:D:3245:ARG:NH2	1:D:3326:GLU:HG2	2.14	0.61
1:C:2210:PHE:O	1:C:2211:LYS:HG3	2.01	0.61
1:D:3263:PRO:HD3	1:D:3303:THR:HG23	1.82	0.61
1:B:1226:HIS:ND1	1:B:1376:ARG:HD2	2.15	0.61
1:B:1501:MET:HE3	1:B:1505:PRO:HB2	1.82	0.61
1:B:1387:TRP:HZ2	5:B:1701:PGX:H71	1.65	0.61
1:C:2203:GLN:HG2	1:C:2298:LEU:CD1	2.30	0.61
1:C:2241:GLN:HG3	1:C:2242:HIS:N	2.14	0.61
1:B:1191:PRO:CD	1:B:1433:ARG:HG3	2.29	0.61
1:A:295:VAL:HB	1:A:298:LEU:HD22	1.83	0.61
1:C:2306:LEU:HD23	1:C:2307:ARG:N	2.15	0.61
1:A:130:TYR:HB3	1:A:134:TYR:O	2.00	0.61
1:A:136:TYR:CD2	1:B:1327:GLN:NE2	2.69	0.61
1:A:100:TRP:CD1	1:A:356:HIS:HB2	2.35	0.61
1:A:176:GLU:OE1	1:A:180:LYS:HE2	2.00	0.61
1:C:2074:PHE:HA	1:C:2077:ARG:HG3	1.83	0.61
1:D:3465:GLU:HA	1:D:3465:GLU:OE2	2.00	0.61
1:D:3118:THR:HA	1:D:3121:SER:OG	2.01	0.61
1:C:2385:TYR:HB2	5:C:2701:PGX:H101	1.82	0.60
1:D:3095:HIS:HA	6:D:4153:HOH:O	2.01	0.60
1:C:2339:GLU:O	1:C:2342:LYS:HB3	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3389:PRO:CG	1:D:3434:VAL:HG13	2.26	0.60
1:C:2327:GLN:NE2	1:D:3136:TYR:HD2	1.98	0.60
1:A:396:ASN:N	1:A:396:ASN:ND2	2.45	0.60
1:C:2118:THR:HA	1:C:2121:SER:OG	2.00	0.60
1:B:1454:GLN:O	1:B:1457:GLU:HG3	2.02	0.60
1:B:1171:LEU:HD12	1:B:1502:GLU:OE2	2.01	0.60
1:A:120:ARG:NH1	1:A:527:ALA:HB1	2.16	0.60
1:B:1120:ARG:NH1	1:B:1527:ALA:HB1	2.16	0.60
1:B:1076:THR:O	1:B:1080:LEU:HG	2.01	0.60
1:C:2113:MET:CA	1:C:2116:VAL:HG13	2.32	0.60
1:C:2184:ARG:HB2	1:C:2439:ASN:CA	2.31	0.60
1:B:1210:PHE:O	1:B:1211:LYS:HG3	2.01	0.60
1:B:1197:MET:CE	1:B:1423:VAL:HG13	2.31	0.60
1:C:2327:GLN:NE2	1:D:3136:TYR:CD2	2.70	0.60
1:C:2409:TYR:N	1:C:2409:TYR:CD2	2.69	0.60
1:C:2295:VAL:HB	1:C:2298:LEU:HD22	1.82	0.60
1:D:3347:ASP:O	1:D:3348:TYR:C	2.40	0.60
1:B:1501:MET:CE	1:B:1505:PRO:HB2	2.31	0.60
1:D:3171:LEU:HD12	1:D:3502:GLU:OE2	2.01	0.60
1:D:3203:GLN:HG2	1:D:3298:LEU:CD1	2.29	0.60
1:D:3409:TYR:N	1:D:3409:TYR:CD2	2.68	0.60
1:B:1578:THR:CG2	1:B:1579:SER:N	2.64	0.60
1:B:1562:ALA:HA	6:B:4092:HOH:O	2.01	0.60
1:B:1118:THR:HA	1:B:1121:SER:OG	2.01	0.60
1:C:2414:LEU:HD11	1:C:2419:LEU:CD2	2.31	0.60
1:C:2184:ARG:NH2	1:C:2441:PRO:HD3	2.17	0.60
1:D:3181:VAL:HG12	1:D:3487:MET:HG2	1.84	0.60
1:A:526:GLY:CA	5:A:701:PGX:H61	2.30	0.60
1:D:3295:VAL:HB	1:D:3298:LEU:HD22	1.83	0.60
1:C:2184:ARG:HA	1:C:2438:ARG:O	2.02	0.60
1:A:184:ARG:HB2	1:A:439:ASN:CA	2.31	0.60
1:B:1241:GLN:HG3	1:B:1242:HIS:N	2.15	0.60
1:A:327:GLN:NE2	1:B:1136:TYR:HD2	2.00	0.60
1:D:3072:PRO:HG2	1:D:3077:ARG:HE	1.65	0.60
1:A:203:GLN:HG2	1:A:298:LEU:CD1	2.30	0.60
1:B:1124:ILE:HD11	1:B:1528:PRO:HB2	1.84	0.60
1:B:1453:ASP:O	1:B:1456:ARG:HB2	2.01	0.60
1:A:409:TYR:N	1:A:409:TYR:CD2	2.69	0.60
1:C:2105(C):ILE:HG21	1:C:2108:LEU:HD12	1.84	0.59
1:C:2501:MET:HE3	1:C:2505:PRO:HB2	1.84	0.59
1:A:180:LYS:HD2	1:A:490:GLU:OE1	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1180:LYS:O	1:B:1181:VAL:HG13	2.02	0.59
1:B:1074:PHE:HA	1:B:1077:ARG:HG3	1.84	0.59
1:A:343:ILE:O	1:A:347:ASP:HB2	2.02	0.59
1:A:197:MET:CE	1:A:423:VAL:HG13	2.32	0.59
1:A:389:PRO:HG3	1:A:508:LEU:HD22	1.84	0.59
1:B:1089:VAL:HA	1:B:1092:ILE:CG1	2.32	0.59
1:B:1495:TYR:HE2	1:B:1502:GLU:HG3	1.67	0.59
1:A:244:LEU:HD23	1:A:271:VAL:HG21	1.82	0.59
1:C:2184:ARG:NH1	1:C:2441:PRO:HG3	2.18	0.59
1:B:1193:GLY:O	1:B:1582:VAL:HG12	2.02	0.59
1:B:1184:ARG:HD3	1:B:1187:PHE:CA	2.29	0.59
1:D:3504:TYR:HA	1:D:3507:LEU:HD12	1.84	0.59
1:D:3136:TYR:O	1:D:3136:TYR:HD1	1.85	0.59
1:A:78:ILE:O	1:A:82:LEU:HD12	2.01	0.59
1:B:1267:LYS:O	1:B:1267:LYS:HG2	2.03	0.59
1:C:2306:LEU:C	1:C:2306:LEU:HD23	2.23	0.59
1:A:501:MET:CE	1:A:505:PRO:HB2	2.32	0.59
1:D:3193:GLY:O	1:D:3582:VAL:HG12	2.02	0.59
1:B:1343:ILE:O	1:B:1347:ASP:HB2	2.01	0.59
1:A:276:PRO:O	1:A:279:ILE:HG12	2.02	0.59
1:C:2276:PRO:HD2	1:C:2279:ILE:CG1	2.32	0.59
1:D:3341:ILE:HG23	1:D:3534:LEU:HD12	1.85	0.59
1:B:1213:ASP:HB2	1:B:1222:ARG:HG3	1.85	0.59
1:D:3192:GLN:OE1	1:D:3517:ILE:HG22	2.02	0.59
1:D:3442:ILE:HD12	1:D:3442:ILE:N	2.18	0.59
1:A:293:GLY:HA2	1:A:299:MET:HE3	1.84	0.59
1:B:1130:TYR:HB3	1:B:1134:TYR:O	2.02	0.59
1:D:3076:THR:O	1:D:3080:LEU:HG	2.03	0.59
1:A:57:CYS:HB3	1:A:69:CYS:SG	2.43	0.59
1:D:3447:VAL:HG12	1:D:3448:ALA:N	2.17	0.59
1:C:2578:THR:HG22	1:C:2579:SER:H	1.66	0.59
1:A:306:LEU:HD23	1:A:307:ARG:N	2.18	0.59
1:B:1388:HIS:HB3	1:B:1444:VAL:HG11	1.84	0.59
1:D:3391:LEU:HD22	1:D:3404:PHE:CZ	2.38	0.59
1:D:3184:ARG:NH2	1:D:3441:PRO:HD3	2.18	0.59
1:C:2276:PRO:O	1:C:2279:ILE:HG12	2.03	0.59
1:A:562:ALA:HA	6:A:4043:HOH:O	2.02	0.59
1:B:1554:VAL:HG12	1:B:1555:GLY:N	2.18	0.59
1:C:2495:TYR:HE2	1:C:2502:GLU:HG3	1.67	0.58
1:A:347:ASP:O	1:A:348:TYR:C	2.40	0.58
1:D:3128:PRO:HG3	1:D:3376:ARG:HB2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3495:TYR:HE2	1:D:3502:GLU:HG3	1.68	0.58
1:A:72:PRO:HG2	1:A:77:ARG:HE	1.67	0.58
1:C:2362:ASP:O	1:C:2365:LEU:HG	2.01	0.58
1:D:3427:THR:HG21	1:D:3578:THR:HA	1.85	0.58
1:A:74:PHE:HA	1:A:77:ARG:HG3	1.84	0.58
1:A:362:ASP:O	1:A:365:LEU:HG	2.03	0.58
1:A:269:THR:OG1	1:A:271:VAL:HG23	2.02	0.58
1:C:2347:ASP:O	1:C:2348:TYR:C	2.41	0.58
1:D:3097:LYS:HB2	1:D:3356:HIS:CE1	2.38	0.58
1:C:2097:LYS:HB2	1:C:2356:HIS:CE1	2.37	0.58
1:A:387:TRP:CH2	5:A:701:PGX:H121	2.38	0.58
1:D:3205:PHE:HE2	5:D:3701:PGX:H171	1.68	0.58
1:A:276:PRO:HD2	1:A:279:ILE:CG1	2.34	0.58
1:C:2171:LEU:HD12	1:C:2502:GLU:OE2	2.04	0.58
1:C:2507:LEU:HD21	1:C:2521:THR:HG22	1.85	0.58
1:A:191:PRO:HG3	1:A:433:ARG:NH1	2.18	0.58
1:B:1085:THR:O	1:B:1089:VAL:HG23	2.03	0.58
1:C:2120:ARG:NH1	1:C:2527:ALA:HB1	2.19	0.58
1:A:554:VAL:HG12	1:A:555:GLY:N	2.18	0.58
1:B:1255:GLN:HG2	1:B:1263:PRO:O	2.04	0.58
1:B:1306:LEU:HD23	1:B:1306:LEU:C	2.24	0.58
1:C:2414:LEU:HA	1:C:2422:PHE:HE1	1.67	0.58
1:A:341:ILE:HG23	1:A:534:LEU:HD12	1.86	0.58
1:A:389:PRO:HG2	1:A:434:VAL:CG1	2.26	0.58
1:A:184:ARG:NH1	1:A:441:PRO:HG3	2.19	0.58
1:B:1184:ARG:HB2	1:B:1439:ASN:CA	2.34	0.58
1:D:3269:THR:OG1	1:D:3271:VAL:HG23	2.04	0.58
1:C:2263:PRO:HD3	1:C:2303:THR:HG23	1.83	0.58
1:C:2108:LEU:HD23	1:C:2111:LEU:CD2	2.34	0.58
1:D:3113:MET:CA	1:D:3116:VAL:HG13	2.34	0.58
1:A:128:PRO:CG	1:A:376:ARG:NH1	2.67	0.58
1:B:1180:LYS:HD2	1:B:1490:GLU:OE1	2.04	0.58
1:D:3226:HIS:CE1	1:D:3376:ARG:HD2	2.39	0.58
1:A:193:GLY:O	1:A:582:VAL:HG12	2.03	0.58
1:C:2136:TYR:CD2	1:D:3327:GLN:NE2	2.72	0.58
1:D:3554:VAL:HG12	1:D:3555:GLY:N	2.18	0.58
1:B:1131:ASN:ND2	1:B:1147:TYR:CD2	2.72	0.58
1:B:1192:GLN:OE1	1:B:1517:ILE:HG22	2.04	0.58
1:B:1322:GLU:HA	6:B:4068:HOH:O	2.03	0.58
1:C:2173:ASP:O	1:C:2177:VAL:HG23	2.03	0.58
1:D:3482:THR:C	1:D:3511:LYS:HB2	2.24	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2150:ARG:HH22	1:C:2154:PRO:HA	1.69	0.58
1:A:171:LEU:HD12	1:A:502:GLU:OE2	2.04	0.58
1:A:495:TYR:HE2	1:A:502:GLU:HG3	1.68	0.58
1:D:3507:LEU:CD2	1:D:3521:THR:HG22	2.33	0.58
1:D:3074:PHE:HA	1:D:3077:ARG:HG3	1.86	0.58
1:B:1507:LEU:HD21	1:B:1521:THR:HG22	1.86	0.57
1:B:1244:LEU:CD2	1:B:1271:VAL:HG21	2.35	0.57
1:D:3113:MET:HE3	1:D:3117:LEU:HD22	1.86	0.57
1:A:210:PHE:O	1:A:211:LYS:HG3	2.03	0.57
1:A:388:HIS:N	1:A:389:PRO:HD2	2.19	0.57
1:D:3173:ASP:O	1:D:3177:VAL:HG23	2.03	0.57
1:B:1396:ASN:N	1:B:1396:ASN:ND2	2.51	0.57
1:B:1276:PRO:HD2	1:B:1279:ILE:CG1	2.35	0.57
1:C:2100:TRP:CD1	1:C:2356:HIS:HB2	2.39	0.57
1:A:414:LEU:HA	1:A:422:PHE:HE1	1.64	0.57
1:B:1386:HIS:HB3	1:B:1388:HIS:CE1	2.39	0.57
1:B:1293:GLY:HA2	1:B:1299:MET:HE3	1.87	0.57
1:D:3343:ILE:O	1:D:3347:ASP:HB2	2.05	0.57
1:A:113:MET:CA	1:A:116:VAL:HG13	2.34	0.57
1:D:3338:GLY:HA3	1:D:3559:ILE:CD1	2.31	0.57
1:B:1078:ILE:O	1:B:1082:LEU:HD12	2.04	0.57
1:B:1280:PRO:HB2	1:B:1282:ASN:OD1	2.04	0.57
1:C:2183:LEU:HD21	1:C:2445:GLN:HG3	1.86	0.57
1:C:2124:ILE:HD11	1:C:2528:PRO:HB2	1.85	0.57
1:A:267:LYS:HG2	1:A:267:LYS:O	2.03	0.57
1:C:2089:VAL:HA	1:C:2092:ILE:CG1	2.33	0.57
1:C:2201:PHE:O	1:C:2202:ALA:C	2.43	0.57
1:C:2206:THR:HA	1:C:2209:PHE:CZ	2.40	0.57
1:C:2386:HIS:HB3	1:C:2388:HIS:CE1	2.40	0.57
1:B:1097:LYS:HB2	1:B:1356:HIS:CE1	2.39	0.57
1:D:3205:PHE:CE2	1:D:3209:PHE:HZ	2.23	0.57
1:B:1427:THR:HG21	1:B:1578:THR:HA	1.85	0.57
1:A:94:THR:HG22	1:A:354:GLY:O	2.04	0.57
1:C:2507:LEU:CD2	1:C:2521:THR:HG22	2.35	0.57
1:C:2578:THR:CG2	1:C:2579:SER:H	2.17	0.57
1:A:183:LEU:HD21	1:A:445:GLN:HG3	1.87	0.57
1:D:3191:PRO:HG3	1:D:3433:ARG:NH1	2.19	0.57
1:C:2072:PRO:HG2	1:C:2077:ARG:HE	1.70	0.57
1:C:2530:SER:OG	5:C:2701:PGX:H162	2.05	0.57
1:D:3507:LEU:HD21	1:D:3521:THR:HG22	1.87	0.57
1:A:49:SER:HB2	1:B:1322:GLU:OE1	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3131:ASN:ND2	1:D:3147:TYR:CD2	2.72	0.57
1:B:1263:PRO:HD3	1:B:1303:THR:HG23	1.87	0.57
1:B:1308:GLU:O	1:B:1311:ARG:HB3	2.05	0.57
1:C:2388:HIS:N	1:C:2389:PRO:HD2	2.19	0.57
1:C:2180:LYS:HD2	1:C:2490:GLU:OE1	2.04	0.57
1:D:3108:LEU:HD23	1:D:3111:LEU:CD2	2.35	0.57
1:A:578:THR:HG22	1:A:579:SER:H	1.68	0.57
1:B:1464:ASN:OD1	1:B:1499:ASP:HA	2.05	0.57
1:D:3386:HIS:HB3	1:D:3388:HIS:CE1	2.39	0.57
1:D:3124:ILE:HD11	1:D:3528:PRO:HB2	1.87	0.57
1:A:504:TYR:HA	1:A:507:LEU:HD12	1.87	0.57
1:D:3188:ILE:HD12	1:D:3439:ASN:CB	2.34	0.57
1:D:3210:PHE:O	1:D:3211:LYS:HG3	2.05	0.57
1:D:3454:GLN:HA	1:D:3457:GLU:HG3	1.87	0.57
1:D:3396:ASN:ND2	1:D:3396:ASN:N	2.51	0.57
1:A:108:LEU:HD23	1:A:111:LEU:CD2	2.35	0.56
1:B:1173:ASP:O	1:B:1177:VAL:HG23	2.05	0.56
1:D:3184:ARG:HD3	1:D:3187:PHE:CA	2.34	0.56
1:C:2234:TYR:CE1	1:C:2252:LEU:HD11	2.40	0.56
1:D:3362:ASP:O	1:D:3365:LEU:HG	2.05	0.56
1:C:2554:VAL:HG12	1:C:2555:GLY:N	2.20	0.56
1:C:2113:MET:HA	1:C:2116:VAL:HG13	1.87	0.56
1:C:2389:PRO:CB	1:C:2434:VAL:HG22	2.35	0.56
1:D:3235:GLY:HA3	1:D:3240:ARG:HG2	1.86	0.56
1:B:1537:ASN:HB2	6:B:4076:HOH:O	2.04	0.56
1:D:3120:ARG:NH1	1:D:3527:ALA:HB1	2.19	0.56
1:B:1347:ASP:O	1:B:1348:TYR:C	2.43	0.56
1:B:1108:LEU:HD23	1:B:1111:LEU:CD2	2.35	0.56
1:C:2078:ILE:O	1:C:2082:LEU:HD12	2.04	0.56
1:C:2094:THR:HG22	1:C:2354:GLY:O	2.05	0.56
1:A:567:LEU:HD12	1:A:567:LEU:O	2.04	0.56
1:C:2113:MET:HE3	1:C:2117:LEU:HD22	1.87	0.56
1:C:2211:LYS:NZ	1:C:2236:GLU:HG3	2.20	0.56
1:C:2389:PRO:CG	1:C:2434:VAL:HG13	2.29	0.56
1:A:211:LYS:NZ	1:A:236:GLU:HG3	2.21	0.56
1:A:184:ARG:NH2	1:A:441:PRO:HD3	2.19	0.56
1:B:1211:LYS:NZ	1:B:1236:GLU:HG3	2.20	0.56
1:D:3089:VAL:HA	1:D:3092:ILE:CG1	2.34	0.56
1:C:2408:LEU:HD13	1:C:2409:TYR:CE2	2.41	0.56
1:D:3276:PRO:O	1:D:3279:ILE:HG12	2.05	0.56
1:B:1578:THR:HG22	1:B:1579:SER:H	1.69	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:582:VAL:O	1:A:582:VAL:HG13	2.06	0.56
1:B:1265:THR:HG23	1:B:1268:ASP:OD2	2.05	0.56
1:C:2057:CYS:HB3	1:C:2069:CYS:SG	2.45	0.56
1:A:89:VAL:HA	1:A:92:ILE:CG1	2.35	0.56
1:C:2305:TRP:O	1:C:2308:GLU:HB3	2.05	0.56
1:D:3281:GLU:HB3	6:D:4185:HOH:O	2.05	0.56
1:B:1034:ASN:HB3	1:B:1037:CYS:SG	2.46	0.56
1:D:3293:GLY:HA2	1:D:3299:MET:HE3	1.87	0.56
1:A:161:THR:HG23	1:A:165:VAL:HA	1.87	0.56
1:C:2192:GLN:OE1	1:C:2517:ILE:HG22	2.05	0.56
1:A:213:ASP:HB2	1:A:222:ARG:HG3	1.88	0.56
1:C:2389:PRO:HG3	1:C:2508:LEU:HD22	1.87	0.56
1:C:2507:LEU:HD22	1:C:2522:MET:HE2	1.87	0.56
1:B:1454:GLN:HA	1:B:1457:GLU:HG3	1.86	0.56
1:B:1409:TYR:CD2	1:B:1409:TYR:N	2.70	0.56
1:A:447:VAL:HG12	1:A:448:ALA:N	2.20	0.56
1:A:131:ASN:ND2	1:A:147:TYR:CD2	2.73	0.56
1:B:1305:TRP:O	1:B:1308:GLU:HB3	2.06	0.56
1:D:3116:VAL:HA	1:D:3119:SER:OG	2.06	0.56
1:D:3357:PHE:CE2	1:D:3359:LEU:HD23	2.41	0.56
1:B:1184:ARG:NH2	1:B:1441:PRO:HD3	2.20	0.56
1:D:3238:LEU:HD23	1:D:3241:GLN:HG2	1.88	0.56
1:D:3331:THR:O	1:D:3335:ILE:HD12	2.05	0.56
1:D:3113:MET:C	1:D:3116:VAL:HG13	2.25	0.56
1:A:184:ARG:HA	1:A:438:ARG:O	2.05	0.56
1:B:1226:HIS:CE1	1:B:1376:ARG:HD2	2.40	0.56
1:D:3451:SER:HB2	1:D:3504:TYR:CE2	2.40	0.56
1:D:3105(D):ILE:HG21	1:D:3108:LEU:HD12	1.86	0.56
1:A:463:LEU:HG	1:A:463:LEU:O	2.04	0.56
1:D:3389:PRO:HG3	1:D:3508:LEU:HD22	1.87	0.56
1:B:1408:LEU:HD13	1:B:1409:TYR:CE2	2.40	0.56
1:C:2128:PRO:CG	1:C:2376:ARG:NH1	2.68	0.56
1:C:2184:ARG:HD3	1:C:2187:PHE:CA	2.33	0.56
1:C:2454:GLN:HA	1:C:2457:GLU:HG3	1.88	0.56
1:C:2499:ASP:O	1:C:2501:MET:N	2.38	0.56
1:A:128:PRO:HG2	1:A:376:ARG:NH1	2.20	0.56
1:A:128:PRO:HG3	1:A:376:ARG:HB2	1.87	0.56
1:B:1388:HIS:N	1:B:1389:PRO:HD2	2.21	0.56
1:B:1405:LYS:H	1:B:1405:LYS:CD	2.18	0.56
1:B:1184:ARG:HA	1:B:1438:ARG:O	2.06	0.56
1:C:2329:PHE:HD2	1:C:2330:GLN:HG2	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3161:THR:HG23	1:D:3165:VAL:HA	1.87	0.56
1:A:362:ASP:OD1	1:A:364:GLU:HB2	2.06	0.56
1:D:3364:GLU:HA	1:D:3367:PHE:CD1	2.41	0.56
1:C:2265:THR:HG23	1:C:2268:ASP:OD2	2.06	0.56
1:B:1362:ASP:O	1:B:1365:LEU:HG	2.05	0.56
1:A:454:GLN:HA	1:A:457:GLU:HG3	1.86	0.55
1:D:3428:ARG:O	1:D:3430:ILE:N	2.39	0.55
1:D:3582:VAL:HG13	1:D:3582:VAL:O	2.06	0.55
1:C:2267:LYS:O	1:C:2267:LYS:HG2	2.05	0.55
1:A:308:GLU:O	1:A:311:ARG:HB3	2.07	0.55
1:B:1428:ARG:O	1:B:1430:ILE:N	2.38	0.55
1:D:3463:LEU:HB2	1:D:3503:LEU:HA	1.88	0.55
1:B:1113:MET:HE3	1:B:1117:LEU:HD22	1.89	0.55
1:A:578:THR:CG2	1:A:579:SER:H	2.18	0.55
1:D:3185:ARG:HH21	1:D:3438:ARG:CD	2.20	0.55
1:D:3457:GLU:C	1:D:3459:LYS:H	2.10	0.55
1:C:2113:MET:HB2	1:C:2357:PHE:HZ	1.71	0.55
1:C:2343:ILE:O	1:C:2347:ASP:HB2	2.05	0.55
1:C:2501:MET:CE	1:C:2505:PRO:HB2	2.36	0.55
1:D:3389:PRO:CB	1:D:3434:VAL:HG22	2.36	0.55
1:B:1116:VAL:HA	1:B:1119:SER:OG	2.07	0.55
1:A:372:GLN:HE22	1:B:1373:TYR:H	1.52	0.55
1:C:2191:PRO:HG3	1:C:2433:ARG:NH1	2.21	0.55
1:C:2442:ILE:HD12	1:C:2442:ILE:N	2.22	0.55
1:A:104:ASN:ND2	1:A:358:LYS:HB2	2.20	0.55
1:B:1238:LEU:HD23	1:B:1241:GLN:HG2	1.89	0.55
1:B:1113:MET:C	1:B:1116:VAL:HG13	2.26	0.55
1:C:2447:VAL:HG12	1:C:2448:ALA:N	2.20	0.55
1:D:3113:MET:HE3	1:D:3116:VAL:HG22	1.87	0.55
1:A:185:ARG:HH21	1:A:438:ARG:CZ	2.20	0.55
1:B:1184:ARG:CD	1:B:1187:PHE:HA	2.32	0.55
1:D:3274:ILE:HG13	1:D:3290:GLU:C	2.27	0.55
1:D:3211:LYS:NZ	1:D:3236:GLU:HG3	2.21	0.55
1:D:3513:ARG:NH2	1:D:3520:GLU:HB2	2.22	0.55
1:D:3134:TYR:HD2	1:D:3136:TYR:HE1	1.54	0.55
1:B:1578:THR:CG2	1:B:1579:SER:H	2.20	0.55
1:C:2489:ALA:HB2	6:C:4140:HOH:O	2.05	0.55
1:C:2198:PHE:CZ	1:C:2352:LEU:HD13	2.42	0.55
1:C:2308:GLU:O	1:C:2311:ARG:HB3	2.07	0.55
1:B:1113:MET:HB2	1:B:1357:PHE:HZ	1.72	0.55
1:B:1039:ASN:N	1:B:1040:PRO:CD	2.69	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3339:GLU:O	1:D:3342:LYS:HB3	2.07	0.55
1:C:2128:PRO:HG3	1:C:2376:ARG:HB2	1.89	0.55
1:A:454:GLN:O	1:A:457:GLU:HG3	2.07	0.55
1:C:2121:SER:O	1:C:2123:LEU:N	2.40	0.55
1:A:191:PRO:CD	1:A:433:ARG:HG3	2.30	0.55
1:A:507:LEU:HD22	1:A:522:MET:HE2	1.89	0.55
1:D:3208:GLN:NE2	1:D:3232:HIS:NE2	2.55	0.55
1:D:3184:ARG:HB2	1:D:3439:ASN:CA	2.37	0.55
1:D:3464:ASN:OD1	1:D:3499:ASP:HA	2.07	0.55
1:D:3566:SER:HA	1:D:3569:CYS:HB2	1.89	0.55
1:D:3213:ASP:HB2	1:D:3222:ARG:HG3	1.88	0.55
1:C:2387:TRP:CH2	5:C:2701:PGX:H121	2.42	0.54
1:A:387:TRP:CZ2	1:A:518:PHE:CZ	2.95	0.54
1:A:405:LYS:H	1:A:405:LYS:CD	2.18	0.54
1:A:435:ALA:HB3	1:A:512:PRO:HG3	1.88	0.54
1:B:1482:THR:C	1:B:1511:LYS:HB2	2.26	0.54
1:B:1357:PHE:CE2	1:B:1359:LEU:HD23	2.42	0.54
1:A:364:GLU:HA	1:A:367:PHE:CD1	2.42	0.54
1:D:3305:TRP:O	1:D:3308:GLU:HB3	2.08	0.54
1:A:308:GLU:HG3	1:A:336:LEU:CD1	2.32	0.54
1:A:387:TRP:CZ2	5:A:701:PGX:H121	2.41	0.54
1:A:451:SER:HB2	1:A:504:TYR:CE2	2.42	0.54
1:B:1582:VAL:O	1:B:1582:VAL:HG13	2.06	0.54
1:C:2208:GLN:NE2	1:C:2232:HIS:NE2	2.56	0.54
1:C:2514:PRO:O	1:C:2515:ASP:HB2	2.07	0.54
1:D:3100:TRP:CD1	1:D:3356:HIS:HB2	2.42	0.54
1:D:3255:GLN:HG2	1:D:3263:PRO:O	2.07	0.54
1:A:184:ARG:HD3	1:A:187:PHE:CA	2.35	0.54
1:B:1380:GLU:HG3	1:B:1460:TYR:HE2	1.72	0.54
1:A:81:LEU:O	1:A:82:LEU:HG	2.07	0.54
1:D:3265:THR:HG23	1:D:3268:ASP:OD2	2.07	0.54
1:C:2185:ARG:HH21	1:C:2438:ARG:CZ	2.19	0.54
1:A:150:ARG:HH22	1:A:154:PRO:HA	1.73	0.54
1:B:1341:ILE:HG23	1:B:1534:LEU:HD12	1.89	0.54
1:B:1463:LEU:O	1:B:1463:LEU:HG	2.08	0.54
1:B:1507:LEU:CD2	1:B:1521:THR:HG22	2.38	0.54
1:B:1113:MET:HE3	1:B:1116:VAL:HG22	1.89	0.54
1:D:3121:SER:O	1:D:3123:LEU:N	2.41	0.54
1:B:1364:GLU:HA	1:B:1367:PHE:CD1	2.42	0.54
1:A:173:ASP:O	1:A:177:VAL:HG23	2.07	0.54
1:B:1379:SER:O	1:B:1382:ASN:HB3	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1504:TYR:HA	1:B:1507:LEU:HD12	1.88	0.54
1:D:3389:PRO:HG2	1:D:3434:VAL:CG1	2.28	0.54
1:C:2547:PRO:HB3	1:C:2553:GLU:N	2.23	0.54
1:C:2253:LYS:O	1:C:2264:PRO:HG3	2.07	0.54
1:A:162:PRO:HG2	1:A:171:LEU:HD23	1.90	0.54
1:B:1274:ILE:HG13	1:B:1290:GLU:C	2.27	0.54
1:D:3352:LEU:HD21	1:D:3387:TRP:CH2	2.42	0.54
1:A:322:GLU:OE1	1:B:1049:SER:HB2	2.07	0.54
1:A:124:ILE:HD11	1:A:528:PRO:HB2	1.89	0.54
1:D:3408:LEU:HD13	1:D:3409:TYR:CE2	2.43	0.54
1:A:39:ASN:N	1:A:39:ASN:HD22	2.05	0.54
1:C:2113:MET:C	1:C:2116:VAL:HG13	2.28	0.54
1:C:2352:LEU:HD21	1:C:2387:TRP:CH2	2.42	0.54
1:A:116:VAL:HA	1:A:119:SER:OG	2.08	0.54
1:B:1389:PRO:HG3	1:B:1508:LEU:HD22	1.90	0.54
1:D:3267:LYS:HG2	1:D:3267:LYS:O	2.06	0.54
1:C:2341:ILE:HG23	1:C:2534:LEU:HD12	1.89	0.54
1:A:201:PHE:O	1:A:202:ALA:C	2.46	0.54
1:C:2096:PHE:CD1	1:C:2096:PHE:N	2.75	0.54
1:A:403:SER:N	1:A:406:GLN:OE1	2.41	0.54
1:B:1191:PRO:HG3	1:B:1433:ARG:NH1	2.23	0.54
1:B:1463:LEU:HB2	1:B:1503:LEU:HA	1.89	0.54
1:B:1482:THR:HG22	6:B:4081:HOH:O	2.07	0.54
1:D:3208:GLN:O	1:D:3211:LYS:HD3	2.08	0.54
1:A:407:PHE:HZ	1:A:426:PHE:HZ	1.54	0.54
1:C:2128:PRO:HG2	1:C:2376:ARG:NH1	2.23	0.54
1:C:2352:LEU:HD21	1:C:2387:TRP:HH2	1.72	0.54
1:A:357:PHE:CE2	1:A:359:LEU:HD23	2.43	0.54
1:D:3184:ARG:HH12	1:D:3441:PRO:HG3	1.72	0.54
1:C:2136:TYR:HD2	1:D:3327:GLN:NE2	2.05	0.54
1:B:1306:LEU:HD23	1:B:1307:ARG:N	2.23	0.54
1:C:2104:ASN:ND2	1:C:2358:LYS:HB2	2.23	0.54
1:C:2191:PRO:CD	1:C:2433:ARG:HG3	2.29	0.54
1:C:2526:GLY:O	1:C:2530:SER:HB3	2.07	0.54
1:A:568:ILE:HG23	1:A:572:VAL:HG21	1.90	0.54
1:A:457:GLU:C	1:A:459:LYS:H	2.11	0.54
1:B:1482:THR:HB	1:B:1484:GLU:HG3	1.90	0.54
1:D:3219:GLY:HA2	1:D:3458:MET:HE1	1.89	0.54
1:D:3396:ASN:HD22	1:D:3401:GLU:HG2	1.72	0.54
1:B:1201:PHE:O	1:B:1202:ALA:C	2.45	0.54
1:B:1113:MET:CA	1:B:1116:VAL:HG13	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2582:VAL:HG13	1:C:2582:VAL:O	2.08	0.54
1:B:1072:PRO:HG2	1:B:1077:ARG:NE	2.23	0.54
1:C:2152:LEU:HB2	1:C:2466:TYR:CE1	2.43	0.54
1:C:2113:MET:HE3	1:C:2116:VAL:HG22	1.90	0.53
1:C:2357:PHE:CE2	1:C:2359:LEU:HD23	2.42	0.53
1:C:2435:ALA:HB3	1:C:2512:PRO:HG3	1.90	0.53
1:A:113:MET:C	1:A:116:VAL:HG13	2.28	0.53
1:A:113:MET:HA	1:A:116:VAL:HG13	1.90	0.53
1:A:463:LEU:HB2	1:A:503:LEU:HA	1.88	0.53
1:D:3405:LYS:H	1:D:3405:LYS:CD	2.22	0.53
1:D:3467:ARG:NH1	1:D:3520:GLU:OE1	2.37	0.53
1:C:2238:LEU:HD23	1:C:2241:GLN:HG2	1.90	0.53
1:B:1573:LYS:HB2	6:B:4063:HOH:O	2.07	0.53
1:B:1161:THR:HG23	1:B:1165:VAL:HA	1.90	0.53
1:C:2048:MET:HA	6:C:4104:HOH:O	2.07	0.53
1:A:339:GLU:O	1:A:342:LYS:HB3	2.08	0.53
1:C:2142:PHE:CE2	1:D:3538:PRO:HG3	2.43	0.53
1:C:2099:VAL:HG12	1:C:2100:TRP:N	2.23	0.53
1:A:389:PRO:CB	1:A:434:VAL:HG22	2.37	0.53
1:A:454:GLN:O	1:A:457:GLU:N	2.41	0.53
1:B:1184:ARG:NH1	1:B:1441:PRO:HG3	2.23	0.53
1:B:1208:GLN:NE2	1:B:1232:HIS:NE2	2.57	0.53
1:D:3482:THR:HB	1:D:3484:GLU:HG3	1.89	0.53
1:B:1121:SER:O	1:B:1123:LEU:N	2.40	0.53
1:C:2088:THR:O	1:C:2092:ILE:HG12	2.08	0.53
1:C:2274:ILE:HG13	1:C:2290:GLU:C	2.27	0.53
1:D:3201:PHE:O	1:D:3202:ALA:C	2.46	0.53
1:A:105(A):ILE:O	1:A:108:LEU:HB2	2.09	0.53
1:A:208:GLN:NE2	1:A:232:HIS:NE2	2.56	0.53
1:A:498:ILE:O	1:A:501:MET:HB2	2.08	0.53
1:C:2308:GLU:CA	1:C:2571:ASN:HD21	2.20	0.53
1:D:3276:PRO:HD2	1:D:3279:ILE:CG1	2.36	0.53
1:A:330:GLN:HE22	1:B:1140:GLU:HB2	1.73	0.53
1:C:2405:LYS:H	1:C:2405:LYS:CD	2.20	0.53
1:C:2457:GLU:C	1:C:2459:LYS:H	2.11	0.53
1:C:2463:LEU:HB2	1:C:2503:LEU:HA	1.90	0.53
1:D:3108:LEU:O	1:D:3112:ILE:HG12	2.08	0.53
1:A:232:HIS:O	1:A:288:GLY:CA	2.55	0.53
1:A:380:GLU:HG3	1:A:460:TYR:HE2	1.73	0.53
1:A:530:SER:HB2	5:A:701:PGX:H161	1.89	0.53
1:A:88:THR:O	1:A:92:ILE:HG12	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1128:PRO:HG3	1:B:1376:ARG:HB2	1.90	0.53
1:B:1188:ILE:HD12	1:B:1439:ASN:CB	2.38	0.53
1:B:1403:SER:N	1:B:1406:GLN:OE1	2.41	0.53
1:B:1457:GLU:C	1:B:1459:LYS:H	2.11	0.53
1:D:3180:LYS:HD2	1:D:3490:GLU:OE1	2.08	0.53
1:D:3481:LEU:CD1	1:D:3510:GLU:HA	2.39	0.53
1:B:1362:ASP:OD1	1:B:1364:GLU:HB2	2.08	0.53
1:D:3039:ASN:N	1:D:3039:ASN:HD22	2.06	0.53
1:C:2116:VAL:HA	1:C:2119:SER:OG	2.09	0.53
1:A:105(A):ILE:HG22	1:A:105(A):ILE:O	2.08	0.53
1:D:3388:HIS:N	1:D:3389:PRO:HD2	2.24	0.53
1:D:3184:ARG:HA	1:D:3438:ARG:O	2.09	0.53
1:B:1329:PHE:HD2	1:B:1330:GLN:HG2	1.74	0.53
1:B:1105(B):ILE:CG2	1:B:1108:LEU:HD12	2.38	0.53
1:C:2039:ASN:N	1:C:2039:ASN:HD22	2.05	0.53
1:B:1254:TYR:C	1:B:1254:TYR:HD1	2.12	0.53
1:C:2188:ILE:HD12	1:C:2439:ASN:CB	2.39	0.53
1:C:2206:THR:HG21	5:C:2701:PGX:H111	1.90	0.53
1:B:1388:HIS:O	1:B:1391:LEU:HB2	2.09	0.53
1:D:3377:ILE:HG13	6:D:4180:HOH:O	2.08	0.53
1:D:3329:PHE:CD2	1:D:3329:PHE:C	2.82	0.53
1:C:2244:LEU:CD2	1:C:2271:VAL:HG21	2.38	0.53
1:C:2255:GLN:HG2	1:C:2263:PRO:O	2.09	0.53
1:C:2380:GLU:HG3	1:C:2460:TYR:HE2	1.74	0.53
1:C:2482:THR:HB	1:C:2484:GLU:HG3	1.90	0.53
1:C:2464:ASN:OD1	1:C:2499:ASP:HA	2.08	0.53
1:A:304:ILE:O	1:A:307:ARG:HB2	2.09	0.53
1:A:261:VAL:O	1:A:307:ARG:NH1	2.42	0.53
1:B:1389:PRO:HG2	1:B:1434:VAL:CG1	2.31	0.53
1:B:1385:TYR:HA	5:B:1701:PGX:O4	2.07	0.53
1:D:3124:ILE:HD11	1:D:3529:PHE:N	2.24	0.53
1:D:3526:GLY:CA	5:D:3701:PGX:H61	2.35	0.53
1:A:566:SER:HA	1:A:569:CYS:HB2	1.90	0.53
1:A:64:PHE:HD2	1:A:70:THR:O	1.91	0.53
1:C:2108:LEU:O	1:C:2112:ILE:HG12	2.09	0.53
1:C:2205:PHE:CE2	1:C:2209:PHE:HZ	2.27	0.53
1:C:2568:ILE:HG23	1:C:2572:VAL:HG21	1.89	0.53
1:A:188:ILE:HD12	1:A:439:ASN:CB	2.37	0.53
1:A:507:LEU:HD21	1:A:521:THR:HG22	1.89	0.53
1:B:1198:PHE:CE1	1:B:1352:LEU:HD13	2.44	0.53
1:D:3403:SER:N	1:D:3406:GLN:OE1	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:245:ARG:HH22	1:A:326:GLU:HA	1.74	0.53
1:A:120:ARG:HD2	1:A:527:ALA:HB1	1.91	0.53
1:A:152:LEU:HB2	1:A:466:TYR:CE1	2.44	0.53
1:D:3407:PHE:HZ	1:D:3426:PHE:HZ	1.57	0.53
1:C:2155:VAL:HG23	1:C:2459:LYS:O	2.09	0.53
1:A:205:PHE:CE2	1:A:209:PHE:HZ	2.26	0.53
1:A:225:GLY:HA3	1:A:229:ASP:OD1	2.07	0.53
1:D:3387:TRP:CH2	5:D:3701:PGX:H121	2.44	0.53
1:D:3414:LEU:HA	1:D:3422:PHE:HE1	1.71	0.53
1:D:3387:TRP:CZ2	1:D:3518:PHE:CZ	2.97	0.53
1:C:2081:LEU:O	1:C:2082:LEU:HG	2.08	0.53
1:A:121:SER:O	1:A:123:LEU:N	2.41	0.53
1:D:3104:ASN:ND2	1:D:3358:LYS:HB2	2.24	0.52
1:A:113:MET:HB2	1:A:357:PHE:HZ	1.74	0.52
1:A:379:SER:O	1:A:382:ASN:HB3	2.08	0.52
1:A:507:LEU:CD2	1:A:521:THR:HG22	2.39	0.52
1:B:1162:PRO:HG2	1:B:1171:LEU:HD23	1.90	0.52
1:D:3128:PRO:CG	1:D:3376:ARG:NH1	2.72	0.52
1:D:3243:LYS:HA	6:D:4189:HOH:O	2.10	0.52
1:B:1105(B):ILE:HG22	1:B:1105(B):ILE:O	2.10	0.52
1:C:2161:THR:HG23	1:C:2165:VAL:HA	1.91	0.52
1:B:1254:TYR:CD1	1:B:1254:TYR:C	2.82	0.52
1:C:2341:ILE:HD13	1:C:2534:LEU:HD12	1.91	0.52
1:B:1467:ARG:NH1	1:B:1520:GLU:OE1	2.41	0.52
1:D:3352:LEU:HD21	1:D:3387:TRP:HH2	1.74	0.52
1:D:3454:GLN:O	1:D:3457:GLU:N	2.42	0.52
1:B:1338:GLY:HA3	1:B:1559:ILE:CD1	2.35	0.52
1:A:124:ILE:HD11	1:A:529:PHE:N	2.24	0.52
1:B:1124:ILE:HD11	1:B:1529:PHE:N	2.25	0.52
1:A:234:TYR:CE1	1:A:252:LEU:HD11	2.44	0.52
1:D:3081:LEU:O	1:D:3082:LEU:HG	2.08	0.52
1:A:265:THR:HG23	1:A:268:ASP:OD2	2.08	0.52
1:A:96:PHE:CD1	1:A:96:PHE:N	2.77	0.52
1:D:3254:TYR:HD1	1:D:3254:TYR:C	2.12	0.52
1:C:2454:GLN:O	1:C:2457:GLU:HG3	2.09	0.52
1:B:1096:PHE:CD1	1:B:1096:PHE:N	2.77	0.52
1:A:347:ASP:O	1:A:350:GLN:HB3	2.09	0.52
1:A:232:HIS:C	1:A:288:GLY:HA3	2.30	0.52
1:B:1182:LEU:C	1:B:1438:ARG:HA	2.29	0.52
1:B:1389:PRO:CG	1:B:1434:VAL:HG13	2.29	0.52
1:D:3088:THR:O	1:D:3092:ILE:HG12	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3435:ALA:HB3	1:D:3512:PRO:HG3	1.91	0.52
1:B:1276:PRO:O	1:B:1279:ILE:HG12	2.08	0.52
1:D:3244:LEU:CD2	1:D:3271:VAL:HG21	2.38	0.52
1:C:2197:MET:CE	1:C:2423:VAL:HG13	2.39	0.52
1:C:2403:SER:N	1:C:2406:GLN:OE1	2.43	0.52
1:C:2498:ILE:HG23	1:C:2499:ASP:N	2.24	0.52
1:B:1435:ALA:HB3	1:B:1512:PRO:HG3	1.90	0.52
1:B:1538:PRO:O	1:B:1540:CYS:N	2.42	0.52
1:D:3495:TYR:CD2	1:D:3501:MET:HA	2.44	0.52
1:C:2308:GLU:HG3	1:C:2336:LEU:CD1	2.33	0.52
1:C:2120:ARG:HD2	1:C:2527:ALA:HB1	1.91	0.52
1:B:1500:VAL:HG12	1:B:1500:VAL:O	2.09	0.52
1:C:2362:ASP:OD1	1:C:2364:GLU:HB2	2.09	0.52
1:D:3039:ASN:N	1:D:3040:PRO:CD	2.72	0.52
1:A:433:ARG:HD3	1:A:436:GLY:H	1.75	0.52
1:B:1389:PRO:CB	1:B:1434:VAL:HG22	2.38	0.52
1:D:3128:PRO:HG2	1:D:3376:ARG:NH1	2.24	0.52
1:D:3162:PRO:HG2	1:D:3171:LEU:HD23	1.92	0.52
1:D:3206:THR:HA	1:D:3209:PHE:CE2	2.44	0.52
1:D:3463:LEU:O	1:D:3463:LEU:HG	2.10	0.52
1:C:2039:ASN:N	1:C:2040:PRO:CD	2.72	0.52
1:D:3254:TYR:CD1	1:D:3254:TYR:C	2.82	0.52
1:B:1566:SER:HA	1:B:1569:CYS:HB2	1.91	0.52
1:C:2407:PHE:HZ	1:C:2426:PHE:HZ	1.58	0.52
1:C:2463:LEU:HG	1:C:2463:LEU:O	2.08	0.52
1:D:3096:PHE:CD1	1:D:3096:PHE:N	2.78	0.52
1:D:3113:MET:CE	1:D:3117:LEU:HD22	2.40	0.52
1:D:3112:ILE:O	1:D:3115:TYR:N	2.43	0.52
1:B:1185:ARG:HH21	1:B:1438:ARG:CZ	2.22	0.52
1:A:235:GLY:HA3	1:A:240:ARG:HG2	1.90	0.52
1:D:3380:GLU:HG3	1:D:3460:TYR:HE2	1.74	0.52
1:D:3363:PRO:C	1:D:3365:LEU:H	2.13	0.52
1:A:39:ASN:N	1:A:40:PRO:CD	2.72	0.52
1:B:1557:LYS:O	1:B:1558:ILE:C	2.47	0.52
1:B:1329:PHE:C	1:B:1329:PHE:CD2	2.82	0.52
1:B:1202:ALA:CA	1:B:1348:TYR:HE1	2.23	0.52
1:D:3050:THR:HG21	1:D:3056:LYS:HB2	1.92	0.52
1:B:1050:THR:HG21	1:B:1056:LYS:HB2	1.90	0.52
1:A:246:LEU:HD23	1:A:251:LYS:HB2	1.91	0.52
1:B:1234:TYR:CE1	1:B:1252:LEU:HD11	2.45	0.52
1:B:1304:ILE:O	1:B:1307:ARG:HB2	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2427:THR:HG21	1:C:2578:THR:HA	1.92	0.52
1:A:464:ASN:OD1	1:A:499:ASP:HA	2.09	0.52
1:A:482:THR:HG23	1:A:509:VAL:HG12	1.92	0.52
1:A:510:GLU:OE1	1:A:519:GLY:HA3	2.10	0.52
1:B:1352:LEU:HD21	1:B:1387:TRP:CH2	2.45	0.52
1:B:1467:ARG:NH1	1:B:1521:THR:OG1	2.42	0.52
1:D:3379:SER:O	1:D:3382:ASN:HB3	2.10	0.52
1:D:3241:GLN:OE1	1:D:3245:ARG:HD2	2.10	0.52
1:C:2349:VAL:HG22	5:C:2701:PGX:O5	2.09	0.52
1:A:255:GLN:HG2	1:A:263:PRO:O	2.09	0.52
1:A:377:ILE:HA	6:A:4037:HOH:O	2.10	0.52
1:A:185:ARG:HH21	1:A:438:ARG:CD	2.22	0.52
1:D:3176:GLU:O	1:D:3177:VAL:C	2.48	0.52
1:A:140:GLU:HB2	1:B:1330:GLN:HE22	1.75	0.52
1:C:2196:MET:CE	1:C:2431:ALA:HB2	2.40	0.52
1:C:2364:GLU:HA	1:C:2367:PHE:CD1	2.44	0.52
1:C:2184:ARG:CD	1:C:2187:PHE:HA	2.35	0.52
1:C:2202:ALA:CA	1:C:2348:TYR:HE1	2.23	0.52
1:C:2347:ASP:O	1:C:2350:GLN:HB3	2.09	0.52
1:D:3306:LEU:HD23	1:D:3307:ARG:N	2.25	0.52
1:A:305:TRP:O	1:A:308:GLU:HB3	2.10	0.52
1:A:308:GLU:CA	1:A:571:ASN:HD21	2.23	0.52
1:A:498:ILE:HG23	1:A:499:ASP:N	2.25	0.52
1:B:1206:THR:HA	1:B:1209:PHE:CE2	2.45	0.52
1:B:1433:ARG:HD3	1:B:1436:GLY:H	1.74	0.52
1:D:3150:ARG:HH22	1:D:3154:PRO:HA	1.75	0.52
1:B:1253:LYS:O	1:B:1264:PRO:HG3	2.10	0.52
1:D:3347:ASP:O	1:D:3350:GLN:N	2.43	0.51
1:B:1232:HIS:C	1:B:1288:GLY:HA3	2.31	0.51
1:C:2330:GLN:HE22	1:D:3140:GLU:HB2	1.75	0.51
1:D:3072:PRO:HG2	1:D:3077:ARG:NE	2.24	0.51
1:A:491:LEU:O	1:A:494:LEU:N	2.42	0.51
1:C:2179:GLU:O	1:C:2181:VAL:N	2.43	0.51
1:B:1099:VAL:HG12	1:B:1100:TRP:N	2.24	0.51
1:D:3225:GLY:HA3	1:D:3229:ASP:OD1	2.10	0.51
1:A:427:THR:HG21	1:A:578:THR:HA	1.91	0.51
1:A:442:ILE:HD12	1:A:442:ILE:N	2.24	0.51
1:A:514:PRO:O	1:A:515:ASP:HB2	2.10	0.51
1:B:1463:LEU:HD12	1:B:1503:LEU:CD1	2.39	0.51
1:B:1577:PHE:C	1:B:1577:PHE:CD2	2.83	0.51
1:C:2198:PHE:CD2	1:C:2198:PHE:C	2.83	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2379:SER:O	1:C:2382:ASN:HB3	2.11	0.51
1:A:261:VAL:H	1:A:307:ARG:NH2	2.07	0.51
1:A:467:ARG:NH1	1:A:521:THR:OG1	2.43	0.51
1:B:1128:PRO:CG	1:B:1376:ARG:NH1	2.74	0.51
1:D:3185:ARG:NH2	6:D:4167:HOH:O	2.43	0.51
1:C:2241:GLN:OE1	1:C:2245:ARG:HD2	2.10	0.51
1:C:2294:LEU:HB3	1:C:2409:TYR:CD2	2.45	0.51
1:A:72:PRO:HG2	1:A:77:ARG:NE	2.25	0.51
1:A:64:PHE:HA	1:A:71:THR:O	2.11	0.51
1:C:2509:VAL:O	1:C:2510:GLU:O	2.28	0.51
1:B:1209:PHE:HB3	1:B:1377:ILE:CD1	2.40	0.51
1:D:3197:MET:HE1	1:D:3423:VAL:HG13	1.92	0.51
1:A:329:PHE:CD2	1:A:329:PHE:C	2.83	0.51
1:B:1152:LEU:HB2	1:B:1466:TYR:CE1	2.46	0.51
1:B:1270:GLN:N	1:B:1270:GLN:OE1	2.43	0.51
1:C:2577:PHE:C	1:C:2577:PHE:CD2	2.83	0.51
1:C:2185:ARG:NH2	6:C:4120:HOH:O	2.44	0.51
1:A:112:ILE:O	1:A:115:TYR:N	2.43	0.51
1:A:526:GLY:O	1:A:530:SER:HB3	2.10	0.51
1:B:1156:ALA:O	1:B:1159:CYS:HB2	2.11	0.51
1:D:3183:LEU:HD21	1:D:3445:GLN:HG3	1.92	0.51
1:A:292:PHE:O	1:A:299:MET:HE2	2.10	0.51
1:D:3568:ILE:HG23	1:D:3572:VAL:HG21	1.92	0.51
1:A:134:TYR:HD2	1:A:136:TYR:HE1	1.57	0.51
1:A:50:THR:CG2	1:A:56:LYS:HB3	2.40	0.51
1:B:1339:GLU:O	1:B:1342:LYS:HB3	2.10	0.51
1:C:2394:THR:O	1:C:2429:GLN:NE2	2.40	0.51
1:A:156:ALA:O	1:A:159:CYS:HB2	2.11	0.51
1:A:209:PHE:N	1:A:209:PHE:CD1	2.78	0.51
1:A:394:THR:HA	1:A:402:TYR:O	2.10	0.51
1:D:3450:ALA:O	1:D:3452:ILE:N	2.43	0.51
1:B:1568:ILE:HG23	1:B:1572:VAL:HG21	1.92	0.51
1:B:1396:ASN:HD22	1:B:1401:GLU:HG2	1.74	0.51
1:B:1120:ARG:HD2	1:B:1527:ALA:HB1	1.92	0.51
1:D:3137:LYS:HD2	6:D:4174:HOH:O	2.10	0.51
1:C:2182:LEU:C	1:C:2438:ARG:HA	2.31	0.51
1:C:2433:ARG:HD3	1:C:2436:GLY:H	1.76	0.51
1:C:2482:THR:HG23	1:C:2509:VAL:HG12	1.91	0.51
1:D:3095:HIS:O	1:D:3097:LYS:N	2.43	0.51
1:A:513:ARG:NH2	1:A:520:GLU:HB2	2.26	0.51
1:B:1444:VAL:CG1	1:B:1444:VAL:O	2.59	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3463:LEU:HD12	1:D:3503:LEU:CD1	2.38	0.51
1:B:1294:LEU:HB3	1:B:1409:TYR:CD2	2.45	0.51
1:C:2547:PRO:O	1:C:2552:GLY:N	2.41	0.51
1:D:3547:PRO:HB3	1:D:3553:GLU:N	2.25	0.51
1:D:3050:THR:CG2	1:D:3056:LYS:HB3	2.41	0.51
1:C:2113:MET:HA	1:C:2116:VAL:CG1	2.41	0.51
1:D:3347:ASP:O	1:D:3350:GLN:HB3	2.11	0.51
1:B:1181:VAL:HG12	1:B:1487:MET:HG2	1.93	0.51
1:D:3156:ALA:O	1:D:3159:CYS:HB2	2.10	0.51
1:A:253:LYS:O	1:A:264:PRO:HG3	2.10	0.51
1:A:547:PRO:HB3	1:A:553:GLU:N	2.26	0.51
1:A:363:PRO:C	1:A:365:LEU:H	2.14	0.51
1:C:2219:GLY:N	1:C:2458:MET:HE2	2.25	0.51
1:C:2185:ARG:HH21	1:C:2438:ARG:CD	2.23	0.51
1:D:3113:MET:HA	1:D:3116:VAL:HG13	1.93	0.51
1:D:3202:ALA:CA	1:D:3348:TYR:HE1	2.23	0.51
1:A:482:THR:HB	1:A:484:GLU:HG3	1.93	0.51
1:A:463:LEU:HD12	1:A:503:LEU:CD1	2.41	0.51
1:B:1208:GLN:O	1:B:1211:LYS:HD3	2.11	0.51
1:D:3509:VAL:O	1:D:3510:GLU:O	2.29	0.51
1:A:428:ARG:O	1:A:430:ILE:N	2.44	0.51
1:C:2566:SER:HA	1:C:2569:CYS:HB2	1.93	0.51
1:C:2232:HIS:C	1:C:2288:GLY:HA3	2.31	0.51
1:B:1183:LEU:HD21	1:B:1445:GLN:HG3	1.93	0.51
1:D:3206:THR:HB	1:D:3210:PHE:CD2	2.46	0.51
1:C:2293:GLY:HA2	1:C:2299:MET:HE3	1.92	0.51
1:C:2124:ILE:HD11	1:C:2529:PHE:N	2.26	0.51
1:D:3465:GLU:OE2	1:D:3468:LYS:CE	2.59	0.51
1:D:3121:SER:C	1:D:3123:LEU:H	2.15	0.51
1:B:1407:PHE:HZ	1:B:1426:PHE:HZ	1.58	0.51
1:A:557:LYS:HA	1:A:560:ASN:HD22	1.76	0.50
1:C:2387:TRP:CZ2	1:C:2518:PHE:CZ	2.99	0.50
1:C:2454:GLN:O	1:C:2457:GLU:N	2.43	0.50
1:C:2463:LEU:HD12	1:C:2503:LEU:CD1	2.40	0.50
1:A:352:LEU:HD21	1:A:387:TRP:CH2	2.46	0.50
1:A:450:ALA:O	1:A:452:ILE:N	2.44	0.50
1:A:433:ARG:HH21	1:A:512:PRO:HB3	1.76	0.50
1:B:1482:THR:HG23	1:B:1509:VAL:HG12	1.93	0.50
1:D:3188:ILE:HB	1:D:3439:ASN:ND2	2.26	0.50
1:D:3433:ARG:HD3	1:D:3436:GLY:H	1.75	0.50
1:D:3526:GLY:O	1:D:3530:SER:HB3	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:238:LEU:HD23	1:A:241:GLN:HG2	1.92	0.50
1:C:2064:PHE:HA	1:C:2071:THR:O	2.11	0.50
1:A:50:THR:HG21	1:A:56:LYS:HB2	1.92	0.50
1:B:1243:LYS:HA	6:B:4095:HOH:O	2.12	0.50
1:A:577:PHE:C	1:A:577:PHE:CD2	2.84	0.50
1:C:2213:ASP:HB2	1:C:2222:ARG:HG3	1.94	0.50
1:A:247:PHE:HA	1:A:325:ASP:OD2	2.12	0.50
1:C:2444:VAL:O	1:C:2444:VAL:CG1	2.60	0.50
1:D:3113:MET:HB2	1:D:3357:PHE:HZ	1.75	0.50
1:A:179:GLU:O	1:A:181:VAL:N	2.44	0.50
1:B:1155:VAL:HG23	1:B:1459:LYS:O	2.11	0.50
1:B:1464:ASN:HD21	1:B:1475:TYR:H	1.59	0.50
1:B:1498:ILE:HG23	1:B:1499:ASP:N	2.26	0.50
1:D:3482:THR:HG23	1:D:3509:VAL:HG12	1.93	0.50
1:B:1120:ARG:O	1:B:1122:TYR:N	2.44	0.50
1:C:2235:GLY:HA3	1:C:2240:ARG:HG2	1.92	0.50
1:B:1363:PRO:C	1:B:1365:LEU:H	2.14	0.50
1:D:3174:SER:O	1:D:3178:LEU:HB2	2.11	0.50
1:D:3514:PRO:O	1:D:3515:ASP:HB2	2.12	0.50
1:C:2363:PRO:C	1:C:2365:LEU:H	2.12	0.50
1:A:329:PHE:HD2	1:A:330:GLN:HG2	1.76	0.50
1:C:2101:ASN:O	1:C:2105:ASN:ND2	2.44	0.50
1:C:2105(C):ILE:HB	1:C:2108:LEU:HB2	1.93	0.50
1:C:2206:THR:HB	1:C:2210:PHE:CE2	2.46	0.50
1:C:2389:PRO:HG2	1:C:2434:VAL:CG1	2.32	0.50
1:D:3099:VAL:HG12	1:D:3100:TRP:N	2.27	0.50
1:A:181:VAL:HG12	1:A:487:MET:HG2	1.93	0.50
1:B:1150:ARG:HH22	1:B:1154:PRO:HA	1.76	0.50
1:A:326:GLU:HB2	6:A:4005:HOH:O	2.10	0.50
1:B:1050:THR:CG2	1:B:1056:LYS:HB3	2.41	0.50
1:C:2121:SER:C	1:C:2123:LEU:H	2.15	0.50
1:C:2270:GLN:OE1	1:C:2270:GLN:N	2.45	0.50
1:C:2219:GLY:HA2	1:C:2458:MET:HE1	1.93	0.50
1:B:1100:TRP:CD1	1:B:1356:HIS:HB2	2.47	0.50
1:D:3300:MET:O	1:D:3304:ILE:HG13	2.12	0.50
1:B:1495:TYR:CD2	1:B:1501:MET:HA	2.46	0.50
1:D:3394:THR:HA	1:D:3402:TYR:O	2.10	0.50
1:B:1347:ASP:O	1:B:1350:GLN:HB3	2.11	0.50
1:D:3500:VAL:HG12	1:D:3500:VAL:O	2.11	0.50
1:C:2202:ALA:HB2	1:C:2348:TYR:CE1	2.47	0.50
1:A:482:THR:C	1:A:511:LYS:HB2	2.31	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1394:THR:HA	1:B:1402:TYR:O	2.12	0.50
1:D:3132:VAL:HG23	6:D:4179:HOH:O	2.12	0.50
1:D:3232:HIS:C	1:D:3288:GLY:HA3	2.32	0.50
1:B:1245:ARG:HD2	1:B:1329:PHE:CE1	2.47	0.50
1:C:2396:ASN:HD22	1:C:2396:ASN:N	2.08	0.50
1:A:546:LYS:HE3	1:B:1137:LYS:NZ	2.26	0.50
1:A:228:VAL:HG23	6:A:4027:HOH:O	2.11	0.50
1:C:2226:HIS:C	1:C:2377:ILE:HD12	2.31	0.50
1:C:2456:ARG:NE	1:C:2502:GLU:OE2	2.44	0.50
1:D:3308:GLU:CA	1:D:3571:ASN:HD21	2.24	0.50
1:C:2095:HIS:O	1:C:2097:LYS:N	2.45	0.50
1:A:384:LEU:HB3	1:A:522:MET:CE	2.42	0.50
1:B:1088:THR:O	1:B:1092:ILE:HG12	2.12	0.50
1:B:1209:PHE:HB3	1:B:1377:ILE:HD11	1.93	0.50
1:D:3134:TYR:CD2	1:D:3136:TYR:HE1	2.29	0.50
1:B:1246:LEU:HD23	1:B:1251:LYS:HB2	1.94	0.50
1:D:3491:LEU:O	1:D:3494:LEU:N	2.45	0.50
1:B:1269:THR:OG1	1:B:1271:VAL:HG23	2.12	0.50
1:A:99:VAL:HG12	1:A:100:TRP:N	2.27	0.50
1:C:2451:SER:HB2	1:C:2504:TYR:CE2	2.46	0.50
1:C:2449:LYS:CA	1:C:2452:ILE:HD12	2.36	0.50
1:C:2464:ASN:ND2	1:C:2475:TYR:H	2.10	0.50
1:A:148:TYR:HB2	1:A:219:GLY:O	2.12	0.50
1:A:182:LEU:C	1:A:438:ARG:HA	2.32	0.50
1:A:198:PHE:CE1	1:A:352:LEU:HD13	2.47	0.50
1:A:331:THR:O	1:A:335:ILE:HD12	2.11	0.50
1:C:2428:ARG:O	1:C:2430:ILE:N	2.45	0.50
1:B:1169:LYS:O	1:B:1170:GLU:HG3	2.12	0.50
1:C:2254:TYR:C	1:C:2254:TYR:HD1	2.15	0.50
1:C:2388:HIS:O	1:C:2391:LEU:HB2	2.11	0.49
1:A:209:PHE:HB3	1:A:377:ILE:CD1	2.41	0.49
1:B:1198:PHE:HA	1:B:1580:PHE:CD2	2.46	0.49
1:B:1113:MET:O	1:B:1116:VAL:HG13	2.12	0.49
1:D:3577:PHE:CD2	1:D:3577:PHE:C	2.84	0.49
1:A:408:LEU:HD13	1:A:409:TYR:CE2	2.46	0.49
1:D:3077:ARG:O	1:D:3081:LEU:HG	2.11	0.49
1:D:3465:GLU:OE2	1:D:3468:LYS:HE2	2.12	0.49
1:A:169:LYS:O	1:A:170:GLU:HG3	2.12	0.49
1:C:2132:VAL:HG23	6:C:4132:HOH:O	2.11	0.49
1:C:2464:ASN:HD21	1:C:2475:TYR:H	1.58	0.49
1:B:1174:SER:O	1:B:1178:LEU:HB2	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:274:ILE:HG13	1:A:290:GLU:C	2.31	0.49
1:D:3196:MET:CE	1:D:3431:ALA:HB2	2.42	0.49
1:B:1108:LEU:O	1:B:1112:ILE:HG12	2.12	0.49
1:B:1151:ALA:HB2	1:B:1529:PHE:HZ	1.77	0.49
1:C:2225:GLY:HA3	1:C:2229:ASP:OD1	2.12	0.49
1:A:43:ASN:ND2	1:A:69:CYS:O	2.45	0.49
1:B:1064:PHE:HA	1:B:1071:THR:O	2.12	0.49
1:C:2246:LEU:HD23	1:C:2251:LYS:HB2	1.94	0.49
1:D:3557:LYS:HA	1:D:3560:ASN:HD22	1.77	0.49
1:B:1308:GLU:CA	1:B:1571:ASN:HD21	2.24	0.49
1:C:2287:VAL:HG23	1:C:2289:GLN:H	1.77	0.49
1:C:2394:THR:HA	1:C:2402:TYR:O	2.12	0.49
1:C:2499:ASP:C	1:C:2501:MET:H	2.15	0.49
1:B:1229:ASP:HA	1:B:1337:ILE:HD11	1.94	0.49
1:B:1196:MET:CE	1:B:1431:ALA:HB2	2.42	0.49
1:B:1347:ASP:O	1:B:1350:GLN:N	2.45	0.49
1:C:2049:SER:HB2	1:D:3322:GLU:OE1	2.13	0.49
1:A:196:MET:CE	1:A:431:ALA:HB2	2.42	0.49
1:A:121:SER:C	1:A:123:LEU:H	2.16	0.49
1:B:1081:LEU:O	1:B:1082:LEU:HG	2.12	0.49
1:D:3087:ASN:HB3	4:D:3702:BOG:H3	1.93	0.49
1:D:3209:PHE:CD1	1:D:3209:PHE:N	2.79	0.49
1:D:3464:ASN:HD21	1:D:3475:TYR:H	1.59	0.49
1:D:3245:ARG:HH22	1:D:3326:GLU:HA	1.78	0.49
1:A:190:ASP:HB2	1:A:517:ILE:HD12	1.94	0.49
1:D:3523:VAL:HG12	1:D:3524:GLU:OE2	2.12	0.49
1:B:1039:ASN:HD22	1:B:1039:ASN:N	2.10	0.49
1:D:3545:TRP:CE3	1:D:3545:TRP:HA	2.47	0.49
1:A:545:TRP:CE3	1:A:545:TRP:HA	2.46	0.49
1:D:3064:PHE:HD2	1:D:3070:THR:O	1.96	0.49
1:C:2435:ALA:O	1:C:2510:GLU:O	2.30	0.49
1:C:2504:TYR:HA	1:C:2507:LEU:HD12	1.93	0.49
1:A:352:LEU:HD21	1:A:387:TRP:HH2	1.78	0.49
1:A:241:GLN:OE1	1:A:245:ARG:HD2	2.11	0.49
1:B:1107:PHE:O	1:B:1111:LEU:HB3	2.12	0.49
1:D:3276:PRO:HG3	1:D:3409:TYR:CD1	2.48	0.49
1:B:1121:SER:C	1:B:1123:LEU:H	2.15	0.49
1:C:2050:THR:HG21	1:C:2056:LYS:HB2	1.94	0.49
1:A:34:ASN:HB3	1:A:37:CYS:SG	2.52	0.49
1:C:2128:PRO:HG3	1:C:2376:ARG:NH1	2.27	0.49
1:C:2150:ARG:NH2	1:C:2154:PRO:HA	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2184:ARG:HH12	1:C:2441:PRO:HG3	1.77	0.49
1:A:302:ALA:O	1:A:303:THR:C	2.51	0.49
1:A:155:VAL:HG23	1:A:459:LYS:O	2.12	0.49
1:A:495:TYR:CD2	1:A:501:MET:HA	2.47	0.49
1:A:90:HIS:CD2	1:A:513:ARG:HG2	2.46	0.49
1:D:3510:GLU:OE1	1:D:3519:GLY:HA3	2.13	0.49
1:D:3131:ASN:C	1:D:3131:ASN:OD1	2.50	0.49
1:D:3064:PHE:HA	1:D:3071:THR:O	2.12	0.49
1:D:3246:LEU:HD23	1:D:3251:LYS:HB2	1.93	0.49
1:D:3557:LYS:O	1:D:3558:ILE:C	2.51	0.49
1:C:2156:ALA:O	1:C:2159:CYS:HB2	2.12	0.49
1:C:2162:PRO:HG2	1:C:2171:LEU:HD23	1.94	0.49
1:C:2209:PHE:HB3	1:C:2377:ILE:HD11	1.94	0.49
1:A:244:LEU:CD2	1:A:271:VAL:HG21	2.42	0.49
1:B:1465:GLU:OE2	1:B:1468:LYS:CE	2.61	0.49
1:C:2254:TYR:C	1:C:2254:TYR:CD1	2.85	0.49
1:C:2195:ASN:OD1	1:C:2197:MET:HB2	2.13	0.49
1:C:2395:PHE:O	1:C:2402:TYR:HD2	1.95	0.49
1:C:2482:THR:C	1:C:2511:LYS:HB2	2.33	0.49
1:C:2433:ARG:HH21	1:C:2512:PRO:HB3	1.78	0.49
1:D:3096:PHE:O	1:D:3099:VAL:N	2.46	0.49
1:D:3113:MET:O	1:D:3116:VAL:HG13	2.12	0.49
1:A:206:THR:HB	1:A:210:PHE:CD2	2.48	0.49
1:B:1206:THR:HB	1:B:1210:PHE:CD2	2.48	0.49
1:B:1456:ARG:NE	1:B:1502:GLU:OE2	2.45	0.49
1:B:1535:MET:O	1:B:1537:ASN:N	2.45	0.49
1:D:3219:GLY:HA2	1:D:3458:MET:CE	2.43	0.49
1:B:1241:GLN:OE1	1:B:1245:ARG:HD2	2.13	0.49
1:A:500:VAL:HG12	1:A:500:VAL:O	2.12	0.49
1:C:2120:ARG:O	1:C:2122:TYR:N	2.46	0.49
1:D:3563:SER:O	1:D:3564:ILE:C	2.51	0.49
1:A:523:VAL:HG12	1:A:524:GLU:OE2	2.13	0.49
1:C:2206:THR:HB	1:C:2210:PHE:CD2	2.48	0.49
1:C:2347:ASP:O	1:C:2350:GLN:N	2.46	0.49
1:C:2450:ALA:O	1:C:2451:SER:C	2.51	0.49
1:A:347:ASP:O	1:A:350:GLN:N	2.46	0.49
1:A:128:PRO:HG3	1:A:376:ARG:NH1	2.28	0.49
1:B:1205:PHE:CE2	5:B:1701:PGX:H171	2.48	0.49
1:B:1202:ALA:HB2	1:B:1348:TYR:CE1	2.48	0.49
1:C:2322:GLU:HB3	1:D:3052:PHE:CD2	2.48	0.49
1:D:3136:TYR:CD1	1:D:3136:TYR:O	2.66	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2072:PRO:HG2	1:C:2077:ARG:NE	2.27	0.49
1:B:1545:TRP:CE3	1:B:1545:TRP:HA	2.48	0.49
1:A:270:GLN:N	1:A:270:GLN:OE1	2.45	0.49
1:B:1339:GLU:OE2	1:B:1558:ILE:CG2	2.61	0.49
1:A:95:HIS:O	1:A:97:LYS:N	2.46	0.49
1:C:2107:PHE:O	1:C:2111:LEU:HB3	2.13	0.49
1:C:2209:PHE:HB3	1:C:2377:ILE:CD1	2.43	0.49
1:C:2467:ARG:NH1	1:C:2521:THR:OG1	2.44	0.49
1:B:1195:ASN:OD1	1:B:1197:MET:HB2	2.13	0.49
1:B:1513:ARG:NH2	1:B:1520:GLU:HB2	2.28	0.49
1:D:3253:LYS:O	1:D:3264:PRO:HG3	2.12	0.49
1:B:1523:VAL:HG12	1:B:1524:GLU:OE2	2.13	0.49
1:C:2301:TYR:O	1:C:2302:ALA:C	2.49	0.48
1:C:2112:ILE:O	1:C:2115:TYR:N	2.46	0.48
1:C:2450:ALA:O	1:C:2452:ILE:N	2.46	0.48
1:D:3537:ASN:HB2	6:D:4170:HOH:O	2.13	0.48
1:A:403:SER:HB2	1:A:405:LYS:HZ2	1.78	0.48
1:A:219:GLY:N	1:A:458:MET:HE2	2.28	0.48
1:A:464:ASN:HD21	1:A:475:TYR:H	1.60	0.48
1:A:513:ARG:HB2	1:A:516:ALA:HB3	1.95	0.48
1:B:1449:LYS:CA	1:B:1452:ILE:HD12	2.40	0.48
1:B:1507:LEU:HD22	1:B:1522:MET:HB2	1.95	0.48
1:B:1530:SER:OG	5:B:1701:PGX:H162	2.13	0.48
1:D:3198:PHE:CE1	1:D:3352:LEU:HD13	2.48	0.48
1:D:3151:ALA:HB2	1:D:3529:PHE:HZ	1.78	0.48
1:B:1547:PRO:HB3	1:B:1553:GLU:N	2.28	0.48
1:C:2151:ALA:HB2	1:C:2529:PHE:HZ	1.78	0.48
1:C:2495:TYR:CD2	1:C:2501:MET:HA	2.48	0.48
1:A:371:PHE:HZ	1:A:536:GLY:N	2.11	0.48
1:B:1352:LEU:HD21	1:B:1387:TRP:HH2	1.76	0.48
1:D:3198:PHE:HA	1:D:3580:PHE:CD2	2.48	0.48
1:D:3294:LEU:HB3	1:D:3409:TYR:CD2	2.47	0.48
1:D:3362:ASP:OD1	1:D:3364:GLU:HB2	2.13	0.48
1:B:1038:SER:C	1:B:1040:PRO:HD3	2.34	0.48
1:B:1064:PHE:HD2	1:B:1070:THR:O	1.96	0.48
1:C:2187:PHE:HB2	1:C:2393:ASP:OD1	2.12	0.48
1:C:2467:ARG:NH1	1:C:2520:GLU:OE1	2.42	0.48
1:D:3403:SER:OG	1:D:3405:LYS:HD2	2.13	0.48
1:C:2545:TRP:HA	1:C:2545:TRP:CE3	2.47	0.48
1:C:2495:TYR:CE2	1:C:2502:GLU:HG3	2.48	0.48
1:A:103:VAL:C	1:A:105:ASN:H	2.16	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:564:ILE:O	1:A:568:ILE:HD12	2.14	0.48
1:A:176:GLU:O	1:A:177:VAL:C	2.51	0.48
1:B:1176:GLU:O	1:B:1177:VAL:C	2.51	0.48
1:B:1344:VAL:HG12	1:B:1345:ILE:N	2.27	0.48
1:B:1535:MET:C	1:B:1537:ASN:H	2.16	0.48
1:D:3198:PHE:C	1:D:3198:PHE:CD2	2.87	0.48
1:C:2140:GLU:HB2	1:D:3330:GLN:HE22	1.78	0.48
1:D:3130:TYR:CE2	1:D:3135:GLY:O	2.66	0.48
1:B:1331:THR:O	1:B:1335:ILE:HD12	2.13	0.48
1:C:2316:LEU:O	1:C:2319:GLU:N	2.47	0.48
1:B:1235:GLY:HA3	1:B:1240:ARG:HG2	1.94	0.48
1:D:3169:LYS:O	1:D:3170:GLU:HG3	2.13	0.48
1:B:1394:THR:O	1:B:1429:GLN:NE2	2.44	0.48
1:B:1454:GLN:O	1:B:1457:GLU:N	2.46	0.48
1:D:3182:LEU:C	1:D:3438:ARG:HA	2.32	0.48
1:D:3152:LEU:HB2	1:D:3466:TYR:CE1	2.47	0.48
1:C:2389:PRO:HB2	1:C:2433:ARG:O	2.13	0.48
1:D:3538:PRO:O	1:D:3540:CYS:N	2.46	0.48
1:D:3113:MET:HA	1:D:3116:VAL:CG1	2.44	0.48
1:C:2315:ILE:HD13	1:C:2558:ILE:HD11	1.95	0.48
1:A:116:VAL:HG22	1:A:117:LEU:N	2.27	0.48
1:A:464:ASN:ND2	1:A:475:TYR:H	2.12	0.48
1:A:538:PRO:HG2	1:B:1139:TRP:HZ3	1.78	0.48
1:B:1190:ASP:HB2	1:B:1517:ILE:HD12	1.95	0.48
1:B:1387:TRP:CZ2	1:B:1518:PHE:CZ	3.01	0.48
1:D:3187:PHE:HB2	1:D:3393:ASP:OD1	2.13	0.48
1:D:3450:ALA:O	1:D:3451:SER:C	2.52	0.48
1:D:3090:HIS:CD2	1:D:3513:ARG:HG2	2.49	0.48
1:D:3371:PHE:CE1	1:D:3532:LYS:HE2	2.49	0.48
1:A:120:ARG:O	1:A:122:TYR:N	2.47	0.48
1:C:2316:LEU:CD1	1:C:2331:THR:HB	2.44	0.48
1:C:2077:ARG:O	1:C:2081:LEU:HG	2.14	0.48
1:B:1523:VAL:HG11	6:B:4064:HOH:O	2.12	0.48
1:C:2131:ASN:C	1:C:2131:ASN:OD1	2.52	0.48
1:D:3034:ASN:HB3	1:D:3037:CYS:SG	2.53	0.48
1:A:254:TYR:HD1	1:A:254:TYR:C	2.17	0.48
1:B:1303:THR:O	1:B:1307:ARG:HG3	2.14	0.48
1:C:2463:LEU:CD1	1:C:2503:LEU:HA	2.44	0.48
1:A:206:THR:HB	1:A:210:PHE:CE2	2.48	0.48
1:B:1092:ILE:HG12	1:B:1092:ILE:H	1.36	0.48
1:B:1206:THR:HB	1:B:1210:PHE:CE2	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1232:HIS:O	1:B:1288:GLY:CA	2.61	0.48
1:B:1467:ARG:O	1:B:1472:LEU:HB2	2.13	0.48
1:B:1090:HIS:CD2	1:B:1513:ARG:HG2	2.49	0.48
1:D:3120:ARG:O	1:D:3122:TYR:N	2.46	0.48
1:D:3185:ARG:HH21	1:D:3438:ARG:CZ	2.27	0.48
1:D:3513:ARG:HB2	1:D:3516:ALA:HB3	1.96	0.48
1:D:3120:ARG:HD2	1:D:3527:ALA:HB1	1.95	0.48
1:A:396:ASN:HD22	1:A:396:ASN:N	2.10	0.48
1:B:1131:ASN:C	1:B:1131:ASN:OD1	2.52	0.48
1:C:2137:LYS:NZ	1:D:3546:LYS:HE3	2.28	0.48
1:A:185:ARG:NH2	6:A:4024:HOH:O	2.45	0.48
1:A:388:HIS:O	1:A:391:LEU:HB2	2.14	0.48
1:B:1196:MET:CE	1:B:1196:MET:HA	2.44	0.48
1:A:229:ASP:OD2	1:A:229:ASP:C	2.51	0.48
1:D:3148:TYR:HB2	1:D:3219:GLY:O	2.12	0.48
1:D:3206:THR:HB	1:D:3210:PHE:CE2	2.48	0.48
1:D:3344:VAL:HG12	1:D:3345:ILE:N	2.28	0.48
1:D:3388:HIS:O	1:D:3391:LEU:HB2	2.13	0.48
1:D:3498:ILE:HG23	1:D:3499:ASP:N	2.29	0.48
1:D:3521:THR:HG22	1:D:3522:MET:N	2.29	0.48
1:B:1113:MET:CE	1:B:1117:LEU:HD22	2.43	0.48
1:A:524:GLU:CA	1:A:524:GLU:OE2	2.60	0.48
1:D:3234:TYR:CE1	1:D:3252:LEU:HD11	2.48	0.48
1:C:2050:THR:CG2	1:C:2056:LYS:HB3	2.44	0.48
1:D:3247:PHE:HA	1:D:3325:ASP:OD2	2.13	0.48
1:C:2384:LEU:HB3	1:C:2522:MET:HE2	1.96	0.48
1:B:1187:PHE:HB2	1:B:1393:ASP:OD1	2.14	0.48
1:B:1451:SER:HB2	1:B:1504:TYR:CE2	2.49	0.48
1:D:3209:PHE:HB3	1:D:3377:ILE:CD1	2.43	0.48
1:C:2196:MET:CE	1:C:2196:MET:HA	2.44	0.48
1:C:2428:ARG:HB3	6:C:4126:HOH:O	2.13	0.48
1:B:1308:GLU:HG3	1:B:1336:LEU:CD1	2.35	0.48
1:A:209:PHE:HB3	1:A:377:ILE:HD11	1.96	0.48
1:A:191:PRO:HG2	1:A:515:ASP:O	2.13	0.48
1:A:192:GLN:OE1	1:A:517:ILE:HG22	2.14	0.48
1:C:2134:TYR:HD2	1:C:2136:TYR:HE1	1.59	0.48
1:B:1272:GLU:HA	6:B:4061:HOH:O	2.13	0.48
1:A:373:TYR:H	1:B:1372:GLN:HE22	1.62	0.48
1:B:1301:TYR:O	1:B:1302:ALA:C	2.52	0.47
1:B:1197:MET:O	1:B:1198:PHE:C	2.52	0.47
1:B:1499:ASP:O	1:B:1501:MET:N	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3387:TRP:HZ2	5:D:3701:PGX:H71	1.79	0.47
1:C:2329:PHE:C	1:C:2329:PHE:CD2	2.87	0.47
1:C:2381:PHE:HB2	1:C:2529:PHE:CD1	2.49	0.47
1:A:462:SER:CB	1:A:465:GLU:HG2	2.43	0.47
1:A:462:SER:HB3	1:A:465:GLU:HG2	1.96	0.47
1:C:2304:ILE:O	1:C:2307:ARG:HB2	2.14	0.47
1:C:2155:VAL:HG12	1:C:2159:CYS:SG	2.54	0.47
1:A:208:GLN:O	1:A:211:LYS:HD3	2.14	0.47
1:B:1185:ARG:HH21	1:B:1438:ARG:CD	2.26	0.47
1:A:287:VAL:HG23	1:A:289:GLN:H	1.78	0.47
1:D:3463:LEU:CD1	1:D:3503:LEU:HA	2.44	0.47
1:B:1108:LEU:HA	1:B:1111:LEU:HD23	1.95	0.47
1:B:1116:VAL:HG22	1:B:1117:LEU:N	2.30	0.47
1:B:1056:LYS:HG3	1:B:1057:CYS:N	2.29	0.47
1:D:3080:LEU:C	1:D:3082:LEU:H	2.18	0.47
1:A:254:TYR:C	1:A:254:TYR:CD1	2.87	0.47
1:C:2208:GLN:O	1:C:2211:LYS:HD3	2.14	0.47
1:A:202:ALA:CA	1:A:348:TYR:HE1	2.27	0.47
1:A:198:PHE:CD2	1:A:198:PHE:C	2.87	0.47
1:B:1404:PHE:H	1:B:1405:LYS:HZ2	1.61	0.47
1:B:1197:MET:HE1	1:B:1423:VAL:HG13	1.96	0.47
1:D:3179:GLU:O	1:D:3181:VAL:N	2.47	0.47
1:B:1309:HIS:HD2	1:B:1310:ASN:OD1	1.97	0.47
1:C:2183:LEU:HD21	1:C:2445:GLN:CG	2.44	0.47
1:C:2463:LEU:HB3	6:C:4112:HOH:O	2.15	0.47
1:A:108:LEU:O	1:A:112:ILE:HG12	2.15	0.47
1:A:113:MET:HA	1:A:116:VAL:CG1	2.43	0.47
1:A:303:THR:O	1:A:307:ARG:HG3	2.15	0.47
1:A:198:PHE:HA	1:A:580:PHE:CD2	2.50	0.47
1:B:1128:PRO:HG2	1:B:1376:ARG:NH1	2.30	0.47
1:B:1150:ARG:NH2	1:B:1154:PRO:HA	2.29	0.47
1:B:1295:VAL:CB	1:B:1298:LEU:HD22	2.43	0.47
1:A:338:GLY:HA3	1:A:559:ILE:CD1	2.39	0.47
1:B:1316:LEU:CD1	1:B:1331:THR:HB	2.45	0.47
1:C:2090:HIS:CD2	1:C:2513:ARG:HG2	2.49	0.47
1:C:2403:SER:OG	1:C:2405:LYS:HD2	2.13	0.47
1:A:205:PHE:HE2	5:A:701:PGX:H171	1.78	0.47
1:A:481:LEU:CD1	1:A:510:GLU:HA	2.44	0.47
1:A:499:ASP:C	1:A:501:MET:H	2.18	0.47
1:B:1287:VAL:HG23	1:B:1289:GLN:H	1.80	0.47
1:B:1463:LEU:CD1	1:B:1503:LEU:HA	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3435:ALA:O	1:D:3510:GLU:O	2.32	0.47
1:D:3245:ARG:O	1:D:3253:LYS:HG3	2.15	0.47
1:C:2080:LEU:C	1:C:2082:LEU:H	2.17	0.47
1:C:2169:LYS:O	1:C:2170:GLU:HG3	2.13	0.47
1:C:2178:LEU:HD22	1:C:2183:LEU:CD1	2.45	0.47
1:C:2387:TRP:CZ2	5:C:2701:PGX:C7	2.95	0.47
1:C:2191:PRO:HG2	1:C:2515:ASP:O	2.15	0.47
1:A:150:ARG:NH2	1:A:154:PRO:HA	2.29	0.47
1:A:175:LYS:O	1:A:179:GLU:HG3	2.14	0.47
1:B:1190:ASP:OD2	1:B:1193:GLY:N	2.48	0.47
1:B:1273:MET:CE	1:B:1287:VAL:H	2.28	0.47
1:B:1450:ALA:O	1:B:1454:GLN:HG3	2.15	0.47
1:B:1532:LYS:C	1:B:1534:LEU:N	2.68	0.47
1:D:3487:MET:O	1:D:3490:GLU:HB3	2.13	0.47
1:B:1564:ILE:O	1:B:1568:ILE:HD12	2.15	0.47
1:A:120:ARG:HH11	1:A:527:ALA:HB1	1.80	0.47
1:B:1302:ALA:O	1:B:1303:THR:C	2.51	0.47
1:C:2232:HIS:O	1:C:2288:GLY:CA	2.61	0.47
1:C:2481:LEU:CD1	1:C:2510:GLU:HA	2.45	0.47
1:C:2532:LYS:C	1:C:2534:LEU:N	2.68	0.47
1:C:2181:VAL:HG12	1:C:2487:MET:HG2	1.97	0.47
1:D:3096:PHE:O	1:D:3098:GLY:N	2.47	0.47
1:D:3304:ILE:HG22	1:D:3571:ASN:HD22	1.79	0.47
1:C:2557:LYS:O	1:C:2558:ILE:C	2.51	0.47
1:A:458:MET:O	1:A:459:LYS:C	2.53	0.47
1:B:1142:PHE:O	1:B:1376:ARG:NH2	2.36	0.47
1:B:1183:LEU:HD22	1:B:1442:ILE:HG13	1.96	0.47
1:D:3219:GLY:N	1:D:3458:MET:HE2	2.29	0.47
1:D:3183:LEU:HD21	1:D:3445:GLN:CG	2.45	0.47
1:C:2396:ASN:HD22	1:C:2401:GLU:HG2	1.79	0.47
1:B:1108:LEU:HD23	1:B:1111:LEU:HD23	1.97	0.47
1:B:1276:PRO:HB2	1:B:1278:HIS:CE1	2.49	0.47
1:B:1050:THR:HG21	1:B:1056:LYS:CB	2.44	0.47
1:A:50:THR:HG21	1:A:56:LYS:CB	2.45	0.47
1:C:2546:LYS:HE3	1:D:3137:LYS:NZ	2.29	0.47
1:B:1247:PHE:HA	1:B:1325:ASP:OD2	2.15	0.47
1:C:2491:LEU:O	1:C:2494:LEU:N	2.47	0.47
1:C:2543:GLN:H	1:C:2543:GLN:CD	2.18	0.47
1:A:107:PHE:O	1:A:111:LEU:HB3	2.15	0.47
1:D:3150:ARG:NH2	1:D:3154:PRO:HA	2.30	0.47
1:D:3209:PHE:HB3	1:D:3377:ILE:HD11	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3449:LYS:CA	1:D:3452:ILE:HD12	2.39	0.47
1:D:3481:LEU:HD12	1:D:3481:LEU:O	2.14	0.47
1:C:2573:LYS:HB2	6:C:4110:HOH:O	2.14	0.47
1:A:134:TYR:CD2	1:A:136:TYR:HE1	2.33	0.47
1:C:2056:LYS:HE2	6:C:4097:HOH:O	2.14	0.47
1:B:1240:ARG:HH12	1:B:1272:GLU:HB2	1.80	0.47
1:B:1086:PRO:HG2	6:B:4096:HOH:O	2.14	0.47
1:C:2132:VAL:HG21	1:C:2219:GLY:HA3	1.97	0.47
1:D:3095:HIS:O	1:D:3100:TRP:CD1	2.68	0.47
1:D:3308:GLU:HG3	1:D:3336:LEU:CD1	2.35	0.47
1:A:206:THR:HA	1:A:209:PHE:CE2	2.50	0.47
1:A:433:ARG:HH21	1:A:512:PRO:CB	2.28	0.47
1:B:1403:SER:OG	1:B:1405:LYS:HD2	2.15	0.47
1:B:1389:PRO:HG2	1:B:1434:VAL:HG22	1.97	0.47
1:B:1509:VAL:O	1:B:1510:GLU:O	2.31	0.47
1:B:1514:PRO:O	1:B:1515:ASP:HB2	2.14	0.47
1:D:3467:ARG:NH1	1:D:3521:THR:OG1	2.47	0.47
1:A:316:LEU:CD1	1:A:331:THR:HB	2.45	0.47
1:B:1316:LEU:O	1:B:1319:GLU:N	2.48	0.47
1:B:1076:THR:O	1:B:1079:LYS:HB2	2.14	0.47
1:B:1372:GLN:O	1:B:1374:GLN:N	2.47	0.47
1:D:3270:GLN:N	1:D:3270:GLN:OE1	2.47	0.47
1:D:3215:LYS:HG2	1:D:3215:LYS:H	1.51	0.47
1:C:2261:VAL:H	1:C:2307:ARG:NH2	2.13	0.47
1:C:2105(C):ILE:O	1:C:2108:LEU:HB2	2.15	0.47
1:C:2403:SER:HB2	1:C:2405:LYS:HZ2	1.80	0.47
1:C:2510:GLU:OE1	1:C:2519:GLY:HA3	2.15	0.47
1:D:3229:ASP:OD2	1:D:3229:ASP:C	2.53	0.47
1:D:3108:LEU:HD23	1:D:3111:LEU:HD23	1.97	0.47
1:D:3116:VAL:HG22	1:D:3117:LEU:N	2.30	0.47
1:A:184:ARG:CD	1:A:187:PHE:HA	2.38	0.47
1:A:429:GLN:HG2	1:A:429:GLN:O	2.14	0.47
1:A:509:VAL:O	1:A:510:GLU:O	2.32	0.47
1:A:229:ASP:HA	1:A:337:ILE:HD11	1.97	0.47
1:A:547:PRO:O	1:A:552:GLY:N	2.43	0.47
1:C:2113:MET:CE	1:C:2117:LEU:HD22	2.44	0.46
1:C:2176:GLU:O	1:C:2179:GLU:N	2.48	0.46
1:C:2209:PHE:CD1	1:C:2209:PHE:N	2.79	0.46
1:B:1225:GLY:HA3	1:B:1229:ASP:OD1	2.15	0.46
1:A:386:HIS:HB2	1:A:504:TYR:CE1	2.50	0.46
1:B:1444:VAL:HG12	1:B:1444:VAL:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1219:GLY:N	1:B:1458:MET:HE2	2.29	0.46
1:C:2295:VAL:CB	1:C:2298:LEU:HD22	2.46	0.46
1:A:465:GLU:OE2	1:A:468:LYS:CE	2.63	0.46
1:C:2302:ALA:O	1:C:2303:THR:C	2.53	0.46
1:C:2303:THR:O	1:C:2307:ARG:HG3	2.15	0.46
1:C:2450:ALA:O	1:C:2454:GLN:HG3	2.15	0.46
1:D:3535:MET:C	1:D:3537:ASN:H	2.19	0.46
1:D:3107:PHE:O	1:D:3111:LEU:HB3	2.15	0.46
1:A:219:GLY:HA2	1:A:458:MET:HE1	1.96	0.46
1:A:444:VAL:CG1	1:A:444:VAL:O	2.62	0.46
1:A:538:PRO:HG2	1:B:1139:TRP:CZ3	2.50	0.46
1:B:1205:PHE:CE2	1:B:1209:PHE:HZ	2.33	0.46
1:B:1386:HIS:HD2	1:B:1451:SER:HB3	1.79	0.46
1:B:1134:TYR:HD2	1:B:1136:TYR:HE1	1.61	0.46
1:D:3543:GLN:H	1:D:3543:GLN:CD	2.18	0.46
1:C:2103:VAL:C	1:C:2105:ASN:H	2.19	0.46
1:D:3303:THR:O	1:D:3307:ARG:HG3	2.16	0.46
1:A:183:LEU:HD21	1:A:445:GLN:CG	2.45	0.46
1:B:1526:GLY:O	1:B:1530:SER:HB3	2.15	0.46
1:D:3403:SER:HB2	1:D:3405:LYS:HZ2	1.80	0.46
1:B:1124:ILE:H	1:B:1124:ILE:HG12	1.59	0.46
1:D:3553:GLU:OE1	1:D:3553:GLU:CA	2.63	0.46
1:A:80:LEU:C	1:A:82:LEU:H	2.18	0.46
1:C:2344:VAL:HG12	1:C:2345:ILE:N	2.30	0.46
1:A:137:LYS:HZ1	1:B:1546:LYS:HE3	1.80	0.46
1:B:1300:MET:O	1:B:1304:ILE:HG13	2.14	0.46
1:C:2187:PHE:CD1	1:C:2187:PHE:C	2.89	0.46
1:C:2433:ARG:HH21	1:C:2512:PRO:CB	2.29	0.46
1:C:2513:ARG:NH2	1:C:2520:GLU:HB2	2.31	0.46
1:D:3304:ILE:O	1:D:3307:ARG:HB2	2.16	0.46
1:A:456:ARG:NE	1:A:502:GLU:OE2	2.48	0.46
1:B:1435:ALA:HB2	1:B:1518:PHE:HA	1.97	0.46
1:D:3190:ASP:OD2	1:D:3193:GLY:N	2.49	0.46
1:D:3567:LEU:HD12	1:D:3567:LEU:C	2.35	0.46
1:C:2429:GLN:O	1:C:2429:GLN:HG2	2.15	0.46
1:A:341:ILE:HD13	1:A:534:LEU:HD12	1.97	0.46
1:B:1389:PRO:HB2	1:B:1433:ARG:O	2.15	0.46
1:B:1414:LEU:HA	1:B:1422:PHE:HE1	1.73	0.46
1:B:1481:LEU:CD1	1:B:1510:GLU:HA	2.46	0.46
1:A:274:ILE:HD12	1:A:291:VAL:HA	1.96	0.46
1:D:3174:SER:N	6:D:4188:HOH:O	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3232:HIS:O	1:D:3288:GLY:CA	2.63	0.46
1:D:3435:ALA:HB2	1:D:3518:PHE:HA	1.96	0.46
1:A:295:VAL:CB	1:A:298:LEU:HD22	2.44	0.46
1:D:3245:ARG:HD2	1:D:3329:PHE:CE1	2.50	0.46
1:A:381:PHE:CD1	1:A:529:PHE:CB	2.97	0.46
1:C:2547:PRO:C	1:C:2552:GLY:HA2	2.36	0.46
1:B:1077:ARG:O	1:B:1081:LEU:HG	2.15	0.46
1:C:2056:LYS:HG3	1:C:2057:CYS:N	2.30	0.46
1:C:2583:GLN:N	1:C:2583:GLN:CD	2.69	0.46
1:C:2174:SER:O	1:C:2178:LEU:HB2	2.16	0.46
1:C:2197:MET:O	1:C:2198:PHE:C	2.54	0.46
1:C:2514:PRO:O	1:C:2515:ASP:CB	2.63	0.46
1:B:1095:HIS:O	1:B:1097:LYS:N	2.49	0.46
1:D:3301:TYR:O	1:D:3302:ALA:C	2.54	0.46
1:D:3261:VAL:O	1:D:3307:ARG:NH1	2.49	0.46
1:A:113:MET:HE3	1:A:116:VAL:HG22	1.97	0.46
1:A:176:GLU:O	1:A:179:GLU:N	2.49	0.46
1:A:499:ASP:O	1:A:501:MET:N	2.49	0.46
1:A:384:LEU:HB3	1:A:522:MET:HE2	1.97	0.46
1:B:1198:PHE:C	1:B:1198:PHE:CD2	2.89	0.46
1:D:3405:LYS:HE3	1:D:3405:LYS:H	1.81	0.46
1:D:3513:ARG:O	1:D:3515:ASP:N	2.49	0.46
1:D:3276:PRO:HB2	1:D:3278:HIS:CE1	2.50	0.46
1:C:2105(C):ILE:CB	1:C:2108:LEU:HD12	2.46	0.46
1:C:2116:VAL:HG22	1:C:2117:LEU:N	2.31	0.46
1:C:2176:GLU:O	1:C:2177:VAL:C	2.54	0.46
1:C:2219:GLY:HA2	1:C:2458:MET:CE	2.46	0.46
1:C:2490:GLU:O	1:C:2493:ALA:HB3	2.16	0.46
1:A:456:ARG:NH1	6:A:4045:HOH:O	2.48	0.46
1:A:513:ARG:O	1:A:515:ASP:N	2.48	0.46
1:B:1179:GLU:O	1:B:1181:VAL:N	2.48	0.46
1:B:1395:PHE:O	1:B:1402:TYR:HD2	1.99	0.46
1:D:3162:PRO:HB2	1:D:3171:LEU:CD2	2.46	0.46
1:A:124:ILE:HD11	1:A:528:PRO:C	2.36	0.46
1:B:1137:LYS:N	6:B:4080:HOH:O	2.49	0.46
1:A:489:ALA:HB2	6:A:4044:HOH:O	2.14	0.46
1:C:2105(C):ILE:CG2	1:C:2108:LEU:HD12	2.46	0.46
1:C:2513:ARG:HB2	1:C:2516:ALA:HB3	1.98	0.46
1:D:3261:VAL:H	1:D:3307:ARG:NH2	2.14	0.46
1:A:383:THR:O	1:A:385:TYR:N	2.49	0.46
1:B:1391:LEU:HD13	1:B:1404:PHE:HE2	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1499:ASP:C	1:B:1501:MET:H	2.18	0.46
1:D:3175:LYS:O	1:D:3178:LEU:HB3	2.16	0.46
1:C:2381:PHE:CD1	1:C:2529:PHE:CB	2.99	0.46
1:A:61:ARG:NH2	1:B:1545:TRP:O	2.48	0.46
1:C:2273:MET:CE	1:C:2287:VAL:H	2.28	0.46
1:D:3274:ILE:HD12	1:D:3291:VAL:HA	1.98	0.46
1:D:3089:VAL:O	1:D:3092:ILE:HG12	2.16	0.46
1:D:3532:LYS:C	1:D:3534:LEU:N	2.69	0.46
1:B:1116:VAL:O	1:B:1119:SER:OG	2.34	0.46
1:C:2065:TYR:CD2	1:C:2065:TYR:N	2.84	0.46
1:B:1323:TRP:CE3	1:B:1327:GLN:HG2	2.51	0.46
1:D:3078:ILE:HD13	1:D:3078:ILE:N	2.30	0.46
1:D:3076:THR:O	1:D:3079:LYS:HB2	2.16	0.46
1:C:2504:TYR:O	1:C:2507:LEU:HB2	2.16	0.46
1:A:405:LYS:HE3	1:A:405:LYS:H	1.81	0.46
1:A:463:LEU:CD1	1:A:503:LEU:HA	2.46	0.46
1:D:3287:VAL:HG23	1:D:3289:GLN:H	1.80	0.46
1:D:3195:ASN:OD1	1:D:3197:MET:HB2	2.15	0.46
1:D:3421:GLN:O	1:D:3422:PHE:C	2.54	0.46
1:B:1245:ARG:HH22	1:B:1326:GLU:HA	1.81	0.46
1:B:1113:MET:HA	1:B:1116:VAL:HG13	1.96	0.46
1:B:1120:ARG:HH11	1:B:1527:ALA:HB1	1.80	0.46
1:C:2064:PHE:HD2	1:C:2070:THR:O	1.99	0.46
1:B:1567:LEU:C	1:B:1567:LEU:HD12	2.37	0.46
1:C:2546:LYS:HE3	1:D:3137:LYS:HZ1	1.80	0.46
1:D:3059:CYS:HB3	1:D:3064:PHE:O	2.16	0.46
1:D:3315:ILE:HD13	1:D:3558:ILE:HD11	1.97	0.45
1:B:1308:GLU:OE2	1:B:1308:GLU:HA	2.16	0.45
1:C:2183:LEU:HD22	1:C:2442:ILE:HG13	1.98	0.45
1:C:2273:MET:CE	1:C:2287:VAL:HG22	2.26	0.45
1:C:2464:ASN:HD21	1:C:2475:TYR:N	2.14	0.45
1:A:532:LYS:C	1:A:534:LEU:N	2.68	0.45
1:D:3187:PHE:C	1:D:3187:PHE:CD1	2.90	0.45
1:D:3190:ASP:HB2	1:D:3517:ILE:HD12	1.97	0.45
1:C:2276:PRO:HG3	1:C:2409:TYR:CD1	2.51	0.45
1:D:3309:HIS:HD2	1:D:3310:ASN:OD1	1.98	0.45
1:A:131:ASN:C	1:A:131:ASN:OD1	2.53	0.45
1:C:2549:THR:HG23	1:D:3137:LYS:HD3	1.98	0.45
1:B:1543:GLN:CD	1:B:1543:GLN:H	2.19	0.45
1:A:187:PHE:HB2	1:A:393:ASP:OD1	2.16	0.45
1:A:371:PHE:CE1	1:A:532:LYS:HE2	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:VAL:O	1:A:90:HIS:C	2.54	0.45
1:B:1380:GLU:HG3	1:B:1460:TYR:CE2	2.50	0.45
1:B:1151:ALA:HB2	1:B:1529:PHE:CZ	2.51	0.45
1:D:3043:ASN:ND2	1:D:3069:CYS:O	2.49	0.45
1:C:2247:PHE:HA	1:C:2325:ASP:OD2	2.15	0.45
1:A:256:VAL:HA	1:A:260:GLU:O	2.17	0.45
1:C:2089:VAL:O	1:C:2090:HIS:C	2.53	0.45
1:D:3230:LEU:CG	1:D:3337:ILE:HG13	2.41	0.45
1:D:3301:TYR:O	1:D:3304:ILE:HB	2.16	0.45
1:A:357:PHE:HE2	1:A:359:LEU:HD23	1.81	0.45
1:A:148:TYR:HD2	1:A:219:GLY:O	1.98	0.45
1:B:1495:TYR:CE2	1:B:1502:GLU:HG3	2.48	0.45
1:A:240:ARG:HH12	1:A:272:GLU:HB2	1.81	0.45
1:D:3173:ASP:OD2	1:D:3175:LYS:N	2.49	0.45
1:D:3381:PHE:O	5:D:3701:PGX:H101	2.17	0.45
1:D:3191:PRO:HG2	1:D:3515:ASP:O	2.16	0.45
1:B:1105(B):ILE:HG21	1:B:1108:LEU:CD1	2.42	0.45
1:C:2331:THR:O	1:C:2335:ILE:HD12	2.16	0.45
1:C:2043:ASN:ND2	1:C:2069:CYS:O	2.49	0.45
1:C:2108:LEU:HA	1:C:2111:LEU:HD23	1.98	0.45
1:C:2142:PHE:O	1:C:2376:ARG:NH2	2.37	0.45
1:C:2387:TRP:HZ2	5:C:2701:PGX:C7	2.24	0.45
1:C:2395:PHE:CD1	1:C:2407:PHE:CD2	3.04	0.45
1:C:2534:LEU:HD13	1:C:2534:LEU:HA	1.87	0.45
1:A:347:ASP:OD2	1:A:564:ILE:HG22	2.17	0.45
1:A:184:ARG:CB	1:A:439:ASN:HA	2.44	0.45
1:A:184:ARG:HH12	1:A:441:PRO:HG3	1.80	0.45
1:B:1148:TYR:HB2	1:B:1219:GLY:O	2.17	0.45
1:B:1455:SER:HA	1:B:1460:TYR:CD1	2.51	0.45
1:B:1464:ASN:ND2	1:B:1475:TYR:H	2.14	0.45
1:D:3380:GLU:HG3	1:D:3460:TYR:CE2	2.52	0.45
1:D:3404:PHE:H	1:D:3405:LYS:HZ2	1.63	0.45
1:D:3386:HIS:HB2	1:D:3504:TYR:CE1	2.50	0.45
1:A:196:MET:CE	1:A:196:MET:HA	2.47	0.45
1:A:65:TYR:CD2	1:A:65:TYR:N	2.84	0.45
1:B:1065:TYR:CD2	1:B:1065:TYR:N	2.84	0.45
1:C:2148:TYR:HB2	1:C:2219:GLY:O	2.16	0.45
1:C:2371:PHE:HZ	1:C:2536:GLY:N	2.14	0.45
1:C:2380:GLU:HG3	1:C:2460:TYR:CE2	2.51	0.45
1:D:3095:HIS:O	1:D:3100:TRP:HD1	1.99	0.45
1:A:538:PRO:HG3	1:B:1142:PHE:CE2	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1209:PHE:N	1:B:1209:PHE:CD1	2.79	0.45
1:B:1405:LYS:H	1:B:1405:LYS:HE3	1.82	0.45
1:B:1191:PRO:HG2	1:B:1515:ASP:O	2.17	0.45
1:D:3176:GLU:O	1:D:3179:GLU:N	2.50	0.45
1:D:3389:PRO:HB2	1:D:3433:ARG:O	2.16	0.45
1:D:3464:ASN:ND2	1:D:3475:TYR:H	2.14	0.45
1:C:2245:ARG:HH22	1:C:2326:GLU:HA	1.82	0.45
1:B:1216:ARG:HB3	1:B:1220:PHE:HD1	1.76	0.45
1:C:2523:VAL:HG12	1:C:2524:GLU:OE2	2.16	0.45
1:D:3050:THR:HG21	1:D:3056:LYS:CB	2.46	0.45
1:B:1080:LEU:C	1:B:1082:LEU:H	2.19	0.45
1:C:2137:LYS:HZ1	1:D:3546:LYS:HE3	1.81	0.45
1:C:2215:LYS:HG2	1:C:2215:LYS:H	1.50	0.45
1:C:2498:ILE:O	1:C:2501:MET:HB2	2.16	0.45
1:C:2198:PHE:HA	1:C:2580:PHE:CD2	2.52	0.45
1:D:3535:MET:O	1:D:3537:ASN:N	2.49	0.45
1:B:1095:HIS:O	1:B:1100:TRP:CD1	2.70	0.45
1:D:3302:ALA:O	1:D:3303:THR:C	2.53	0.45
1:A:564:ILE:O	1:A:568:ILE:CD1	2.65	0.45
1:A:218:PRO:C	1:A:458:MET:CE	2.85	0.45
1:A:389:PRO:HB2	1:A:433:ARG:O	2.17	0.45
1:A:435:ALA:O	1:A:510:GLU:O	2.34	0.45
1:A:530:SER:OG	5:A:701:PGX:H162	2.17	0.45
1:B:1128:PRO:HG3	1:B:1376:ARG:NH1	2.30	0.45
1:D:3151:ALA:HB2	1:D:3529:PHE:CZ	2.51	0.45
1:D:3198:PHE:CZ	1:D:3352:LEU:HD13	2.51	0.45
1:D:3369:GLN:O	1:D:3371:PHE:N	2.49	0.45
1:C:2190:ASP:OD1	1:C:2192:GLN:HG3	2.17	0.45
1:A:190:ASP:OD1	1:A:192:GLN:HG3	2.16	0.45
1:A:465:GLU:OE2	1:A:468:LYS:HE2	2.17	0.45
1:C:2363:PRO:C	1:C:2365:LEU:N	2.70	0.45
1:A:246:LEU:HB3	1:A:251:LYS:O	2.16	0.45
1:C:2168:ASN:C	1:C:2170:GLU:N	2.70	0.45
1:D:3065:TYR:N	1:D:3065:TYR:CD2	2.85	0.45
1:C:2383:THR:O	1:C:2385:TYR:N	2.49	0.45
1:C:2568:ILE:HG23	1:C:2572:VAL:CG2	2.46	0.45
1:A:174:SER:O	1:A:178:LEU:HB2	2.17	0.45
1:B:1176:GLU:O	1:B:1179:GLU:N	2.50	0.45
1:B:1198:PHE:CZ	1:B:1352:LEU:HD13	2.51	0.45
1:A:276:PRO:HB2	1:A:278:HIS:CE1	2.51	0.45
1:B:1276:PRO:HG3	1:B:1409:TYR:CD1	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2535:MET:O	1:C:2537:ASN:N	2.50	0.45
1:C:2523:VAL:HG12	1:C:2524:GLU:N	2.31	0.45
1:C:2347:ASP:O	1:C:2348:TYR:O	2.35	0.45
1:C:2455:SER:HA	1:C:2460:TYR:CD1	2.51	0.45
1:C:2513:ARG:O	1:C:2515:ASP:N	2.50	0.45
1:D:3229:ASP:HA	1:D:3337:ILE:HD11	1.98	0.45
1:A:197:MET:HE1	1:A:423:VAL:HG13	1.99	0.45
1:B:1173:ASP:OD2	1:B:1173:ASP:C	2.55	0.45
1:B:1274:ILE:HD12	1:B:1291:VAL:HG23	1.98	0.45
1:B:1504:TYR:O	1:B:1507:LEU:HB2	2.17	0.45
1:D:3404:PHE:CD1	1:D:3404:PHE:N	2.85	0.45
1:D:3433:ARG:HH21	1:D:3512:PRO:HB3	1.81	0.45
1:D:3386:HIS:HD2	1:D:3451:SER:HB3	1.81	0.45
1:D:3155:VAL:HG23	1:D:3459:LYS:O	2.17	0.45
1:D:3161:THR:O	1:D:3164:GLY:N	2.48	0.45
1:C:2538:PRO:O	1:C:2540:CYS:N	2.49	0.45
1:C:2190:ASP:OD2	1:C:2193:GLY:N	2.50	0.45
1:D:3563:SER:C	1:D:3565:GLN:N	2.69	0.45
1:B:1168:ASN:C	1:B:1170:GLU:N	2.70	0.45
1:C:2357:PHE:HE2	1:C:2359:LEU:HD23	1.81	0.45
1:D:3201:PHE:O	1:D:3204:HIS:N	2.50	0.45
1:B:1175:LYS:O	1:B:1178:LEU:HB3	2.16	0.45
5:B:1701:PGX:H202	6:B:4074:HOH:O	2.17	0.45
1:D:3197:MET:O	1:D:3198:PHE:C	2.55	0.45
1:A:294:LEU:HB3	1:A:409:TYR:CD2	2.52	0.45
1:A:381:PHE:HB2	1:A:529:PHE:CD1	2.51	0.45
1:C:2190:ASP:HB2	1:C:2517:ILE:HD12	1.97	0.45
1:C:2059:CYS:HB3	1:C:2064:PHE:O	2.16	0.45
1:D:3034:ASN:HA	1:D:3035:PRO:HD2	1.86	0.45
1:D:3415:LEU:HD23	1:D:3415:LEU:HA	1.82	0.45
1:C:2261:VAL:O	1:C:2307:ARG:NH1	2.50	0.45
1:C:2184:ARG:CB	1:C:2439:ASN:HA	2.44	0.45
1:C:2487:MET:O	1:C:2490:GLU:HB3	2.17	0.45
1:D:3103:VAL:C	1:D:3105:ASN:H	2.21	0.45
1:A:107:PHE:HD2	1:A:107:PHE:H	1.65	0.45
1:A:535:MET:C	1:A:537:ASN:H	2.20	0.45
1:D:3162:PRO:HB2	1:D:3171:LEU:HD21	1.99	0.45
1:D:3481:LEU:HD12	1:D:3510:GLU:HA	1.98	0.45
1:D:3507:LEU:HD22	1:D:3522:MET:HB2	1.98	0.45
1:D:3295:VAL:CB	1:D:3298:LEU:HD22	2.47	0.45
1:B:1201:PHE:O	1:B:1204:HIS:N	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2276:PRO:HB2	1:C:2278:HIS:CE1	2.52	0.45
1:B:1465:GLU:OE2	1:B:1468:LYS:HE2	2.17	0.45
1:A:300:MET:O	1:A:304:ILE:HG13	2.16	0.44
1:B:1229:ASP:C	1:B:1229:ASP:OD2	2.55	0.44
1:C:2099:VAL:HA	1:C:2102:ILE:CD1	2.28	0.44
1:A:195:ASN:OD1	1:A:197:MET:HB2	2.17	0.44
1:A:404:PHE:CD1	1:A:404:PHE:N	2.85	0.44
1:A:449:LYS:CA	1:A:452:ILE:HD12	2.41	0.44
1:D:3532:LYS:C	1:D:3534:LEU:H	2.21	0.44
1:D:3530:SER:HB2	5:D:3701:PGX:H161	1.99	0.44
1:C:2566:SER:O	1:C:2567:LEU:C	2.56	0.44
1:A:183:LEU:HD22	1:A:442:ILE:HG13	1.98	0.44
1:A:383:THR:C	1:A:385:TYR:N	2.71	0.44
1:A:405:LYS:H	1:A:405:LYS:CE	2.30	0.44
1:A:454:GLN:O	1:A:455:SER:C	2.55	0.44
1:B:1226:HIS:C	1:B:1377:ILE:HD12	2.38	0.44
1:B:1188:ILE:HB	1:B:1439:ASN:ND2	2.33	0.44
1:B:1458:MET:O	1:B:1459:LYS:C	2.56	0.44
1:D:3381:PHE:CD1	1:D:3529:PHE:CB	2.99	0.44
1:B:1381:PHE:HB2	1:B:1529:PHE:CD1	2.52	0.44
1:D:3065:TYR:HB2	1:D:3066:GLY:H	1.64	0.44
1:C:2389:PRO:HG2	1:C:2434:VAL:HG22	1.98	0.44
1:C:2507:LEU:HD22	1:C:2522:MET:HB2	2.00	0.44
1:A:108:LEU:HD23	1:A:111:LEU:HD23	1.99	0.44
1:A:113:MET:CE	1:A:117:LEU:HD22	2.47	0.44
1:A:219:GLY:HA2	1:A:458:MET:CE	2.46	0.44
1:B:1162:PRO:HB2	1:B:1171:LEU:CD2	2.47	0.44
1:B:1369:GLN:O	1:B:1371:PHE:N	2.50	0.44
1:B:1405:LYS:H	1:B:1405:LYS:CE	2.30	0.44
1:B:1513:ARG:HB2	1:B:1516:ALA:HB3	1.99	0.44
1:D:3329:PHE:HD2	1:D:3330:GLN:HG2	1.82	0.44
1:A:462:SER:O	1:A:465:GLU:HB2	2.16	0.44
1:A:168:ASN:C	1:A:170:GLU:N	2.69	0.44
1:D:3246:LEU:HB3	1:D:3251:LYS:O	2.17	0.44
1:C:2112:ILE:O	1:C:2115:TYR:HB3	2.17	0.44
1:B:1095:HIS:O	1:B:1100:TRP:HD1	2.00	0.44
1:D:3308:GLU:HA	1:D:3308:GLU:OE2	2.17	0.44
1:C:2339:GLU:OE2	1:C:2558:ILE:CG2	2.66	0.44
1:A:538:PRO:O	1:A:540:CYS:N	2.51	0.44
1:B:1273:MET:HE2	1:B:1285:PHE:O	2.18	0.44
1:B:1389:PRO:HB2	1:B:1434:VAL:HA	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1487:MET:O	1:B:1490:GLU:HB3	2.18	0.44
1:B:1205:PHE:HE2	5:B:1701:PGX:H171	1.82	0.44
1:D:3352:LEU:HG	1:D:3518:PHE:HE2	1.83	0.44
1:D:3371:PHE:HZ	1:D:3536:GLY:N	2.15	0.44
1:B:1381:PHE:CD1	1:B:1529:PHE:CB	3.00	0.44
1:A:136:TYR:O	1:A:136:TYR:HD1	2.01	0.44
1:C:2050:THR:HG21	1:C:2056:LYS:CB	2.47	0.44
1:A:37:CYS:O	1:A:39:ASN:ND2	2.50	0.44
1:C:2405:LYS:H	1:C:2405:LYS:HE3	1.83	0.44
1:C:2532:LYS:C	1:C:2534:LEU:H	2.20	0.44
1:D:3202:ALA:HB2	1:D:3348:TYR:CE1	2.52	0.44
1:A:395:PHE:O	1:A:402:TYR:HD2	2.00	0.44
1:B:1187:PHE:CD1	1:B:1187:PHE:C	2.90	0.44
1:B:1490:GLU:O	1:B:1493:ALA:HB3	2.17	0.44
1:D:3196:MET:HG2	1:D:3429:GLN:HG2	2.00	0.44
1:D:3513:ARG:HH21	1:D:3520:GLU:HB2	1.83	0.44
1:D:3316:LEU:CD1	1:D:3331:THR:HB	2.47	0.44
1:C:2524:GLU:CA	1:C:2524:GLU:OE2	2.62	0.44
1:A:323:TRP:CE3	1:A:327:GLN:HG2	2.53	0.44
1:A:548:SER:O	1:A:550:PHE:N	2.50	0.44
1:A:315:ILE:HD13	1:A:558:ILE:HD11	1.99	0.44
1:A:339:GLU:OE2	1:A:558:ILE:CG2	2.66	0.44
1:C:2103:VAL:O	1:C:2105:ASN:N	2.51	0.44
1:C:2206:THR:HA	1:C:2209:PHE:CE2	2.52	0.44
1:C:2369:GLN:O	1:C:2371:PHE:N	2.50	0.44
1:A:435:ALA:HB2	1:A:518:PHE:HA	1.99	0.44
1:A:450:ALA:O	1:A:451:SER:C	2.55	0.44
1:B:1173:ASP:OD2	1:B:1175:LYS:N	2.51	0.44
1:B:1371:PHE:HZ	1:B:1536:GLY:N	2.15	0.44
1:B:1436:GLY:HA2	1:B:1512:PRO:HG2	2.00	0.44
1:B:1513:ARG:O	1:B:1515:ASP:N	2.50	0.44
1:D:3198:PHE:HB2	1:D:3580:PHE:HB3	1.99	0.44
1:A:295:VAL:HB	1:A:298:LEU:HB2	1.99	0.44
1:B:1107:PHE:HD2	1:B:1107:PHE:H	1.64	0.44
1:C:2134:TYR:CD2	1:C:2136:TYR:HE1	2.35	0.44
1:D:3056:LYS:HA	6:D:4150:HOH:O	2.17	0.44
1:B:1462:SER:HB3	1:B:1465:GLU:HG2	1.99	0.44
1:B:1261:VAL:O	1:B:1307:ARG:NH1	2.51	0.44
1:C:2454:GLN:O	1:C:2455:SER:C	2.54	0.44
1:D:3108:LEU:HA	1:D:3111:LEU:HD23	1.99	0.44
1:A:568:ILE:HG23	1:A:572:VAL:CG2	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:198:PHE:CZ	1:A:352:LEU:HD13	2.52	0.44
1:A:150:ARG:HD2	1:A:380:GLU:OE1	2.17	0.44
1:A:521:THR:HG22	1:A:522:MET:N	2.32	0.44
1:B:1175:LYS:O	1:B:1179:GLU:HG3	2.18	0.44
1:B:1386:HIS:HB2	1:B:1504:TYR:CE1	2.52	0.44
1:D:3173:ASP:OD2	1:D:3173:ASP:C	2.55	0.44
1:D:3352:LEU:HD12	1:D:3352:LEU:HA	1.81	0.44
1:D:3396:ASN:HD22	1:D:3396:ASN:N	2.16	0.44
1:C:2124:ILE:H	1:C:2124:ILE:HG12	1.61	0.44
1:B:1136:TYR:HD1	1:B:1136:TYR:O	2.00	0.44
1:B:1461:GLN:H	1:B:1466:TYR:HE2	1.65	0.44
1:C:2373:TYR:H	1:D:3372:GLN:HE22	1.65	0.44
1:B:1548:SER:O	1:B:1550:PHE:N	2.50	0.44
1:A:470:PHE:N	1:A:470:PHE:CD2	2.85	0.44
1:A:583:GLN:N	1:A:583:GLN:CD	2.70	0.44
1:C:2352:LEU:HG	1:C:2518:PHE:HE2	1.83	0.44
1:A:112:ILE:O	1:A:115:TYR:HB3	2.17	0.44
1:A:507:LEU:HD22	1:A:522:MET:HB2	1.99	0.44
1:B:1178:LEU:HD22	1:B:1183:LEU:CD1	2.48	0.44
1:B:1482:THR:CG2	1:B:1509:VAL:HG12	2.48	0.44
1:D:3444:VAL:CG1	1:D:3444:VAL:O	2.65	0.44
1:D:3444:VAL:O	1:D:3445:GLN:C	2.56	0.44
1:D:3292:PHE:O	1:D:3299:MET:HE2	2.18	0.44
1:B:1113:MET:HA	1:B:1116:VAL:CG1	2.47	0.44
1:C:2269:THR:OG1	1:C:2271:VAL:HG23	2.17	0.44
1:C:2161:THR:O	1:C:2164:GLY:N	2.46	0.44
1:D:3363:PRO:C	1:D:3365:LEU:N	2.70	0.44
1:A:59:CYS:HB3	1:A:64:PHE:O	2.18	0.44
1:C:2567:LEU:C	1:C:2567:LEU:HD12	2.37	0.44
1:C:2274:ILE:HD11	1:C:2290:GLU:HG3	2.00	0.44
1:C:2482:THR:HG22	6:C:4128:HOH:O	2.17	0.44
1:D:3105(D):ILE:CG2	1:D:3108:LEU:HD12	2.48	0.44
1:A:532:LYS:C	1:A:534:LEU:H	2.21	0.44
1:A:535:MET:O	1:A:537:ASN:N	2.51	0.44
1:B:1435:ALA:O	1:B:1510:GLU:O	2.36	0.44
1:D:3405:LYS:CE	1:D:3405:LYS:H	2.30	0.44
1:C:2323:TRP:CE3	1:C:2327:GLN:HG2	2.52	0.44
1:A:77:ARG:O	1:A:81:LEU:HG	2.18	0.44
1:A:137:LYS:NZ	1:B:1546:LYS:HE3	2.32	0.44
1:C:2105(C):ILE:O	1:C:2108:LEU:N	2.50	0.43
1:C:2112:ILE:HB	1:C:2357:PHE:CE1	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:112:ILE:HB	1:A:357:PHE:CE1	2.53	0.43
1:A:187:PHE:CD1	1:A:187:PHE:C	2.91	0.43
1:A:352:LEU:HA	1:A:352:LEU:HD12	1.81	0.43
1:A:467:ARG:NH1	1:A:520:GLU:OE1	2.44	0.43
1:B:1429:GLN:O	1:B:1429:GLN:HG2	2.18	0.43
1:D:3178:LEU:HD22	1:D:3183:LEU:CD1	2.48	0.43
1:D:3182:LEU:O	1:D:3438:ARG:CA	2.61	0.43
1:D:3381:PHE:HB2	1:D:3529:PHE:CD1	2.53	0.43
1:D:3184:ARG:CB	1:D:3439:ASN:HA	2.48	0.43
1:D:3499:ASP:O	1:D:3501:MET:N	2.51	0.43
1:B:1292:PHE:O	1:B:1299:MET:HE2	2.18	0.43
1:A:322:GLU:HB3	1:B:1052:PHE:CD2	2.52	0.43
1:D:3524:GLU:OE2	1:D:3524:GLU:CA	2.65	0.43
1:A:543:GLN:O	1:B:1137:LYS:HE2	2.18	0.43
1:B:1363:PRO:C	1:B:1365:LEU:N	2.72	0.43
1:B:1160:PRO:HD2	1:B:1164:GLY:O	2.18	0.43
1:A:415:LEU:HD23	1:A:415:LEU:HA	1.85	0.43
1:D:3583:GLN:N	1:D:3583:GLN:CD	2.72	0.43
1:B:1304:ILE:HG22	1:B:1571:ASN:HD22	1.82	0.43
1:C:2503:LEU:O	1:C:2504:TYR:C	2.55	0.43
1:C:2557:LYS:HA	1:C:2560:ASN:HD22	1.82	0.43
1:A:185:ARG:HE	1:A:438:ARG:HD3	1.83	0.43
1:B:1442:ILE:N	1:B:1442:ILE:CD1	2.81	0.43
1:D:3495:TYR:CE2	1:D:3502:GLU:HG3	2.51	0.43
1:D:3532:LYS:HB3	1:D:3533:GLY:H	1.70	0.43
1:C:2052:PHE:CD2	1:D:3322:GLU:HB3	2.53	0.43
1:B:1112:ILE:O	1:B:1116:VAL:HG13	2.18	0.43
1:C:2252:LEU:HD12	1:C:2309:HIS:CG	2.53	0.43
1:B:1524:GLU:CA	1:B:1524:GLU:OE2	2.65	0.43
1:A:546:LYS:HE3	1:B:1137:LYS:HZ1	1.82	0.43
1:A:461:GLN:H	1:A:466:TYR:HE2	1.65	0.43
1:A:248:LYS:N	1:A:325:ASP:OD1	2.51	0.43
1:D:3461:GLN:H	1:D:3466:TYR:HE2	1.66	0.43
1:D:3339:GLU:OE2	1:D:3558:ILE:CG2	2.66	0.43
1:A:557:LYS:O	1:A:558:ILE:C	2.56	0.43
1:C:2175:LYS:O	1:C:2179:GLU:HG3	2.19	0.43
1:C:2371:PHE:CE1	1:C:2532:LYS:HE2	2.53	0.43
1:B:1229:ASP:OD2	1:B:1231:ASN:N	2.51	0.43
1:A:495:TYR:CE2	1:A:502:GLU:HG3	2.50	0.43
1:B:1190:ASP:OD1	1:B:1192:GLN:HG3	2.18	0.43
1:B:1219:GLY:HA2	1:B:1458:MET:CE	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1352:LEU:HA	1:B:1352:LEU:HD12	1.79	0.43
1:D:3148:TYR:HD2	1:D:3219:GLY:O	2.01	0.43
1:D:3482:THR:CA	1:D:3511:LYS:HB2	2.48	0.43
1:D:3509:VAL:O	1:D:3510:GLU:C	2.56	0.43
1:D:3525:LEU:C	1:D:3528:PRO:HD2	2.38	0.43
1:D:3528:PRO:O	1:D:3529:PHE:C	2.56	0.43
1:B:1563:SER:C	1:B:1565:GLN:N	2.70	0.43
1:B:1112:ILE:O	1:B:1115:TYR:HB3	2.18	0.43
1:C:2124:ILE:HG22	1:C:2125:ASP:N	2.33	0.43
1:D:3126:SER:HA	1:D:3127:PRO:C	2.39	0.43
1:C:2304:ILE:HG22	1:C:2567:LEU:HD11	2.01	0.43
1:C:2463:LEU:HD12	1:C:2503:LEU:HA	2.00	0.43
1:A:173:ASP:OD2	1:A:173:ASP:C	2.57	0.43
1:A:188:ILE:HB	1:A:439:ASN:ND2	2.34	0.43
1:B:1507:LEU:CD2	1:B:1522:MET:HB2	2.47	0.43
1:D:3185:ARG:HH21	1:D:3438:ARG:HD3	1.81	0.43
1:D:3298:LEU:HD12	1:D:3298:LEU:HA	1.76	0.43
1:B:1104:ASN:ND2	1:B:1358:LYS:HB2	2.33	0.43
1:C:2327:GLN:HB2	1:D:3136:TYR:HE2	1.83	0.43
1:A:161:THR:O	1:A:164:GLY:N	2.50	0.43
1:D:3547:PRO:O	1:D:3552:GLY:N	2.48	0.43
1:D:3249:ASP:HA	1:D:3328:LEU:CD1	2.48	0.43
1:D:3315:ILE:H	1:D:3315:ILE:HG13	1.52	0.43
1:B:1252:LEU:HD12	1:B:1309:HIS:CG	2.53	0.43
1:C:2427:THR:HG23	1:C:2578:THR:HG23	2.00	0.43
1:A:107:PHE:CD2	1:A:107:PHE:N	2.86	0.43
1:A:308:GLU:HA	1:A:308:GLU:OE2	2.18	0.43
1:A:380:GLU:HG3	1:A:460:TYR:CE2	2.52	0.43
1:A:389:PRO:HG2	1:A:434:VAL:HG22	2.01	0.43
1:A:455:SER:HA	1:A:460:TYR:CD1	2.53	0.43
1:B:1183:LEU:HD21	1:B:1445:GLN:CG	2.48	0.43
1:B:1287:VAL:O	1:B:1288:GLY:C	2.56	0.43
1:B:1463:LEU:HD12	1:B:1503:LEU:HA	2.00	0.43
1:B:1532:LYS:C	1:B:1534:LEU:H	2.22	0.43
1:D:3124:ILE:HD11	1:D:3528:PRO:C	2.39	0.43
1:D:3455:SER:HA	1:D:3460:TYR:CD1	2.53	0.43
1:D:3490:GLU:O	1:D:3493:ALA:HB3	2.18	0.43
1:B:1241:GLN:OE1	1:B:1329:PHE:CZ	2.72	0.43
6:C:4113:HOH:O	1:D:3140:GLU:HB2	2.18	0.43
1:D:3130:TYR:CD2	1:D:3135:GLY:O	2.72	0.43
1:A:216:ARG:HB3	1:A:220:PHE:HD1	1.73	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:276:PRO:HG3	1:A:409:TYR:CD1	2.53	0.43
1:C:2240:ARG:HH12	1:C:2272:GLU:HB2	1.83	0.43
1:C:2465:GLU:OE2	1:C:2468:LYS:CE	2.66	0.43
1:A:363:PRO:C	1:A:365:LEU:N	2.71	0.43
1:C:2034:ASN:HB3	1:C:2037:CYS:SG	2.58	0.43
1:A:249:ASP:HA	1:A:328:LEU:CD1	2.48	0.43
1:C:2341:ILE:HD12	1:C:2534:LEU:O	2.18	0.43
1:D:3240:ARG:HH12	1:D:3272:GLU:HB2	1.83	0.43
1:B:1150:ARG:HD2	1:B:1380:GLU:OE1	2.17	0.43
1:B:1482:THR:CA	1:B:1511:LYS:HB2	2.48	0.43
1:D:3124:ILE:HG12	1:D:3124:ILE:H	1.57	0.43
1:B:1564:ILE:O	1:B:1568:ILE:CD1	2.66	0.43
1:C:2320:HIS:C	1:C:2322:GLU:H	2.21	0.43
1:A:396:ASN:HD22	1:A:401:GLU:HG2	1.78	0.43
1:D:3566:SER:O	1:D:3567:LEU:C	2.56	0.43
1:B:1134:TYR:CD2	1:B:1136:TYR:HE1	2.37	0.43
1:C:2462:SER:CB	1:C:2465:GLU:HG2	2.48	0.43
1:D:3368:ASN:N	1:D:3368:ASN:OD1	2.51	0.43
1:C:2444:VAL:O	1:C:2444:VAL:HG12	2.18	0.43
1:D:3112:ILE:HB	1:D:3357:PHE:CE1	2.54	0.43
1:A:301:TYR:O	1:A:302:ALA:C	2.56	0.43
1:B:1230:LEU:CG	1:B:1337:ILE:HG13	2.46	0.43
1:B:1155:VAL:HG12	1:B:1159:CYS:SG	2.58	0.43
1:D:3089:VAL:O	1:D:3090:HIS:C	2.56	0.43
1:D:3456:ARG:NE	1:D:3502:GLU:OE2	2.51	0.43
1:D:3564:ILE:O	1:D:3568:ILE:HD12	2.18	0.43
1:B:1320:HIS:CD2	1:B:1323:TRP:CE2	3.06	0.43
1:B:1130:TYR:CE2	1:B:1135:GLY:O	2.72	0.43
1:D:3469:ARG:HD2	1:D:3469:ARG:HA	1.77	0.43
1:D:3168:ASN:C	1:D:3170:GLU:N	2.72	0.43
1:C:2108:LEU:HD23	1:C:2111:LEU:HD23	1.99	0.43
1:C:2383:THR:C	1:C:2385:TYR:N	2.70	0.43
1:C:2563:SER:O	1:C:2564:ILE:C	2.57	0.43
1:C:2564:ILE:O	1:C:2568:ILE:CD1	2.66	0.43
1:B:1096:PHE:O	1:B:1098:GLY:N	2.52	0.43
1:B:1089:VAL:O	1:B:1092:ILE:HG12	2.19	0.43
1:B:1184:ARG:HH12	1:B:1441:PRO:HG3	1.82	0.43
1:B:1481:LEU:HD12	1:B:1481:LEU:O	2.19	0.43
1:B:1498:ILE:O	1:B:1501:MET:HB2	2.18	0.43
1:D:3274:ILE:HD11	1:D:3290:GLU:HG3	2.00	0.43
1:D:3434:VAL:HG13	1:D:3508:LEU:CD2	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2320:HIS:C	1:C:2322:GLU:N	2.72	0.43
1:B:1577:PHE:CG	1:B:1578:THR:N	2.87	0.43
1:C:2535:MET:C	1:C:2537:ASN:H	2.21	0.43
1:B:1124:ILE:HG22	1:B:1125:ASP:N	2.33	0.43
1:C:2231:ASN:OD1	1:C:2231:ASN:C	2.56	0.43
1:D:3462:SER:CB	1:D:3465:GLU:HG2	2.48	0.43
1:B:1566:SER:HA	1:B:1569:CYS:CB	2.48	0.43
1:C:2546:LYS:HA	6:C:4145:HOH:O	2.19	0.43
1:B:1065:TYR:HB2	1:B:1066:GLY:H	1.61	0.43
1:D:3531:LEU:HD12	1:D:3531:LEU:HA	1.82	0.43
1:C:2301:TYR:O	1:C:2302:ALA:O	2.36	0.43
1:C:2139:TRP:CZ3	1:D:3538:PRO:HG2	2.53	0.43
1:C:2386:HIS:HB2	1:C:2504:TYR:CE1	2.54	0.43
1:A:301:TYR:O	1:A:304:ILE:HB	2.18	0.43
1:A:403:SER:H	1:A:406:GLN:HB2	1.84	0.43
1:B:1341:ILE:HD13	1:B:1534:LEU:HD12	2.00	0.43
1:A:274:ILE:HD12	1:A:291:VAL:CA	2.49	0.43
1:A:151:ALA:HB2	1:A:529:PHE:HZ	1.82	0.43
1:C:2078:ILE:HD13	1:C:2078:ILE:N	2.33	0.43
1:A:327:GLN:CG	1:B:1136:TYR:CE2	3.02	0.43
1:C:2243:LYS:O	1:C:2253:LYS:HE3	2.18	0.43
1:A:38:SER:C	1:A:40:PRO:HD3	2.39	0.43
1:D:3372:GLN:O	1:D:3374:GLN:N	2.50	0.43
1:B:1315:ILE:HD13	1:B:1558:ILE:HD11	1.99	0.43
1:C:2173:ASP:OD2	1:C:2175:LYS:N	2.51	0.43
1:C:2099:VAL:CA	1:C:2102:ILE:HD12	2.28	0.43
1:D:3124:ILE:HG22	1:D:3125:ASP:N	2.34	0.43
1:D:3442:ILE:N	1:D:3442:ILE:CD1	2.81	0.43
1:D:3566:SER:HA	1:D:3569:CYS:CB	2.48	0.43
1:A:130:TYR:CE2	1:A:135:GLY:O	2.72	0.43
1:B:1078:ILE:HD13	1:B:1078:ILE:N	2.34	0.43
1:D:3038:SER:C	1:D:3040:PRO:HD3	2.38	0.43
1:B:1301:TYR:O	1:B:1304:ILE:HB	2.19	0.42
1:C:2405:LYS:CE	1:C:2405:LYS:H	2.31	0.42
1:D:3112:ILE:O	1:D:3115:TYR:HB3	2.19	0.42
1:A:262:TYR:HA	1:A:303:THR:HG23	2.00	0.42
1:A:427:THR:O	1:A:427:THR:HG22	2.19	0.42
1:A:427:THR:HG23	1:A:578:THR:HG23	2.01	0.42
1:A:185:ARG:NH2	1:A:438:ARG:NE	2.61	0.42
1:B:1273:MET:HE1	1:B:1287:VAL:H	1.83	0.42
1:B:1475:TYR:CD2	1:B:1480:GLU:HG2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1467:ARG:NH2	1:B:1520:GLU:OE1	2.49	0.42
1:D:3226:HIS:C	1:D:3377:ILE:HD12	2.39	0.42
1:A:245:ARG:NH2	1:A:326:GLU:HA	2.33	0.42
1:D:3267:LYS:HB3	6:D:4185:HOH:O	2.17	0.42
1:A:76:THR:O	1:A:79:LYS:HB2	2.19	0.42
1:B:1059:CYS:HB3	1:B:1064:PHE:O	2.18	0.42
1:A:202:ALA:HB2	1:A:348:TYR:CE1	2.55	0.42
1:A:142:PHE:O	1:A:376:ARG:NH2	2.40	0.42
1:A:507:LEU:CD2	1:A:522:MET:HB2	2.49	0.42
1:A:531:LEU:HD12	1:A:531:LEU:HA	1.80	0.42
1:A:229:ASP:OD2	1:A:231:ASN:N	2.50	0.42
1:D:3150:ARG:HD2	1:D:3380:GLU:OE1	2.19	0.42
1:A:243:LYS:O	1:A:253:LYS:HE3	2.19	0.42
1:C:2322:GLU:HA	6:C:4115:HOH:O	2.19	0.42
1:D:3160:PRO:HD2	1:D:3164:GLY:O	2.19	0.42
1:B:1427:THR:CG2	1:B:1578:THR:HA	2.48	0.42
1:C:2280:PRO:HG2	1:C:2283:LEU:HG	2.01	0.42
1:C:2462:SER:O	1:C:2465:GLU:HB2	2.19	0.42
1:B:1073:GLU:O	1:B:1077:ARG:HG2	2.19	0.42
1:C:2246:LEU:HG	1:C:2248:LYS:HB2	2.01	0.42
1:D:3094:THR:HG22	1:D:3354:GLY:O	2.18	0.42
1:C:2274:ILE:HD12	1:C:2291:VAL:HA	2.01	0.42
1:C:2404:PHE:H	1:C:2404:PHE:HD1	1.67	0.42
1:C:2435:ALA:HB2	1:C:2518:PHE:HA	2.00	0.42
1:D:3107:PHE:N	1:D:3107:PHE:CD2	2.87	0.42
1:A:201:PHE:N	1:A:301:TYR:HE2	2.17	0.42
1:A:302:ALA:O	1:A:304:ILE:N	2.52	0.42
1:A:197:MET:O	1:A:198:PHE:C	2.56	0.42
1:A:380:GLU:N	1:A:460:TYR:OH	2.52	0.42
1:A:481:LEU:HD12	1:A:481:LEU:O	2.19	0.42
1:B:1184:ARG:CB	1:B:1439:ASN:HA	2.47	0.42
1:D:3181:VAL:HG12	1:D:3487:MET:CG	2.50	0.42
1:C:2308:GLU:HA	1:C:2308:GLU:OE2	2.19	0.42
1:B:1275:TYR:CE2	1:B:1284:GLN:CA	3.00	0.42
1:B:1563:SER:O	1:B:1564:ILE:C	2.57	0.42
1:C:2547:PRO:CB	1:C:2552:GLY:HA2	2.48	0.42
1:C:2073:GLU:O	1:C:2077:ARG:HG2	2.19	0.42
1:A:309:HIS:HD2	1:A:310:ASN:OD1	2.02	0.42
1:B:1261:VAL:H	1:B:1307:ARG:NH2	2.17	0.42
1:C:2458:MET:O	1:C:2459:LYS:C	2.56	0.42
1:D:3202:ALA:HA	1:D:3348:TYR:HE1	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:113:MET:O	1:A:116:VAL:HG13	2.20	0.42
1:A:534:LEU:HD13	1:A:534:LEU:HA	1.90	0.42
1:B:1089:VAL:O	1:B:1090:HIS:C	2.57	0.42
1:B:1196:MET:HG2	1:B:1429:GLN:O	2.19	0.42
1:B:1444:VAL:O	1:B:1445:GLN:C	2.58	0.42
1:D:3395:PHE:O	1:D:3402:TYR:HD2	2.02	0.42
1:D:3530:SER:C	1:D:3532:LYS:H	2.23	0.42
1:C:2245:ARG:HD2	1:C:2329:PHE:CE1	2.54	0.42
1:D:3323:TRP:CE3	1:D:3327:GLN:HG2	2.54	0.42
1:C:2548:SER:O	1:C:2550:PHE:N	2.53	0.42
1:A:469:ARG:HA	1:A:469:ARG:HD2	1.77	0.42
1:B:1099:VAL:O	1:B:1102:ILE:HB	2.19	0.42
1:D:3357:PHE:HE2	1:D:3359:LEU:HD23	1.81	0.42
1:C:2095:HIS:O	1:C:2100:TRP:HD1	2.02	0.42
1:A:173:ASP:OD2	1:A:175:LYS:N	2.53	0.42
1:B:1162:PRO:HB2	1:B:1171:LEU:HD21	2.01	0.42
1:B:1190:ASP:OD2	1:B:1192:GLN:HB2	2.18	0.42
1:B:1421:GLN:O	1:B:1422:PHE:C	2.58	0.42
1:D:3155:VAL:HG12	1:D:3159:CYS:SG	2.59	0.42
1:D:3128:PRO:HG3	1:D:3376:ARG:NH1	2.34	0.42
1:A:124:ILE:HG22	1:A:125:ASP:N	2.34	0.42
1:C:2500:VAL:HG12	1:C:2500:VAL:O	2.19	0.42
1:D:3568:ILE:HG23	1:D:3572:VAL:CG2	2.48	0.42
1:A:56:LYS:HA	6:A:4007:HOH:O	2.18	0.42
1:B:1094:THR:HG22	1:B:1354:GLY:O	2.20	0.42
1:C:2531:LEU:HA	1:C:2531:LEU:HD12	1.80	0.42
1:C:2150:ARG:HD2	1:C:2380:GLU:OE1	2.19	0.42
1:C:2481:LEU:HD12	1:C:2510:GLU:HA	2.02	0.42
1:C:2521:THR:HG22	1:C:2522:MET:N	2.33	0.42
1:A:404:PHE:H	1:A:405:LYS:HZ2	1.67	0.42
1:A:404:PHE:N	1:A:404:PHE:HD1	2.18	0.42
1:B:1182:LEU:O	1:B:1438:ARG:CA	2.62	0.42
1:B:1205:PHE:CZ	1:B:1344:VAL:HG21	2.54	0.42
1:D:3184:ARG:CD	1:D:3187:PHE:HA	2.37	0.42
1:D:3211:LYS:O	1:D:3212:THR:C	2.58	0.42
1:D:3185:ARG:HE	1:D:3438:ARG:HD3	1.85	0.42
1:D:3458:MET:O	1:D:3459:LYS:C	2.58	0.42
1:D:3467:ARG:NH2	1:D:3520:GLU:OE1	2.52	0.42
1:B:1245:ARG:O	1:B:1253:LYS:HG3	2.19	0.42
1:B:1396:ASN:N	1:B:1396:ASN:HD22	2.17	0.42
1:B:1105(B):ILE:O	1:B:1108:LEU:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1124:ILE:HD11	1:B:1528:PRO:C	2.40	0.42
1:C:2390:LEU:HD21	1:C:2517:ILE:HD11	2.01	0.42
1:C:2462:SER:HB3	1:C:2465:GLU:HG2	2.02	0.42
1:D:3470:PHE:N	1:D:3470:PHE:CD2	2.87	0.42
1:A:344:VAL:HG12	1:A:345:ILE:N	2.34	0.42
1:A:95:HIS:O	1:A:100:TRP:CD1	2.73	0.42
1:C:2391:LEU:HD13	1:C:2404:PHE:HE2	1.84	0.42
1:C:2467:ARG:O	1:C:2472:LEU:HB2	2.19	0.42
1:C:2564:ILE:O	1:C:2568:ILE:HD12	2.19	0.42
1:B:1230:LEU:HD11	1:B:1337:ILE:HA	2.02	0.42
1:A:155:VAL:HG12	1:A:159:CYS:SG	2.59	0.42
1:A:404:PHE:HD1	1:A:404:PHE:H	1.67	0.42
1:A:482:THR:CG2	1:A:509:VAL:HG12	2.49	0.42
1:A:92:ILE:H	1:A:92:ILE:HG12	1.34	0.42
1:B:1198:PHE:HB2	1:B:1580:PHE:HB3	2.00	0.42
1:B:1531:LEU:HD12	1:B:1531:LEU:HA	1.79	0.42
1:D:3467:ARG:O	1:D:3472:LEU:HB2	2.19	0.42
1:D:3503:LEU:O	1:D:3504:TYR:C	2.58	0.42
1:A:320:HIS:C	1:A:322:GLU:H	2.22	0.42
1:A:151:ALA:HB2	1:A:529:PHE:CZ	2.55	0.42
1:C:2302:ALA:O	1:C:2304:ILE:N	2.52	0.42
1:C:2348:TYR:HD2	1:C:2349:VAL:N	2.18	0.42
1:C:2532:LYS:HB3	1:C:2533:GLY:H	1.68	0.42
1:C:2564:ILE:HG23	1:C:2565:GLN:N	2.35	0.42
1:B:1099:VAL:CA	1:B:1102:ILE:HD12	2.29	0.42
1:B:1274:ILE:HD12	1:B:1291:VAL:HA	2.01	0.42
1:B:1404:PHE:N	1:B:1404:PHE:CD1	2.88	0.42
1:D:3530:SER:O	1:D:3532:LYS:N	2.52	0.42
1:B:1112:ILE:HB	1:B:1357:PHE:CE1	2.55	0.42
1:C:2528:PRO:O	1:C:2529:PHE:C	2.58	0.42
1:D:3141:ALA:O	1:D:3143:SER:N	2.53	0.42
1:C:2110:SER:O	1:C:2111:LEU:C	2.57	0.42
1:C:2113:MET:O	1:C:2117:LEU:HD22	2.20	0.42
1:C:2197:MET:HG3	1:C:2578:THR:HG21	2.01	0.42
1:C:2211:LYS:O	1:C:2212:THR:C	2.59	0.42
1:A:563:SER:C	1:A:565:GLN:N	2.72	0.42
1:A:503:LEU:O	1:A:504:TYR:C	2.56	0.42
1:A:532:LYS:O	1:A:535:MET:N	2.53	0.42
1:B:1389:PRO:CB	1:B:1434:VAL:HA	2.49	0.42
1:D:3404:PHE:HD1	1:D:3404:PHE:N	2.17	0.42
1:D:3433:ARG:HH21	1:D:3512:PRO:CB	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3384:LEU:HB2	5:D:3701:PGX:O3	2.19	0.42
1:C:2230:LEU:CG	1:C:2337:ILE:HG13	2.44	0.42
1:D:3295:VAL:HB	1:D:3298:LEU:HB2	2.02	0.42
1:B:1568:ILE:HG23	1:B:1572:VAL:CG2	2.50	0.42
1:D:3577:PHE:CG	1:D:3578:THR:N	2.87	0.42
1:D:3564:ILE:HG22	6:D:4157:HOH:O	2.19	0.42
1:A:523:VAL:HG12	1:A:524:GLU:N	2.33	0.42
1:D:3074:PHE:O	1:D:3077:ARG:N	2.53	0.42
1:D:3256:VAL:HA	1:D:3260:GLU:O	2.20	0.42
1:A:315:ILE:HG13	1:A:315:ILE:H	1.56	0.42
1:C:2404:PHE:CD1	1:C:2404:PHE:N	2.85	0.42
1:C:2507:LEU:CD2	1:C:2522:MET:HB2	2.50	0.42
1:D:3231:ASN:O	1:D:3235:GLY:N	2.52	0.42
1:D:3105(D):ILE:CB	1:D:3108:LEU:HD12	2.49	0.42
1:D:3357:PHE:CD2	1:D:3359:LEU:HD23	2.55	0.42
1:A:103:VAL:C	1:A:105:ASN:N	2.73	0.42
1:A:116:VAL:CG2	1:A:117:LEU:N	2.82	0.42
1:A:350:GLN:NE2	1:A:359:LEU:H	2.18	0.42
1:A:185:ARG:HH21	1:A:438:ARG:HD3	1.85	0.42
1:A:226:HIS:C	1:A:377:ILE:HD12	2.40	0.42
1:A:478:PHE:O	1:A:482:THR:OG1	2.37	0.42
1:A:487:MET:O	1:A:490:GLU:HB3	2.20	0.42
1:B:1384:LEU:HB3	1:B:1522:MET:CE	2.50	0.42
1:B:1450:ALA:O	1:B:1451:SER:C	2.57	0.42
1:B:1530:SER:C	1:B:1532:LYS:H	2.23	0.42
1:D:3481:LEU:O	1:D:3511:LYS:N	2.53	0.42
1:D:3295:VAL:HG12	1:D:3298:LEU:H	1.85	0.42
1:D:3427:THR:HG23	1:D:3578:THR:HG23	2.02	0.42
1:A:160:PRO:HD2	1:A:164:GLY:O	2.20	0.42
1:C:2553:GLU:OE1	1:C:2553:GLU:CA	2.62	0.42
1:C:2538:PRO:HG2	1:D:3139:TRP:HZ3	1.85	0.42
1:B:1528:PRO:O	1:B:1529:PHE:C	2.58	0.42
1:A:234:TYR:HB2	1:A:333:ARG:NH1	2.35	0.42
1:A:48:MET:HE1	1:B:1551:GLY:O	2.19	0.42
1:D:3318:GLN:OE1	1:D:3318:GLN:HA	2.19	0.42
1:B:1126:SER:HA	1:B:1127:PRO:C	2.38	0.42
1:C:2262:TYR:HA	1:C:2303:THR:HG23	2.02	0.41
1:C:2173:ASP:C	1:C:2173:ASP:OD2	2.58	0.41
1:C:2530:SER:O	1:C:2532:LYS:N	2.52	0.41
1:D:3229:ASP:OD2	1:D:3231:ASN:N	2.53	0.41
1:D:3099:VAL:O	1:D:3102:ILE:HB	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:454:GLN:O	1:A:456:ARG:N	2.52	0.41
1:B:1371:PHE:CE1	1:B:1532:LYS:HE2	2.55	0.41
1:D:3092:ILE:H	1:D:3092:ILE:HG12	1.36	0.41
1:D:3345:ILE:CG1	1:D:3534:LEU:HG	2.50	0.41
1:B:1141:ALA:O	1:B:1143:SER:N	2.52	0.41
1:B:1465:GLU:CA	1:B:1465:GLU:OE2	2.68	0.41
1:D:3073:GLU:O	1:D:3076:THR:HB	2.20	0.41
1:C:2038:SER:C	1:C:2040:PRO:HD3	2.40	0.41
1:D:3548:SER:O	1:D:3550:PHE:N	2.53	0.41
1:C:2249:ASP:HA	1:C:2328:LEU:CD1	2.50	0.41
1:B:1557:LYS:HA	1:B:1560:ASN:HD22	1.85	0.41
1:C:2404:PHE:H	1:C:2405:LYS:HZ2	1.66	0.41
1:B:1099:VAL:HA	1:B:1102:ILE:CD1	2.29	0.41
1:A:403:SER:OG	1:A:405:LYS:HD2	2.20	0.41
1:A:444:VAL:HG12	1:A:444:VAL:O	2.20	0.41
1:B:1535:MET:O	1:B:1540:CYS:HB2	2.20	0.41
1:D:3274:ILE:HD12	1:D:3291:VAL:CA	2.49	0.41
1:C:2064:PHE:CE2	1:C:2072:PRO:HB3	2.54	0.41
1:B:1368:ASN:OD1	1:B:1368:ASN:N	2.53	0.41
1:B:1301:TYR:O	1:B:1302:ALA:O	2.38	0.41
1:C:2350:GLN:NE2	1:C:2359:LEU:H	2.17	0.41
1:C:2404:PHE:HD1	1:C:2404:PHE:N	2.18	0.41
1:C:2184:ARG:NE	1:C:2439:ASN:OD1	2.48	0.41
1:C:2504:TYR:HB3	1:C:2505:PRO:CD	2.45	0.41
1:A:531:LEU:O	1:A:535:MET:HB2	2.21	0.41
1:B:1275:TYR:HE2	1:B:1284:GLN:CA	2.34	0.41
1:B:1202:ALA:HA	1:B:1348:TYR:HE1	1.85	0.41
1:D:3316:LEU:O	1:D:3319:GLU:N	2.52	0.41
1:B:1136:TYR:HB2	6:B:4080:HOH:O	2.20	0.41
1:A:372:GLN:O	1:A:374:GLN:N	2.51	0.41
1:A:108:LEU:HA	1:A:111:LEU:HD23	2.02	0.41
1:C:2096:PHE:O	1:C:2098:GLY:N	2.53	0.41
1:A:352:LEU:HG	1:A:518:PHE:HE2	1.86	0.41
1:A:394:THR:O	1:A:429:GLN:NE2	2.47	0.41
1:A:386:HIS:HD2	1:A:451:SER:HB3	1.85	0.41
1:A:509:VAL:O	1:A:510:GLU:C	2.59	0.41
1:A:532:LYS:HB3	1:A:533:GLY:H	1.70	0.41
1:B:1403:SER:HB2	1:B:1405:LYS:HZ2	1.86	0.41
1:B:1517:ILE:O	1:B:1517:ILE:HG13	2.20	0.41
1:B:1532:LYS:O	1:B:1535:MET:N	2.53	0.41
1:A:274:ILE:HD11	1:A:290:GLU:HG3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3383:THR:C	1:D:3385:TYR:N	2.74	0.41
1:D:3404:PHE:HD1	1:D:3404:PHE:H	1.68	0.41
1:A:295:VAL:HG12	1:A:297:GLY:H	1.85	0.41
1:C:2275:TYR:CE2	1:C:2284:GLN:CA	3.03	0.41
1:C:2275:TYR:HE2	1:C:2284:GLN:HA	1.84	0.41
1:B:1347:ASP:OD2	1:B:1564:ILE:HG22	2.20	0.41
1:B:1427:THR:HG23	1:B:1578:THR:HG23	2.02	0.41
1:C:2151:ALA:HB2	1:C:2529:PHE:CZ	2.53	0.41
1:C:2120:ARG:HH11	1:C:2527:ALA:HB1	1.83	0.41
1:C:2074:PHE:O	1:C:2077:ARG:N	2.53	0.41
1:B:1523:VAL:HG12	1:B:1524:GLU:N	2.36	0.41
1:A:74:PHE:O	1:A:75:LEU:C	2.59	0.41
1:D:3059:CYS:HA	1:D:3062:THR:HG21	2.01	0.41
1:B:1308:GLU:OE2	1:B:1311:ARG:HD3	2.21	0.41
1:C:2139:TRP:HZ3	1:D:3538:PRO:HG2	1.86	0.41
1:C:2185:ARG:HH21	1:C:2438:ARG:HD3	1.85	0.41
1:C:2384:LEU:HB3	1:C:2522:MET:CE	2.50	0.41
1:C:2389:PRO:CB	1:C:2434:VAL:HA	2.51	0.41
1:A:103:VAL:O	1:A:105:ASN:N	2.53	0.41
1:B:1383:THR:O	1:B:1385:TYR:N	2.54	0.41
1:B:1464:ASN:HD21	1:B:1475:TYR:N	2.19	0.41
1:B:1530:SER:O	1:B:1532:LYS:N	2.53	0.41
1:D:3274:ILE:HD12	1:D:3291:VAL:HG23	2.01	0.41
1:D:3196:MET:HA	1:D:3196:MET:CE	2.51	0.41
1:D:3148:TYR:CZ	1:D:3221:THR:HB	2.55	0.41
1:D:3394:THR:O	1:D:3429:GLN:NE2	2.46	0.41
1:D:3380:GLU:N	1:D:3460:TYR:OH	2.53	0.41
1:B:1295:VAL:HG12	1:B:1298:LEU:H	1.85	0.41
1:C:2309:HIS:HD2	1:C:2310:ASN:OD1	2.03	0.41
1:A:73:GLU:O	1:A:77:ARG:HG2	2.20	0.41
1:A:50:THR:CG2	1:A:56:LYS:CB	2.98	0.41
1:B:1246:LEU:HG	1:B:1248:LYS:HB2	2.02	0.41
1:B:1583:GLN:N	1:B:1583:GLN:CD	2.74	0.41
1:C:2156:ALA:C	1:C:2158:ASP:N	2.73	0.41
1:C:2389:PRO:HB2	1:C:2434:VAL:HA	2.03	0.41
1:C:2530:SER:C	1:C:2532:LYS:H	2.23	0.41
1:B:1096:PHE:O	1:B:1097:LYS:C	2.58	0.41
1:D:3112:ILE:O	1:D:3116:VAL:HG13	2.21	0.41
1:B:1383:THR:C	1:B:1385:TYR:N	2.72	0.41
1:B:1434:VAL:HG13	1:B:1508:LEU:CD2	2.50	0.41
1:D:3377:ILE:HA	6:D:4180:HOH:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3450:ALA:O	1:D:3454:GLN:HG3	2.21	0.41
1:D:3507:LEU:CD2	1:D:3522:MET:HB2	2.51	0.41
1:C:2295:VAL:HB	1:C:2298:LEU:HB2	2.03	0.41
1:D:3056:LYS:HG3	1:D:3057:CYS:N	2.36	0.41
1:A:327:GLN:HG3	1:B:1136:TYR:CE2	2.55	0.41
1:D:3123:LEU:O	1:D:3469:ARG:NH2	2.54	0.41
1:A:39:ASN:ND2	1:A:39:ASN:N	2.68	0.41
1:C:2186:GLU:N	6:C:4100:HOH:O	2.52	0.41
1:A:95:HIS:O	1:A:100:TRP:HD1	2.02	0.41
1:C:2454:GLN:O	1:C:2456:ARG:N	2.53	0.41
1:D:3096:PHE:O	1:D:3097:LYS:C	2.59	0.41
1:D:3105(D):ILE:CG2	1:D:3108:LEU:HB2	2.51	0.41
1:A:178:LEU:HD22	1:A:183:LEU:CD1	2.50	0.41
1:A:514:PRO:O	1:A:515:ASP:CB	2.66	0.41
1:A:197:MET:HG3	1:A:578:THR:HG21	2.03	0.41
1:B:1481:LEU:O	1:B:1511:LYS:N	2.53	0.41
1:B:1535:MET:C	1:B:1537:ASN:N	2.74	0.41
1:D:3190:ASP:OD1	1:D:3192:GLN:HG3	2.20	0.41
1:A:137:LYS:HD3	1:B:1549:THR:HG23	2.02	0.41
1:A:551:GLY:O	1:B:1048:MET:HE1	2.21	0.41
1:B:1309:HIS:O	1:B:1312:VAL:N	2.53	0.41
1:C:2185:ARG:HE	1:C:2438:ARG:HD3	1.86	0.41
1:D:3535:MET:O	1:D:3540:CYS:HB2	2.21	0.41
1:A:184:ARG:NH2	1:A:391:LEU:O	2.48	0.41
1:A:516:ALA:HB1	6:A:4048:HOH:O	2.21	0.41
1:B:1487:MET:O	1:B:1488:ALA:C	2.59	0.41
1:B:1522:MET:O	1:B:1522:MET:HG3	2.21	0.41
1:D:3218:PRO:C	1:D:3458:MET:CE	2.88	0.41
1:D:3486:GLU:HB3	1:D:3487:MET:H	1.73	0.41
1:D:3514:PRO:O	1:D:3515:ASP:CB	2.69	0.41
1:D:3243:LYS:O	1:D:3253:LYS:HE3	2.21	0.41
1:C:2065:TYR:N	1:C:2071:THR:O	2.49	0.41
1:C:2229:ASP:OD2	1:C:2229:ASP:C	2.58	0.41
1:D:3462:SER:HB3	1:D:3465:GLU:HG2	2.03	0.41
1:A:366:LEU:C	1:A:368:ASN:H	2.24	0.41
1:C:2372:GLN:O	1:C:2374:GLN:N	2.50	0.41
1:C:2415:LEU:HA	1:C:2415:LEU:HD23	1.83	0.41
1:C:2089:VAL:O	1:C:2092:ILE:HG12	2.21	0.41
1:C:2162:PRO:HB2	1:C:2171:LEU:CD2	2.51	0.41
1:C:2341:ILE:HD13	1:C:2534:LEU:CD1	2.50	0.41
1:C:2449:LYS:HA	1:C:2452:ILE:CD1	2.44	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2218:PRO:C	1:C:2458:MET:CE	2.89	0.41
1:C:2482:THR:CG2	1:C:2509:VAL:HG12	2.51	0.41
1:C:2509:VAL:O	1:C:2510:GLU:C	2.59	0.41
1:C:2366:LEU:HA	1:C:2369:GLN:CG	2.51	0.41
1:C:2185:ARG:NH2	1:C:2438:ARG:NE	2.63	0.41
1:C:2347:ASP:OD2	1:C:2564:ILE:HG22	2.21	0.41
1:D:3103:VAL:C	1:D:3105:ASN:N	2.75	0.41
1:A:117:LEU:HA	1:A:117:LEU:HD13	1.81	0.41
1:C:2096:PHE:O	1:C:2099:VAL:N	2.54	0.41
1:A:156:ALA:HB3	1:A:159:CYS:SG	2.61	0.41
1:A:530:SER:C	1:A:532:LYS:H	2.24	0.41
1:B:1132:VAL:HG21	1:B:1219:GLY:HA3	2.03	0.41
1:A:132:VAL:HG23	6:A:4038:HOH:O	2.21	0.41
1:A:464:ASN:HD21	1:A:475:TYR:N	2.18	0.41
1:B:1503:LEU:O	1:B:1504:TYR:C	2.59	0.41
1:D:3124:ILE:HG22	1:D:3125:ASP:H	1.85	0.41
1:D:3175:LYS:O	1:D:3179:GLU:HG3	2.21	0.41
1:D:3429:GLN:HG2	1:D:3429:GLN:O	2.20	0.41
1:D:3499:ASP:C	1:D:3501:MET:H	2.23	0.41
1:D:3504:TYR:O	1:D:3507:LEU:HB2	2.20	0.41
1:B:1110:SER:O	1:B:1111:LEU:C	2.59	0.41
1:A:553:GLU:OE1	1:A:553:GLU:CA	2.60	0.41
1:A:56:LYS:HG3	1:A:57:CYS:N	2.35	0.41
1:C:2039:ASN:N	1:C:2039:ASN:ND2	2.69	0.41
1:D:3152:LEU:HD12	1:D:3466:TYR:CD1	2.56	0.41
1:A:368:ASN:N	1:A:368:ASN:OD1	2.54	0.41
1:D:3479:GLU:O	1:D:3483:GLY:N	2.49	0.41
1:C:2287:VAL:O	1:C:2288:GLY:C	2.58	0.41
1:D:3105(D):ILE:HG22	1:D:3108:LEU:H	1.86	0.41
1:A:563:SER:O	1:A:564:ILE:C	2.59	0.41
1:A:486:GLU:HB3	1:A:487:MET:H	1.70	0.41
1:B:1273:MET:CE	1:B:1287:VAL:HG22	2.34	0.41
1:B:1509:VAL:O	1:B:1510:GLU:C	2.59	0.41
1:D:3444:VAL:HG12	1:D:3444:VAL:O	2.21	0.41
1:C:2295:VAL:HG12	1:C:2298:LEU:H	1.86	0.41
1:C:2216:ARG:HB3	1:C:2220:PHE:HD1	1.76	0.41
1:A:428:ARG:O	1:A:582:VAL:HG21	2.21	0.41
1:D:3280:PRO:HG2	1:D:3283:LEU:HG	2.03	0.41
1:D:3252:LEU:HD12	1:D:3309:HIS:CG	2.56	0.41
1:D:3073:GLU:O	1:D:3077:ARG:HG2	2.21	0.41
1:C:2465:GLU:OE2	1:C:2468:LYS:HE2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2256:VAL:HA	1:C:2260:GLU:O	2.21	0.41
1:B:1249:ASP:HA	1:B:1328:LEU:CD1	2.50	0.41
1:B:1470:PHE:N	1:B:1470:PHE:CD2	2.88	0.41
1:C:2300:MET:O	1:C:2304:ILE:HG13	2.21	0.40
1:C:2128:PRO:HG3	1:C:2376:ARG:HH11	1.86	0.40
1:C:2498:ILE:CG2	1:C:2499:ASP:N	2.83	0.40
1:C:2534:LEU:HD22	5:C:2701:PGX:C18	2.43	0.40
1:A:105(A):ILE:O	1:A:108:LEU:N	2.55	0.40
1:A:110:SER:O	1:A:111:LEU:C	2.60	0.40
1:A:113:MET:O	1:A:116:VAL:HG22	2.21	0.40
1:A:162:PRO:HB2	1:A:171:LEU:CD2	2.51	0.40
1:A:421:GLN:O	1:A:422:PHE:C	2.59	0.40
1:A:530:SER:O	1:A:532:LYS:N	2.54	0.40
1:D:3205:PHE:CZ	1:D:3344:VAL:HG21	2.56	0.40
1:D:3436:GLY:HA2	1:D:3512:PRO:HG2	2.02	0.40
1:D:3475:TYR:CD1	1:D:3481:LEU:HB2	2.56	0.40
1:A:295:VAL:HG12	1:A:298:LEU:H	1.86	0.40
1:C:2076:THR:O	1:C:2079:LYS:HB2	2.21	0.40
1:B:1268:ASP:OD1	1:B:1268:ASP:N	2.53	0.40
1:A:268:ASP:N	1:A:268:ASP:OD1	2.54	0.40
1:B:1302:ALA:O	1:B:1304:ILE:N	2.54	0.40
1:C:2148:TYR:HD2	1:C:2219:GLY:O	2.04	0.40
1:C:2503:LEU:HG	1:C:2507:LEU:CD1	2.51	0.40
1:C:2563:SER:C	1:C:2565:GLN:N	2.72	0.40
1:D:3103:VAL:HG12	1:D:3104:ASN:N	2.37	0.40
1:A:132:VAL:HG21	1:A:219:GLY:HA3	2.03	0.40
1:A:341:ILE:HD13	1:A:534:LEU:CD1	2.51	0.40
1:A:383:THR:O	1:A:384:LEU:C	2.59	0.40
1:A:389:PRO:HB2	1:A:434:VAL:HA	2.02	0.40
1:A:454:GLN:CA	1:A:457:GLU:HG3	2.51	0.40
1:B:1388:HIS:NE2	1:B:1447:VAL:CG1	2.85	0.40
1:B:1209:PHE:CZ	5:B:1701:PGX:H192	2.56	0.40
1:D:3402:TYR:OH	1:D:3417:HIS:CE1	2.74	0.40
1:C:2280:PRO:HG2	1:C:2283:LEU:CG	2.52	0.40
1:B:1320:HIS:CD2	1:B:1323:TRP:CZ2	3.09	0.40
1:B:1407:PHE:HD1	1:B:1413:ILE:HD13	1.87	0.40
1:C:2470:PHE:CD2	1:C:2470:PHE:N	2.88	0.40
1:C:2085:THR:O	1:C:2088:THR:HB	2.21	0.40
1:C:2162:PRO:HB2	1:C:2171:LEU:HD21	2.04	0.40
1:C:2481:LEU:HD12	1:C:2481:LEU:O	2.21	0.40
1:D:3095:HIS:C	1:D:3097:LYS:N	2.74	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:369:GLN:O	1:A:371:PHE:N	2.54	0.40
1:A:481:LEU:O	1:A:511:LYS:N	2.55	0.40
1:B:1274:ILE:HD11	1:B:1290:GLU:HG3	2.04	0.40
1:B:1433:ARG:HH21	1:B:1512:PRO:CB	2.35	0.40
1:D:3498:ILE:O	1:D:3501:MET:HB2	2.21	0.40
1:C:2308:GLU:OE2	1:C:2311:ARG:HD3	2.21	0.40
1:C:2336:LEU:O	1:C:2337:ILE:C	2.59	0.40
1:B:1245:ARG:NH2	1:B:1326:GLU:HA	2.37	0.40
1:A:204:HIS:CD2	1:A:292:PHE:CE2	3.09	0.40
1:D:3427:THR:CG2	1:D:3578:THR:HA	2.50	0.40
1:C:2428:ARG:O	1:C:2582:VAL:HG21	2.22	0.40
1:D:3050:THR:CG2	1:D:3056:LYS:CB	2.99	0.40
1:A:65:TYR:N	1:A:71:THR:O	2.52	0.40
1:C:2093:LEU:HB3	1:C:2355:TYR:CD1	2.56	0.40
1:B:1262:TYR:HA	1:B:1303:THR:HG23	2.02	0.40
1:C:2301:TYR:O	1:C:2304:ILE:HB	2.21	0.40
1:C:2454:GLN:C	1:C:2456:ARG:N	2.74	0.40
1:D:3201:PHE:N	1:D:3301:TYR:HE2	2.19	0.40
1:A:304:ILE:HG22	1:A:571:ASN:HD22	1.86	0.40
1:A:223:GLY:HA2	1:A:236:GLU:OE1	2.21	0.40
1:B:1437:GLY:O	1:B:1438:ARG:C	2.59	0.40
1:B:1450:ALA:O	1:B:1452:ILE:N	2.54	0.40
1:B:1514:PRO:O	1:B:1515:ASP:CB	2.70	0.40
1:A:273:MET:CE	1:A:287:VAL:H	2.34	0.40
1:A:274:ILE:HD12	1:A:291:VAL:HG23	2.04	0.40
1:D:3198:PHE:O	1:D:3199:ALA:C	2.60	0.40
1:D:3132:VAL:HG21	1:D:3219:GLY:HA3	2.03	0.40
1:D:3383:THR:O	1:D:3385:TYR:N	2.54	0.40
1:D:3464:ASN:HD21	1:D:3475:TYR:N	2.19	0.40
1:B:1295:VAL:O	1:B:1297:GLY:N	2.55	0.40
1:B:1112:ILE:O	1:B:1115:TYR:N	2.54	0.40
1:B:1357:PHE:CD2	1:B:1359:LEU:HD23	2.56	0.40
1:C:2124:ILE:HD11	1:C:2528:PRO:C	2.41	0.40
1:A:75:LEU:O	1:A:75:LEU:HD12	2.21	0.40
1:A:47:CYS:SG	1:A:55:TYR:HD1	2.44	0.40
1:A:99:VAL:O	1:A:102:ILE:HB	2.21	0.40
1:C:2112:ILE:O	1:C:2116:VAL:HG13	2.21	0.40
1:A:142:PHE:CE2	1:B:1538:PRO:HG3	2.56	0.40
1:A:454:GLN:C	1:A:456:ARG:N	2.75	0.40
1:A:498:ILE:CG2	1:A:499:ASP:N	2.84	0.40
1:A:481:LEU:HD12	1:A:510:GLU:HA	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1211:LYS:O	1:B:1212:THR:C	2.59	0.40
1:B:1531:LEU:O	1:B:1535:MET:HB2	2.21	0.40
1:A:231:ASN:O	1:A:235:GLY:N	2.55	0.40
1:D:3273:MET:CE	1:D:3287:VAL:H	2.34	0.40
1:D:3475:TYR:CD2	1:D:3480:GLU:HG2	2.56	0.40
1:D:3428:ARG:O	1:D:3582:VAL:HG21	2.22	0.40
1:A:295:VAL:O	1:A:298:LEU:N	2.55	0.40
1:A:245:ARG:O	1:A:253:LYS:HG3	2.21	0.40
1:B:1348:TYR:HD2	1:B:1349:VAL:N	2.20	0.40
1:C:2320:HIS:CD2	1:C:2323:TRP:CE2	3.10	0.40
1:D:3136:TYR:CD1	1:D:3136:TYR:C	2.94	0.40
1:D:3216:ARG:HB3	1:D:3220:PHE:HD1	1.79	0.40
1:A:525:LEU:C	1:A:528:PRO:HD2	2.41	0.40
1:C:2535:MET:O	1:C:2540:CYS:HB2	2.22	0.40
1:C:2538:PRO:HG2	1:D:3139:TRP:CZ3	2.57	0.40
1:D:3564:ILE:HG13	1:D:3568:ILE:HD13	2.02	0.40
1:B:1034:ASN:HA	1:B:1035:PRO:HD2	1.86	0.40
1:C:2461:GLN:H	1:C:2466:TYR:HE2	1.67	0.40
1:D:3036:CYS:O	1:D:3037:CYS:C	2.60	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	550/552 (100%)	374 (68%)	124 (22%)	52 (10%)	1	3
1	B	550/552 (100%)	379 (69%)	119 (22%)	52 (10%)	1	3
1	C	550/552 (100%)	372 (68%)	120 (22%)	58 (10%)	1	3
1	D	550/552 (100%)	376 (68%)	121 (22%)	53 (10%)	1	3
All	All	2200/2208 (100%)	1501 (68%)	484 (22%)	215 (10%)	1	3

All (215) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	121	SER
1	A	122	TYR
1	A	176	GLU
1	A	180	LYS
1	A	348	TYR
1	A	386	HIS
1	A	400	GLN
1	A	429	GLN
1	A	486	GLU
1	A	510	GLU
1	A	514	PRO
1	B	1121	SER
1	B	1122	TYR
1	B	1176	GLU
1	B	1180	LYS
1	B	1348	TYR
1	B	1386	HIS
1	B	1400	GLN
1	B	1429	GLN
1	B	1486	GLU
1	B	1510	GLU
1	C	2121	SER
1	C	2122	TYR
1	C	2176	GLU
1	C	2180	LYS
1	C	2181	VAL
1	C	2348	TYR
1	C	2386	HIS
1	C	2400	GLN
1	C	2429	GLN
1	C	2486	GLU
1	C	2500	VAL
1	C	2510	GLU
1	C	2514	PRO
1	D	3121	SER
1	D	3122	TYR
1	D	3176	GLU
1	D	3180	LYS
1	D	3348	TYR
1	D	3386	HIS
1	D	3400	GLN
1	D	3429	GLN

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Mol	Chain	Res	Type
1	D	3486	GLU
1	D	3510	GLU
1	A	96	PHE
1	A	120	ARG
1	A	141	ALA
1	A	142	PHE
1	A	177	VAL
1	A	181	VAL
1	A	292	PHE
1	A	500	VAL
1	A	533	GLY
1	A	536	GLY
1	A	539	ILE
1	A	549	THR
1	B	1096	PHE
1	B	1120	ARG
1	B	1141	ALA
1	B	1142	PHE
1	B	1181	VAL
1	B	1292	PHE
1	B	1302	ALA
1	B	1423	VAL
1	B	1458	MET
1	B	1500	VAL
1	B	1514	PRO
1	B	1533	GLY
1	B	1536	GLY
1	B	1539	ILE
1	B	1549	THR
1	C	2096	PHE
1	C	2120	ARG
1	C	2141	ALA
1	C	2142	PHE
1	C	2177	VAL
1	C	2292	PHE
1	C	2302	ALA
1	C	2459	LYS
1	C	2512	PRO
1	C	2533	GLY
1	C	2539	ILE
1	D	3096	PHE
1	D	3097	LYS

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Mol	Chain	Res	Type
1	D	3141	ALA
1	D	3142	PHE
1	D	3177	VAL
1	D	3181	VAL
1	D	3292	PHE
1	D	3500	VAL
1	D	3514	PRO
1	D	3533	GLY
1	D	3539	ILE
1	A	97	LYS
1	A	106	PRO
1	A	302	ALA
1	A	367	PHE
1	A	451	SER
1	A	458	MET
1	A	459	LYS
1	A	512	PRO
1	B	1097	LYS
1	B	1106	PRO
1	B	1177	VAL
1	B	1373	TYR
1	B	1512	PRO
1	C	2097	LYS
1	C	2104	ASN
1	C	2106	PRO
1	C	2303	THR
1	C	2367	PHE
1	C	2423	VAL
1	C	2458	MET
1	C	2531	LEU
1	C	2536	GLY
1	C	2549	THR
1	D	3120	ARG
1	D	3302	ALA
1	D	3423	VAL
1	D	3451	SER
1	D	3458	MET
1	D	3459	LYS
1	D	3512	PRO
1	D	3536	GLY
1	D	3549	THR
1	A	104	ASN

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Mol	Chain	Res	Type
1	A	303	THR
1	A	373	TYR
1	A	423	VAL
1	A	447	VAL
1	A	506	ALA
1	B	1201	PHE
1	B	1303	THR
1	B	1309	HIS
1	B	1317	LYS
1	B	1367	PHE
1	B	1370	GLN
1	B	1445	GLN
1	B	1459	LYS
1	B	1531	LEU
1	B	1558	ILE
1	C	2370	GLN
1	C	2451	SER
1	C	2496	SER
1	D	3106	PRO
1	D	3201	PHE
1	D	3367	PHE
1	D	3445	GLN
1	D	3454	GLN
1	D	3528	PRO
1	D	3531	LEU
1	D	3558	ILE
1	A	201	PHE
1	A	309	HIS
1	A	445	GLN
1	A	454	GLN
1	A	496	SER
1	A	528	PRO
1	A	531	LEU
1	B	1212	THR
1	B	1284	GLN
1	B	1447	VAL
1	B	1454	GLN
1	B	1496	SER
1	B	1528	PRO
1	C	2037	CYS
1	C	2194	SER
1	C	2201	PHE

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Mol	Chain	Res	Type
1	C	2212	THR
1	C	2309	HIS
1	C	2373	TYR
1	C	2384	LEU
1	C	2445	GLN
1	C	2454	GLN
1	C	2528	PRO
1	D	3228	VAL
1	D	3303	THR
1	D	3309	HIS
1	D	3370	GLN
1	D	3373	TYR
1	D	3447	VAL
1	D	3496	SER
1	D	3554	VAL
1	A	212	THR
1	A	277	PRO
1	A	554	VAL
1	A	558	ILE
1	B	1132	VAL
1	B	1277	PRO
1	B	1554	VAL
1	C	2364	GLU
1	C	2447	VAL
1	C	2506	ALA
1	C	2558	ILE
1	C	2565	GLN
1	D	3277	PRO
1	D	3565	GLN
1	A	132	VAL
1	C	2128	PRO
1	C	2277	PRO
1	C	2554	VAL
1	B	1128	PRO
1	B	1430	ILE
1	C	2132	VAL
1	D	3132	VAL
1	A	430	ILE
1	A	505	PRO
1	B	1538	PRO
1	C	2505	PRO
1	D	3128	PRO

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Mol	Chain	Res	Type
1	D	3430	ILE
1	A	128	PRO
1	C	2538	PRO
1	D	3505	PRO
1	D	3538	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	493/493 (100%)	391 (79%)	102 (21%)	1	7
1	B	493/493 (100%)	391 (79%)	102 (21%)	1	7
1	C	493/493 (100%)	393 (80%)	100 (20%)	1	7
1	D	493/493 (100%)	394 (80%)	99 (20%)	1	8
All	All	1972/1972 (100%)	1569 (80%)	403 (20%)	1	7

All (403) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	46	GLU
1	A	48	MET
1	A	49	SER
1	A	54	GLN
1	A	65	TYR
1	A	70	THR
1	A	77	ARG
1	A	78	ILE
1	A	85	THR
1	A	89	VAL
1	A	90	HIS
1	A	92	ILE
1	A	93	LEU
1	A	107	PHE
1	A	111	LEU
1	A	117	LEU

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Mol	Chain	Res	Type
1	A	119	SER
1	A	120	ARG
1	A	121	SER
1	A	124	ILE
1	A	130	TYR
1	A	136	TYR
1	A	137	LYS
1	A	138	SER
1	A	146	SER
1	A	158	ASP
1	A	161	THR
1	A	165	VAL
1	A	171	LEU
1	A	173	ASP
1	A	177	VAL
1	A	178	LEU
1	A	181	VAL
1	A	185	ARG
1	A	190	ASP
1	A	192	GLN
1	A	197	MET
1	A	203	GLN
1	A	207	HIS
1	A	209	PHE
1	A	215	LYS
1	A	221	THR
1	A	231	ASN
1	A	236	GLU
1	A	241	GLN
1	A	246	LEU
1	A	248	LYS
1	A	249	ASP
1	A	254	TYR
1	A	265	THR
1	A	268	ASP
1	A	274	ILE
1	A	289	GLN
1	A	298	LEU
1	A	300	MET
1	A	301	TYR
1	A	319	GLU
1	A	322	GLU

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Mol	Chain	Res	Type
1	A	326	GLU
1	A	334	LEU
1	A	337	ILE
1	A	353	SER
1	A	358	LYS
1	A	376	ARG
1	A	377	ILE
1	A	385	TYR
1	A	396	ASN
1	A	405	LYS
1	A	407	PHE
1	A	409	TYR
1	A	412	SER
1	A	416	GLU
1	A	419	LEU
1	A	420	THR
1	A	430	ILE
1	A	438	ARG
1	A	445	GLN
1	A	455	SER
1	A	457	GLU
1	A	462	SER
1	A	463	LEU
1	A	469	ARG
1	A	471	SER
1	A	482	THR
1	A	484	GLU
1	A	486	GLU
1	A	496	SER
1	A	501	MET
1	A	520	GLU
1	A	522	MET
1	A	524	GLU
1	A	525	LEU
1	A	531	LEU
1	A	532	LYS
1	A	534	LEU
1	A	535	MET
1	A	539	ILE
1	A	543	GLN
1	A	549	THR
1	A	569	CYS

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Mol	Chain	Res	Type
1	A	575	CYS
1	A	581	ASN
1	B	1046	GLU
1	B	1048	MET
1	B	1049	SER
1	B	1054	GLN
1	B	1065	TYR
1	B	1070	THR
1	B	1077	ARG
1	B	1078	ILE
1	B	1085	THR
1	B	1089	VAL
1	B	1090	HIS
1	B	1092	ILE
1	B	1093	LEU
1	B	1107	PHE
1	B	1111	LEU
1	B	1117	LEU
1	B	1119	SER
1	B	1120	ARG
1	B	1121	SER
1	B	1124	ILE
1	B	1130	TYR
1	B	1136	TYR
1	B	1137	LYS
1	B	1138	SER
1	B	1146	SER
1	B	1158	ASP
1	B	1161	THR
1	B	1165	VAL
1	B	1171	LEU
1	B	1173	ASP
1	B	1177	VAL
1	B	1178	LEU
1	B	1181	VAL
1	B	1185	ARG
1	B	1190	ASP
1	B	1192	GLN
1	B	1197	MET
1	B	1203	GLN
1	B	1207	HIS
1	B	1209	PHE

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Mol	Chain	Res	Type
1	B	1215	LYS
1	B	1221	THR
1	B	1231	ASN
1	B	1236	GLU
1	B	1241	GLN
1	B	1246	LEU
1	B	1248	LYS
1	B	1249	ASP
1	B	1252	LEU
1	B	1254	TYR
1	B	1257	ILE
1	B	1265	THR
1	B	1268	ASP
1	B	1274	ILE
1	B	1298	LEU
1	B	1300	MET
1	B	1301	TYR
1	B	1319	GLU
1	B	1322	GLU
1	B	1326	GLU
1	B	1334	LEU
1	B	1337	ILE
1	B	1353	SER
1	B	1358	LYS
1	B	1376	ARG
1	B	1377	ILE
1	B	1385	TYR
1	B	1396	ASN
1	B	1405	LYS
1	B	1407	PHE
1	B	1409	TYR
1	B	1412	SER
1	B	1416	GLU
1	B	1419	LEU
1	B	1420	THR
1	B	1422	PHE
1	B	1430	ILE
1	B	1438	ARG
1	B	1445	GLN
1	B	1455	SER
1	B	1457	GLU
1	B	1462	SER

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Mol	Chain	Res	Type
1	B	1463	LEU
1	B	1469	ARG
1	B	1471	SER
1	B	1482	THR
1	B	1484	GLU
1	B	1486	GLU
1	B	1496	SER
1	B	1501	MET
1	B	1520	GLU
1	B	1522	MET
1	B	1524	GLU
1	B	1525	LEU
1	B	1531	LEU
1	B	1532	LYS
1	B	1534	LEU
1	B	1535	MET
1	B	1539	ILE
1	B	1543	GLN
1	B	1549	THR
1	B	1581	ASN
1	C	2046	GLU
1	C	2048	MET
1	C	2049	SER
1	C	2054	GLN
1	C	2065	TYR
1	C	2070	THR
1	C	2077	ARG
1	C	2078	ILE
1	C	2085	THR
1	C	2089	VAL
1	C	2090	HIS
1	C	2092	ILE
1	C	2093	LEU
1	C	2107	PHE
1	C	2111	LEU
1	C	2117	LEU
1	C	2119	SER
1	C	2120	ARG
1	C	2121	SER
1	C	2124	ILE
1	C	2130	TYR
1	C	2136	TYR

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Mol	Chain	Res	Type
1	C	2137	LYS
1	C	2138	SER
1	C	2146	SER
1	C	2158	ASP
1	C	2161	THR
1	C	2165	VAL
1	C	2171	LEU
1	C	2173	ASP
1	C	2177	VAL
1	C	2178	LEU
1	C	2181	VAL
1	C	2185	ARG
1	C	2190	ASP
1	C	2192	GLN
1	C	2197	MET
1	C	2203	GLN
1	C	2207	HIS
1	C	2209	PHE
1	C	2215	LYS
1	C	2221	THR
1	C	2231	ASN
1	C	2236	GLU
1	C	2241	GLN
1	C	2246	LEU
1	C	2248	LYS
1	C	2249	ASP
1	C	2254	TYR
1	C	2257	ILE
1	C	2265	THR
1	C	2274	ILE
1	C	2289	GLN
1	C	2298	LEU
1	C	2300	MET
1	C	2319	GLU
1	C	2322	GLU
1	C	2326	GLU
1	C	2334	LEU
1	C	2337	ILE
1	C	2353	SER
1	C	2358	LYS
1	C	2376	ARG
1	C	2377	ILE

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Mol	Chain	Res	Type
1	C	2385	TYR
1	C	2396	ASN
1	C	2405	LYS
1	C	2407	PHE
1	C	2409	TYR
1	C	2412	SER
1	C	2416	GLU
1	C	2419	LEU
1	C	2420	THR
1	C	2430	ILE
1	C	2438	ARG
1	C	2445	GLN
1	C	2455	SER
1	C	2457	GLU
1	C	2462	SER
1	C	2463	LEU
1	C	2469	ARG
1	C	2471	SER
1	C	2482	THR
1	C	2484	GLU
1	C	2486	GLU
1	C	2496	SER
1	C	2501	MET
1	C	2520	GLU
1	C	2522	MET
1	C	2524	GLU
1	C	2525	LEU
1	C	2531	LEU
1	C	2532	LYS
1	C	2534	LEU
1	C	2535	MET
1	C	2539	ILE
1	C	2543	GLN
1	C	2549	THR
1	C	2569	CYS
1	C	2581	ASN
1	D	3046	GLU
1	D	3048	MET
1	D	3049	SER
1	D	3054	GLN
1	D	3065	TYR
1	D	3070	THR

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Mol	Chain	Res	Type
1	D	3077	ARG
1	D	3078	ILE
1	D	3085	THR
1	D	3089	VAL
1	D	3090	HIS
1	D	3092	ILE
1	D	3093	LEU
1	D	3107	PHE
1	D	3111	LEU
1	D	3117	LEU
1	D	3119	SER
1	D	3120	ARG
1	D	3121	SER
1	D	3124	ILE
1	D	3130	TYR
1	D	3136	TYR
1	D	3137	LYS
1	D	3138	SER
1	D	3146	SER
1	D	3158	ASP
1	D	3161	THR
1	D	3165	VAL
1	D	3171	LEU
1	D	3173	ASP
1	D	3178	LEU
1	D	3181	VAL
1	D	3185	ARG
1	D	3190	ASP
1	D	3192	GLN
1	D	3197	MET
1	D	3203	GLN
1	D	3207	HIS
1	D	3209	PHE
1	D	3215	LYS
1	D	3221	THR
1	D	3231	ASN
1	D	3236	GLU
1	D	3241	GLN
1	D	3246	LEU
1	D	3249	ASP
1	D	3254	TYR
1	D	3257	ILE

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Mol	Chain	Res	Type
1	D	3265	THR
1	D	3274	ILE
1	D	3289	GLN
1	D	3298	LEU
1	D	3300	MET
1	D	3301	TYR
1	D	3319	GLU
1	D	3322	GLU
1	D	3326	GLU
1	D	3334	LEU
1	D	3337	ILE
1	D	3353	SER
1	D	3358	LYS
1	D	3376	ARG
1	D	3377	ILE
1	D	3385	TYR
1	D	3396	ASN
1	D	3405	LYS
1	D	3407	PHE
1	D	3409	TYR
1	D	3412	SER
1	D	3416	GLU
1	D	3419	LEU
1	D	3420	THR
1	D	3430	ILE
1	D	3438	ARG
1	D	3445	GLN
1	D	3455	SER
1	D	3457	GLU
1	D	3462	SER
1	D	3463	LEU
1	D	3469	ARG
1	D	3471	SER
1	D	3482	THR
1	D	3484	GLU
1	D	3486	GLU
1	D	3496	SER
1	D	3501	MET
1	D	3520	GLU
1	D	3522	MET
1	D	3524	GLU
1	D	3525	LEU

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Mol	Chain	Res	Type
1	D	3531	LEU
1	D	3532	LYS
1	D	3534	LEU
1	D	3535	MET
1	D	3539	ILE
1	D	3543	GLN
1	D	3549	THR
1	D	3569	CYS
1	D	3581	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (59) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	204	HIS
1	A	207	HIS
1	A	208	GLN
1	A	320	HIS
1	A	327	GLN
1	A	350	GLN
1	A	372	GLN
1	A	374	GLN
1	A	388	HIS
1	A	396	ASN
1	A	411	ASN
1	A	417	HIS
1	A	560	ASN
1	A	565	GLN
1	A	571	ASN
1	A	581	ASN
1	B	1204	HIS
1	B	1208	GLN
1	B	1320	HIS
1	B	1327	GLN
1	B	1350	GLN
1	B	1356	HIS
1	B	1372	GLN
1	B	1374	GLN
1	B	1396	ASN
1	B	1411	ASN
1	B	1560	ASN
1	B	1565	GLN
1	B	1571	ASN

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Mol	Chain	Res	Type
1	B	1581	ASN
1	C	2043	ASN
1	C	2208	GLN
1	C	2320	HIS
1	C	2327	GLN
1	C	2350	GLN
1	C	2396	ASN
1	C	2411	ASN
1	C	2417	HIS
1	C	2464	ASN
1	C	2560	ASN
1	C	2565	GLN
1	C	2571	ASN
1	C	2581	ASN
1	D	3204	HIS
1	D	3208	GLN
1	D	3320	HIS
1	D	3327	GLN
1	D	3350	GLN
1	D	3372	GLN
1	D	3374	GLN
1	D	3388	HIS
1	D	3396	ASN
1	D	3411	ASN
1	D	3417	HIS
1	D	3464	ASN
1	D	3560	ASN
1	D	3565	GLN
1	D	3571	ASN
1	D	3581	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates

8 carbohydrates are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	NAG	A	661	1,2	14,14,15	0.65	0	15,19,21	0.71	0
2	NAG	A	662	2	14,14,15	0.75	0	15,19,21	0.53	0
2	NAG	B	1661	1,2	14,14,15	0.85	0	15,19,21	0.76	1 (6%)
2	NAG	B	1662	2	14,14,15	0.88	0	15,19,21	0.56	0
2	NAG	C	2661	1,2	14,14,15	0.65	0	15,19,21	0.72	1 (6%)
2	NAG	C	2662	2	14,14,15	0.75	0	15,19,21	0.55	0
2	NAG	D	3661	1,2	14,14,15	0.73	0	15,19,21	0.73	1 (6%)
2	NAG	D	3662	2	14,14,15	0.81	0	15,19,21	0.59	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	A	661	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	662	2	-	0/6/23/26	0/1/1/1
2	NAG	B	1661	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	1662	2	-	0/6/23/26	0/1/1/1
2	NAG	C	2661	1,2	-	0/6/23/26	0/1/1/1
2	NAG	C	2662	2	-	0/6/23/26	0/1/1/1
2	NAG	D	3661	1,2	-	0/6/23/26	0/1/1/1
2	NAG	D	3662	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1661	NAG	C2-N2-C7	-2.28	120.11	123.04
2	C	2661	NAG	C2-N2-C7	-2.15	120.28	123.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	3661	NAG	C2-N2-C7	-2.12	120.32	123.04

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.6 Ligand geometry

16 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	NAG	A	671	1	14,14,15	0.66	0	15,19,21	1.17	2 (13%)
3	NAG	A	681	1	14,14,15	0.69	0	15,19,21	0.74	0
5	PGX	A	701	-	20,26,27	0.94	2 (10%)	17,33,34	1.45	1 (5%)
4	BOG	A	702	-	20,20,20	0.88	2 (10%)	25,25,25	0.65	0
3	NAG	B	1671	1	14,14,15	0.54	0	15,19,21	0.91	1 (6%)
3	NAG	B	1681	1	14,14,15	0.66	0	15,19,21	0.67	0
5	PGX	B	1701	-	20,26,27	0.93	1 (5%)	17,33,34	1.45	1 (5%)
4	BOG	B	1702	-	20,20,20	0.85	2 (10%)	25,25,25	0.66	0
3	NAG	C	2671	1	14,14,15	0.68	0	15,19,21	1.13	1 (6%)
3	NAG	C	2681	1	14,14,15	0.68	0	15,19,21	0.66	0
5	PGX	C	2701	-	20,26,27	0.86	0	17,33,34	1.45	1 (5%)
4	BOG	C	2702	-	20,20,20	0.94	2 (10%)	25,25,25	0.64	0
3	NAG	D	3671	1	14,14,15	0.57	0	15,19,21	1.00	2 (13%)
3	NAG	D	3681	1	14,14,15	0.60	0	15,19,21	0.51	0
5	PGX	D	3701	-	20,26,27	0.92	2 (10%)	17,33,34	1.46	1 (5%)
4	BOG	D	3702	-	20,20,20	0.86	2 (10%)	25,25,25	0.63	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	A	671	1	-	0/6/23/26	0/1/1/1
3	NAG	A	681	1	-	0/6/23/26	0/1/1/1
5	PGX	A	701	-	-	0/17/40/42	0/0/2/2
4	BOG	A	702	-	-	0/11/31/31	0/1/1/1
3	NAG	B	1671	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1681	1	-	0/6/23/26	0/1/1/1
5	PGX	B	1701	-	-	0/17/40/42	0/0/2/2
4	BOG	B	1702	-	-	0/11/31/31	0/1/1/1
3	NAG	C	2671	1	-	0/6/23/26	0/1/1/1
3	NAG	C	2681	1	-	0/6/23/26	0/1/1/1
5	PGX	C	2701	-	-	0/17/40/42	0/0/2/2
4	BOG	C	2702	-	-	0/11/31/31	0/1/1/1
3	NAG	D	3671	1	-	0/6/23/26	0/1/1/1
3	NAG	D	3681	1	-	0/6/23/26	0/1/1/1
5	PGX	D	3701	-	-	0/17/40/42	0/0/2/2
4	BOG	D	3702	-	-	0/11/31/31	0/1/1/1

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	3702	BOG	O5-C1	2.01	1.47	1.41
5	B	1701	PGX	C8-C9	2.06	1.57	1.53
4	C	2702	BOG	O5-C1	2.07	1.47	1.41
5	D	3701	PGX	C12-C11	2.08	1.57	1.53
4	B	1702	BOG	O1-C1	2.11	1.43	1.40
5	A	701	PGX	C12-C11	2.13	1.57	1.53
4	A	702	BOG	O5-C1	2.14	1.47	1.41
5	D	3701	PGX	C8-C9	2.15	1.57	1.53
4	D	3702	BOG	O1-C1	2.18	1.44	1.40
4	A	702	BOG	O1-C1	2.19	1.44	1.40
4	B	1702	BOG	O5-C1	2.21	1.47	1.41
5	A	701	PGX	C8-C9	2.27	1.57	1.53
4	C	2702	BOG	O1-C1	2.72	1.45	1.40

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	3701	PGX	C11-C10-C9	-5.69	85.67	103.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	701	PGX	C11-C10-C9	-5.62	85.86	103.56
5	B	1701	PGX	C11-C10-C9	-5.60	85.95	103.56
5	C	2701	PGX	C11-C10-C9	-5.59	85.99	103.56
3	A	671	NAG	C2-N2-C7	-3.07	119.09	123.04
3	C	2671	NAG	C2-N2-C7	-2.75	119.51	123.04
3	B	1671	NAG	C2-N2-C7	-2.34	120.04	123.04
3	D	3671	NAG	C2-N2-C7	-2.22	120.19	123.04
3	A	671	NAG	C1-O5-C5	2.40	115.30	112.25
3	D	3671	NAG	C1-O5-C5	2.47	115.38	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 48 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	701	PGX	9	0
5	B	1701	PGX	13	0
5	C	2701	PGX	14	0
5	D	3701	PGX	11	0
4	D	3702	BOG	1	0

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	552/552 (100%)	-0.17	5 (0%)	85	64	2, 25, 52, 71	0
1	B	552/552 (100%)	-0.11	5 (0%)	85	64	3, 25, 51, 70	0
1	C	552/552 (100%)	-0.19	5 (0%)	85	64	2, 25, 51, 70	0
1	D	552/552 (100%)	-0.13	6 (1%)	82	58	3, 25, 51, 70	0
All	All	2208/2208 (100%)	-0.15	21 (0%)	84	60	2, 25, 51, 71	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	105	ASN	3.2
1	B	1103	VAL	3.2
1	D	3105(D)	ILE	3.2
1	C	2083	LYS	3.0
1	B	1102	ILE	2.9
1	B	1105	ASN	2.7
1	D	3583	GLN	2.5
1	B	1095	HIS	2.2
1	A	276	PRO	2.2
1	B	1105(B)	ILE	2.2
1	D	3496	SER	2.1
1	C	2357	PHE	2.1
1	D	3063	GLY	2.1
1	C	2105	ASN	2.0
1	A	82	LEU	2.0
1	C	2074	PHE	2.0
1	C	2272	GLU	2.0
1	D	3165	VAL	2.0
1	D	3436	GLY	2.0
1	A	74	PHE	2.0
1	A	98	GLY	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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th 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	LLDF	B-factors(Å ²)	Q<0.9
2	NAG	A	661	14/15	0.83	0.38	3.06	52,59,65,72	0
2	NAG	C	2661	14/15	0.86	0.24	2.71	51,59,64,72	0
2	NAG	D	3661	14/15	0.84	0.36	1.78	51,62,66,71	0
2	NAG	B	1661	14/15	0.79	0.34	1.50	52,60,67,74	0
2	NAG	D	3662	14/15	0.56	0.48	-	77,80,85,86	0
2	NAG	A	662	14/15	0.68	0.63	-	77,81,84,84	0
2	NAG	B	1662	14/15	0.55	0.47	-	78,81,84,84	0
2	NAG	C	2662	14/15	0.60	0.50	-	78,81,85,85	0

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th 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	LLDF	B-factors(Å ²)	Q<0.9
5	PGX	C	2701	25/26	0.63	0.53	7.33	75,79,84,84	0
4	BOG	A	702	20/20	0.76	0.55	6.79	54,58,62,65	0
5	PGX	A	701	25/26	0.72	0.48	6.20	73,78,86,87	0
3	NAG	C	2681	14/15	0.54	0.54	5.61	66,69,73,73	0
5	PGX	D	3701	25/26	0.71	0.43	4.46	74,78,86,87	0
4	BOG	C	2702	20/20	0.76	0.48	4.35	56,60,64,66	0
5	PGX	B	1701	25/26	0.67	0.49	4.06	72,78,84,85	0
3	NAG	B	1681	14/15	0.76	0.39	2.42	66,71,73,75	0
4	BOG	D	3702	20/20	0.75	0.42	2.34	46,53,59,62	0
3	NAG	A	681	14/15	0.70	0.40	1.55	67,70,73,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	BOG	B	1702	20/20	0.79	0.39	1.22	50,54,59,59	0
3	NAG	D	3681	14/15	0.84	0.29	0.42	66,70,72,73	0
3	NAG	C	2671	14/15	0.87	0.18	-0.50	7,10,25,28	0
3	NAG	B	1671	14/15	0.89	0.18	-0.53	5,10,25,26	0
3	NAG	A	671	14/15	0.89	0.18	-0.73	2,9,25,27	0
3	NAG	D	3671	14/15	0.91	0.14	-0.97	2,9,23,25	0

6.5 Other polymers [i](#)

There are no such residues in this entry.