



Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 04:57 am BST

PDB ID : 3K4A
Title : Crystal structure of selenomethionine substituted E. coli beta-glucuronidase
Authors : Wallace, B.D.; Orans, J.; Redinbo, M.R.
Deposited on : 2009-10-05
Resolution : 2.90 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

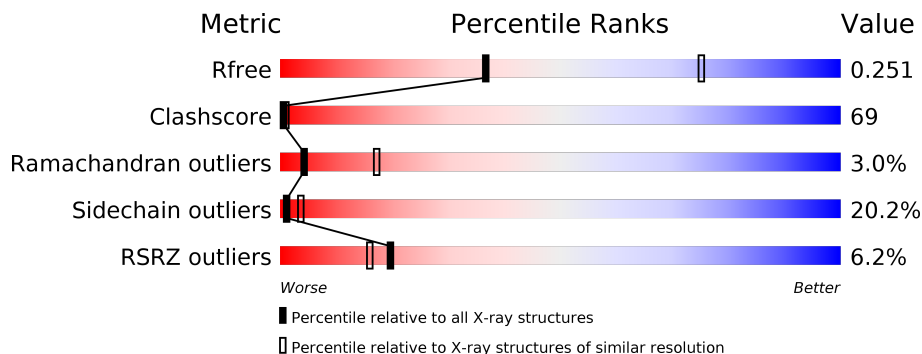
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	605	 5% 33% 51% 14% ..
1	B	605	 7% 25% 55% 16% ..

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9761 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 Beta-glucuronidase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	597	4779	3034	827	896	9	13	0	0	0
1	B	597	4768	3026	826	894	9	13	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	SER	-	EXPRESSION TAG	UNP P05804
A	0	HIS	-	EXPRESSION TAG	UNP P05804
B	-1	SER	-	EXPRESSION TAG	UNP P05804
B	0	HIS	-	EXPRESSION TAG	UNP P05804

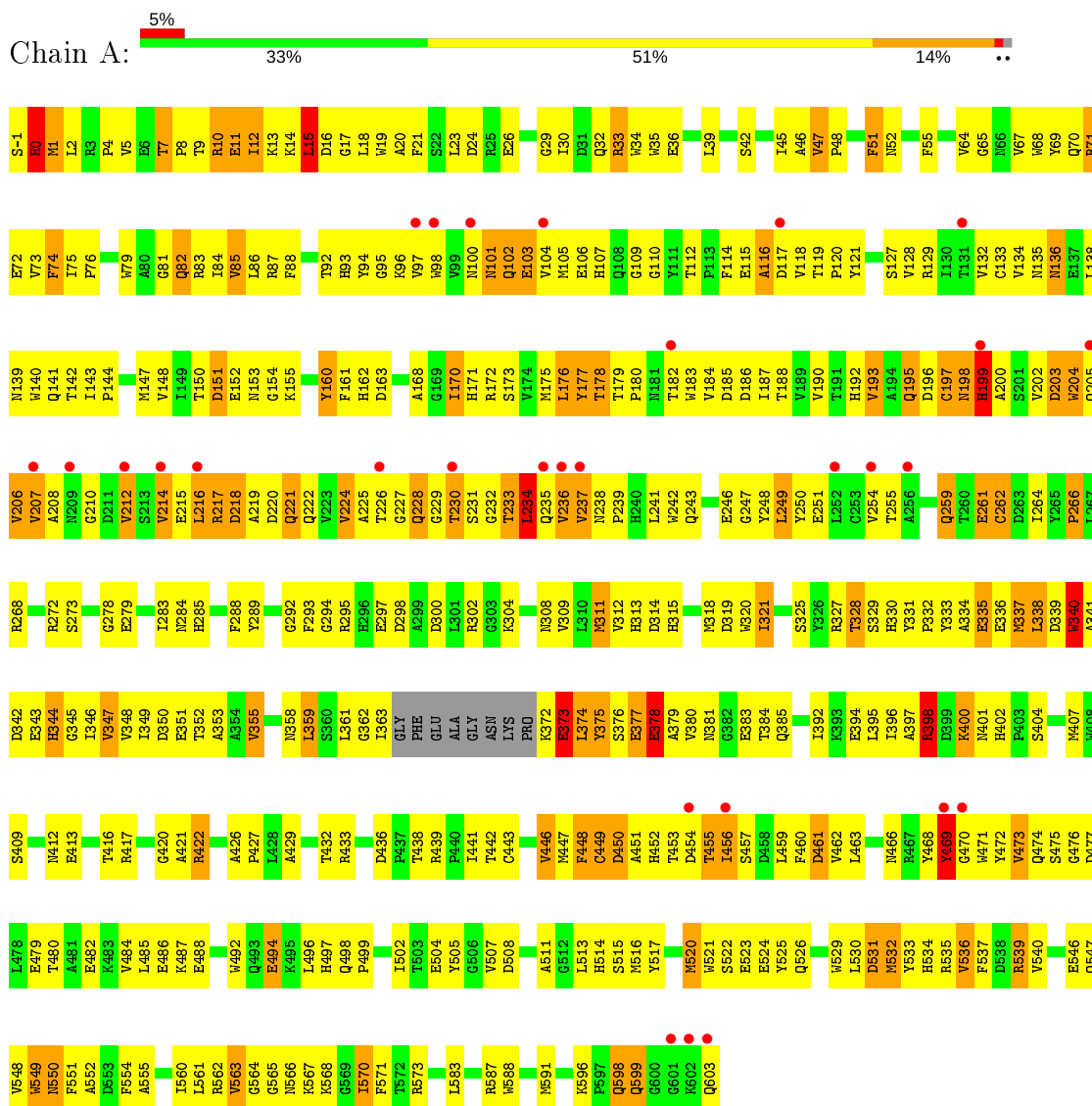
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	123	Total	O	0	0
			123	123		
2	B	91	Total	O	0	0
			91	91		

3 Residue-property plots i

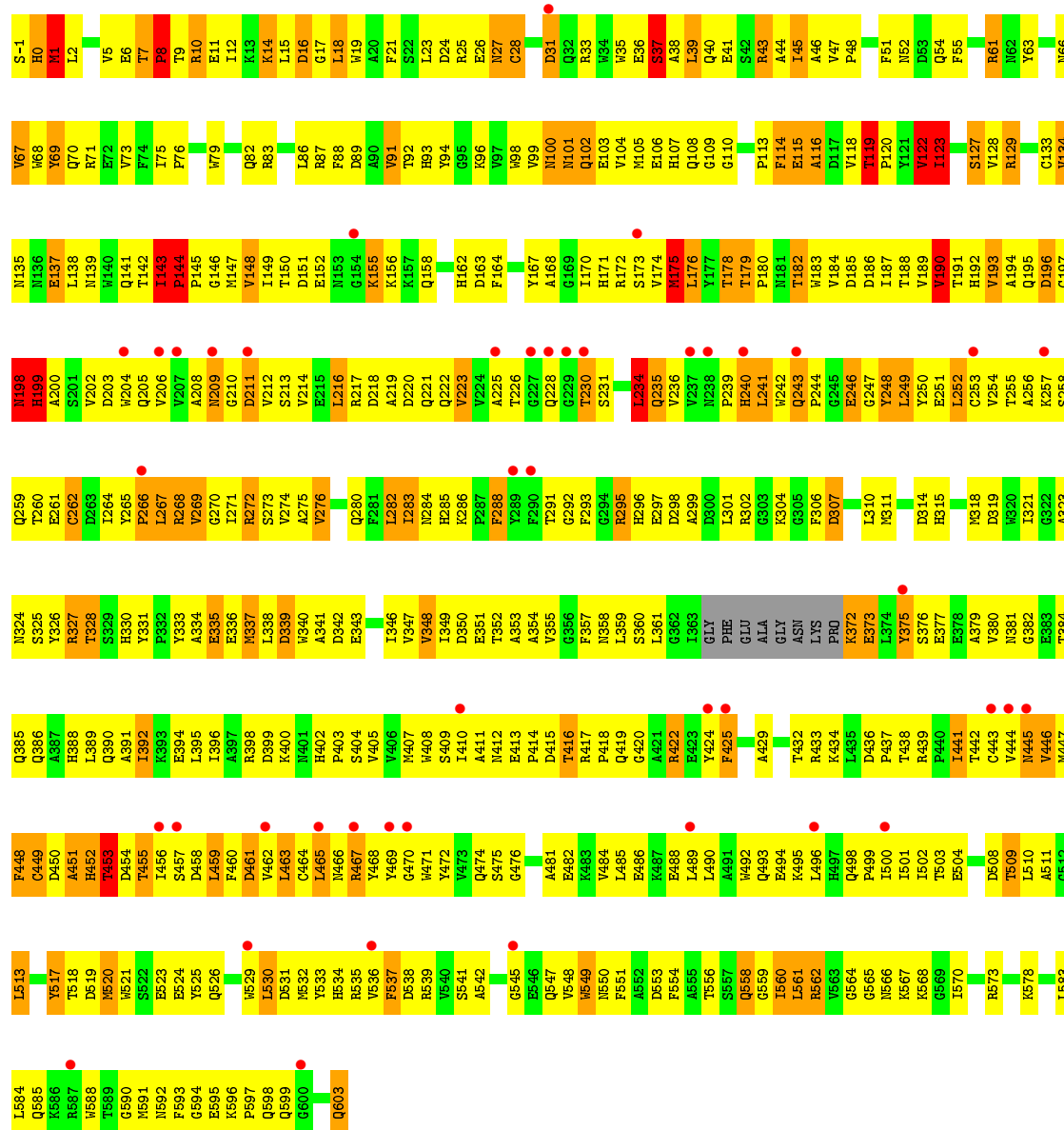
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

- Molecule 1: Beta-glucuronidase



- Molecule 1: Beta-glucuronidase





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	169.00Å 77.26Å 126.58Å 90.00° 125.02° 90.00°	Depositor
Resolution (Å)	32.11 – 2.90 48.11 – 2.90	Depositor EDS
% Data completeness (in resolution range)	100.0 (32.11-2.90) 98.9 (48.11-2.90)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.59 (at 2.91Å)	Xtrriage
Refinement program	REFMAC 5.5.0072	Depositor
R, R_{free}	0.242 , 0.282 0.251 , 0.251	Depositor DCC
R_{free} test set	1495 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	54.2	Xtrriage
Anisotropy	0.687	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 61.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	9761	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.55% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality i

5.1 Standard geometry i

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	0.98	8/4893 (0.2%)	1.05	19/6636 (0.3%)
1	B	0.82	2/4882 (0.0%)	0.94	8/6623 (0.1%)
All	All	0.91	10/9775 (0.1%)	1.00	27/13259 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	6
1	B	0	5
All	All	0	11

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	340	TRP	CB-CG	-9.12	1.33	1.50
1	A	1	MSE	CG-SE	-6.18	1.74	1.95
1	B	1	MSE	CG-SE	-5.88	1.75	1.95
1	A	532	MSE	CG-SE	-5.87	1.75	1.95
1	A	311	MSE	CG-SE	-5.72	1.76	1.95
1	A	443	CYS	CB-SG	-5.63	1.72	1.81
1	A	516	MSE	CG-SE	-5.40	1.77	1.95
1	B	175	MSE	CG-SE	-5.23	1.77	1.95
1	A	337	MSE	CG-SE	-5.18	1.77	1.95
1	A	520	MSE	CG-SE	-5.02	1.78	1.95

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	374	LEU	N-CA-C	8.35	133.55	111.00
1	A	199	HIS	N-CA-C	7.98	132.56	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	573	ARG	NE-CZ-NH1	-7.83	116.38	120.30
1	A	198	ASN	N-CA-C	7.50	131.25	111.00
1	A	294	GLY	N-CA-C	-7.17	95.18	113.10
1	B	453	THR	N-CA-C	-7.04	91.98	111.00
1	A	449	CYS	CA-CB-SG	-7.01	101.39	114.00
1	A	449	CYS	N-CA-C	6.66	128.98	111.00
1	A	448	PHE	CB-CA-C	-5.97	98.45	110.40
1	A	0	HIS	N-CA-C	5.93	127.02	111.00
1	A	398	ARG	NE-CZ-NH1	5.89	123.25	120.30
1	A	446	VAL	CB-CA-C	-5.64	100.68	111.40
1	A	15	LEU	CA-CB-CG	5.54	128.03	115.30
1	B	307	ASP	CB-CG-OD1	5.45	123.21	118.30
1	B	122	VAL	CB-CA-C	5.38	121.62	111.40
1	B	549	TRP	CA-CB-CG	-5.32	103.59	113.70
1	B	199	HIS	N-CA-C	5.28	125.25	111.00
1	A	469	TYR	CB-CA-C	-5.24	99.92	110.40
1	A	196	ASP	N-CA-C	5.21	125.06	111.00
1	A	234	LEU	CA-CB-CG	5.20	127.25	115.30
1	B	234	LEU	CA-CB-CG	5.18	127.23	115.30
1	A	398	ARG	NE-CZ-NH2	-5.04	117.78	120.30
1	B	91	VAL	N-CA-C	-5.03	97.42	111.00
1	B	116	ALA	N-CA-C	5.03	124.58	111.00
1	A	448	PHE	C-N-CA	-5.02	109.15	121.70
1	A	422	ARG	CG-CD-NE	-5.00	101.30	111.80
1	A	599	GLN	N-CA-C	-5.00	97.50	111.00

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	116	ALA	Peptide
1	A	197	CYS	Peptide
1	A	373	GLU	Peptide
1	A	378	GLU	Peptide
1	A	455	THR	Peptide
1	A	549	TRP	Peptide
1	B	143	ILE	Peptide
1	B	17	GLY	Peptide
1	B	37	SER	Peptide
1	B	451	ALA	Peptide
1	B	8	PRO	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4779	0	4554	600	1
1	B	4768	0	4532	690	4
2	A	123	0	0	73	3
2	B	91	0	0	59	0
All	All	9761	0	9086	1279	4

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 69.

All (1279) 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:B:502:ILE:HD12	1:B:537:PHE:CE2	1.49	1.48
1:A:455:THR:CG2	1:A:456:ILE:HG22	1.50	1.41
1:B:198:ASN:CB	1:B:236:VAL:HG22	1.59	1.32
1:B:444:VAL:CG1	1:B:466:ASN:HD21	1.47	1.26
1:A:456:ILE:CG1	1:A:459:LEU:HB2	1.64	1.26
1:B:449:CYS:SG	1:B:488:GLU:OE1	1.97	1.21
1:B:444:VAL:HG13	1:B:466:ASN:ND2	1.55	1.21
1:A:92:THR:HG21	1:A:171:HIS:ND1	1.56	1.20
1:A:238:ASN:CG	1:A:239:PRO:HD3	1.63	1.18
1:B:452:HIS:O	1:B:453:THR:HG23	1.44	1.16
1:B:253:CYS:SG	1:B:264:ILE:HG22	1.85	1.15
1:A:502:ILE:HD13	1:A:537:PHE:CE2	1.80	1.15
1:A:448:PHE:HB3	1:A:452:HIS:HA	1.15	1.15
1:A:402:HIS:CD2	2:A:673:HOH:O	1.94	1.14
1:A:139:ASN:O	1:A:142:THR:HG22	1.46	1.14
1:A:237:VAL:HG12	1:A:238:ASN:N	1.63	1.14
1:B:92:THR:HG22	2:B:680:HOH:O	1.45	1.14
1:A:448:PHE:O	1:A:452:HIS:HB2	1.48	1.13
1:B:416:THR:HG21	1:B:453:THR:HA	1.28	1.13
1:A:237:VAL:CG1	1:A:238:ASN:H	1.61	1.12
1:B:273:SER:HB3	1:B:284:ASN:H	1.09	1.11
1:B:335:GLU:HA	2:B:662:HOH:O	0.94	1.10
1:A:456:ILE:HG13	1:A:459:LEU:HB2	1.27	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:213:SER:HB3	1:B:255:THR:HB	1.31	1.10
1:A:151:ASP:HB2	1:A:155:LYS:HB3	1.23	1.10
1:A:402:HIS:HD2	2:A:673:HOH:O	1.31	1.10
1:B:36:GLU:HG3	1:B:129:ARG:HH22	1.16	1.09
1:A:92:THR:HG21	1:A:171:HIS:CE1	1.88	1.09
1:A:455:THR:CG2	1:A:456:ILE:CG2	2.31	1.09
1:B:198:ASN:HB2	1:B:236:VAL:HG22	1.17	1.09
1:B:466:ASN:HB2	1:B:504:GLU:HB2	1.30	1.09
1:A:151:ASP:CB	1:A:155:LYS:HB3	1.83	1.08
1:A:92:THR:O	1:A:110:GLY:CA	2.01	1.08
1:A:183:TRP:HB3	2:A:715:HOH:O	1.52	1.07
1:B:444:VAL:HG13	1:B:466:ASN:HD21	0.92	1.07
1:B:36:GLU:HG3	1:B:129:ARG:NH2	1.68	1.07
1:B:69:TYR:CD1	1:B:170:ILE:HD12	1.88	1.07
1:A:448:PHE:HB3	1:A:452:HIS:CA	1.85	1.06
1:A:361:LEU:HA	2:A:717:HOH:O	1.52	1.06
1:B:502:ILE:CD1	1:B:537:PHE:HE2	1.68	1.06
1:A:328:THR:C	2:A:711:HOH:O	1.92	1.06
1:B:566:ASN:HB3	1:B:568:LYS:HD2	1.36	1.05
1:A:455:THR:HG22	1:A:456:ILE:HG22	1.09	1.05
1:B:447:MSE:HE3	1:B:467:ARG:HB3	1.34	1.05
1:A:455:THR:HG23	1:A:456:ILE:CG2	1.87	1.05
1:B:502:ILE:CD1	1:B:537:PHE:CE2	2.41	1.04
1:B:144:PRO:HD2	1:B:353:ALA:O	1.55	1.04
1:B:69:TYR:CE1	1:B:170:ILE:HD12	1.91	1.04
1:A:17:GLY:HA2	1:A:47:VAL:HG13	1.04	1.03
1:A:455:THR:HG23	1:A:456:ILE:HG22	1.38	1.03
1:A:494:GLU:HG2	2:A:713:HOH:O	1.57	1.03
1:B:273:SER:O	1:B:283:ILE:HA	1.55	1.03
1:A:14:LYS:HB3	1:A:14:LYS:NZ	1.70	1.02
1:B:416:THR:CG2	1:B:453:THR:HA	1.88	1.02
1:A:338:LEU:HG	1:A:339:ASP:N	1.74	1.02
1:A:335:GLU:HA	2:A:614:HOH:O	0.84	1.01
1:B:92:THR:O	1:B:110:GLY:HA3	1.60	1.01
1:A:92:THR:O	1:A:110:GLY:HA3	1.61	1.00
1:A:83:ARG:HB3	1:A:179:THR:O	1.57	1.00
1:A:343:GLU:OE1	2:A:615:HOH:O	1.77	1.00
1:B:549:TRP:HZ3	1:B:568:LYS:NZ	1.58	1.00
1:B:337:MSE:HE1	1:B:348:VAL:HG21	1.41	0.99
1:A:179:THR:HB	2:A:715:HOH:O	1.61	0.99
1:A:10:ARG:HD2	1:A:79:TRP:HE1	1.24	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:92:THR:CG2	1:A:171:HIS:HD1	1.73	0.99
1:B:172:ARG:HH11	1:B:334:ALA:HB2	1.25	0.99
1:B:143:ILE:HG23	1:B:353:ALA:O	1.62	0.98
1:B:14:LYS:HD3	1:B:174:VAL:O	1.62	0.98
1:B:282:LEU:HD23	1:B:285:HIS:HA	1.43	0.98
1:B:198:ASN:HB3	1:B:236:VAL:HG22	1.43	0.97
1:B:273:SER:HB3	1:B:284:ASN:N	1.79	0.97
1:A:14:LYS:HD2	1:A:176:LEU:HB2	1.45	0.97
1:A:92:THR:HG22	2:A:666:HOH:O	1.62	0.97
1:B:15:LEU:CD2	1:B:173:SER:HB3	1.94	0.97
1:B:559:GLY:H	1:B:562:ARG:HH22	1.05	0.97
1:A:142:THR:HG23	1:A:144:PRO:O	1.65	0.97
1:A:14:LYS:HZ3	1:A:14:LYS:HB3	1.25	0.97
1:A:456:ILE:HG12	1:A:459:LEU:HB2	1.42	0.97
1:A:233:THR:O	1:A:234:LEU:HD23	1.64	0.96
1:B:172:ARG:NH1	1:B:334:ALA:HB2	1.81	0.96
1:A:5:VAL:HG11	1:A:266:PRO:HD2	1.46	0.96
1:A:92:THR:CG2	1:A:171:HIS:ND1	2.28	0.96
1:A:39:LEU:HD22	1:A:70:GLN:HB2	1.45	0.96
1:A:92:THR:O	1:A:110:GLY:HA2	1.66	0.96
1:A:17:GLY:CA	1:A:47:VAL:HG13	1.95	0.95
1:B:36:GLU:HB2	1:B:101:ASN:HD21	1.28	0.95
1:B:96:LYS:HE2	1:B:103:GLU:OE2	1.66	0.95
1:B:15:LEU:HD22	1:B:173:SER:HA	1.48	0.95
1:B:92:THR:O	1:B:110:GLY:CA	2.15	0.95
1:B:299:ALA:HB2	1:B:310:LEU:HD11	1.47	0.94
1:B:502:ILE:HD12	1:B:537:PHE:CZ	2.01	0.94
1:A:237:VAL:HG12	1:A:238:ASN:H	0.78	0.94
1:B:15:LEU:HD22	1:B:173:SER:CB	1.98	0.94
1:A:502:ILE:CD1	1:A:537:PHE:CE2	2.49	0.94
1:B:325:SER:N	2:B:691:HOH:O	2.01	0.94
1:B:272:ARG:HG3	1:B:274:VAL:HG23	1.51	0.93
1:A:199:HIS:CE1	1:A:236:VAL:CG2	2.52	0.93
1:A:8:PRO:HB2	2:A:610:HOH:O	1.68	0.93
1:B:197:CYS:HB3	1:B:198:ASN:CB	1.99	0.93
1:A:118:VAL:HG23	1:A:120:PRO:HD2	1.50	0.92
1:B:10:ARG:H	1:B:178:THR:HG22	1.34	0.92
1:A:101:ASN:OD1	1:A:129:ARG:NH2	2.01	0.92
1:B:15:LEU:HD22	1:B:173:SER:CA	1.99	0.92
1:B:462:VAL:HG22	1:B:499:PRO:HG2	1.52	0.92
1:A:338:LEU:HG	1:A:339:ASP:H	1.35	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:144:PRO:CD	1:B:353:ALA:O	2.19	0.91
1:B:108:GLN:HG3	2:B:617:HOH:O	1.69	0.91
1:B:118:VAL:C	1:B:120:PRO:HD3	1.92	0.90
1:A:449:CYS:SG	1:A:449:CYS:O	2.30	0.90
1:A:378:GLU:HG3	1:A:378:GLU:O	1.71	0.90
1:B:417:ARG:HG2	1:B:418:PRO:HD3	1.53	0.90
1:B:465:LEU:H	1:B:465:LEU:HD12	1.37	0.90
1:A:328:THR:HG22	1:A:333:TYR:CG	2.07	0.90
1:B:198:ASN:CB	1:B:236:VAL:CG2	2.48	0.90
1:B:449:CYS:CB	1:B:488:GLU:OE1	2.20	0.90
1:A:455:THR:HG22	1:A:456:ILE:CG2	1.96	0.89
1:A:548:VAL:HG11	1:A:570:ILE:HD11	1.53	0.89
1:B:96:LYS:NZ	2:B:648:HOH:O	1.98	0.89
1:A:342:ASP:OD2	2:A:673:HOH:O	1.89	0.89
1:A:92:THR:HG21	1:A:171:HIS:HD1	1.22	0.89
1:B:197:CYS:HB3	1:B:198:ASN:ND2	1.87	0.89
1:A:102:GLN:OE1	1:A:102:GLN:HA	1.74	0.88
1:A:110:GLY:O	2:A:666:HOH:O	1.89	0.88
1:B:197:CYS:HB3	1:B:198:ASN:CG	1.93	0.88
1:A:327:ARG:HH21	1:A:412:ASN:HD21	1.15	0.88
1:A:456:ILE:HG13	1:A:459:LEU:CB	2.04	0.88
1:B:429:ALA:O	1:B:433:ARG:HG2	1.74	0.88
1:A:327:ARG:HH21	1:A:412:ASN:ND2	1.70	0.88
1:B:191:THR:HG22	1:B:200:ALA:HB2	1.56	0.88
1:B:197:CYS:HB3	1:B:198:ASN:HB3	1.56	0.87
1:B:10:ARG:HH11	1:B:10:ARG:HB2	1.34	0.87
1:B:382:GLY:O	1:B:386:GLN:HG2	1.74	0.87
1:B:253:CYS:SG	1:B:264:ILE:CG2	2.62	0.86
1:B:101:ASN:N	1:B:101:ASN:HD22	1.73	0.86
1:B:10:ARG:HH11	1:B:10:ARG:CB	1.87	0.86
1:B:311:MSE:HE2	1:B:336:GLU:HG2	1.56	0.86
1:B:470:GLY:H	1:B:529:TRP:HH2	1.23	0.86
1:A:548:VAL:HG11	1:A:570:ILE:CD1	2.06	0.86
1:B:105:MSE:SE	1:B:114:PHE:HB3	2.26	0.85
1:A:95:GLY:HA2	1:A:133:CYS:O	1.76	0.85
1:B:447:MSE:HE3	1:B:467:ARG:CB	2.05	0.85
1:A:15:LEU:HD23	1:A:173:SER:OG	1.77	0.85
1:B:101:ASN:HD22	1:B:101:ASN:H	1.25	0.85
1:B:86:LEU:O	1:B:105:MSE:HE1	1.77	0.85
1:B:302:ARG:HD3	2:B:645:HOH:O	1.77	0.84
1:A:84:ILE:HG22	1:A:176:LEU:HD11	1.57	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:74:PHE:CZ	1:B:7:THR:HA	2.11	0.84
1:A:197:CYS:HB2	1:A:198:ASN:OD1	1.75	0.84
1:B:451:ALA:HB2	2:B:677:HOH:O	1.76	0.84
1:B:15:LEU:CD2	1:B:173:SER:CB	2.54	0.84
1:B:10:ARG:HH12	1:B:79:TRP:HE1	1.26	0.84
1:A:17:GLY:HA3	1:A:47:VAL:H	1.41	0.84
1:B:36:GLU:HB2	1:B:101:ASN:ND2	1.92	0.84
1:B:471:TRP:HZ3	1:B:520:MSE:HG2	1.42	0.84
1:B:184:VAL:HG21	1:B:254:VAL:HG12	1.60	0.84
1:A:33:ARG:HB3	1:A:36:GLU:OE2	1.78	0.84
1:B:172:ARG:HH11	1:B:334:ALA:CB	1.89	0.84
1:B:198:ASN:HB3	1:B:236:VAL:CG2	2.06	0.83
1:B:328:THR:HA	1:B:333:TYR:CZ	2.13	0.83
1:B:45:ILE:HG13	1:B:55:PHE:HZ	1.43	0.83
1:A:186:ASP:HB3	1:A:206:VAL:CG1	2.08	0.83
1:B:10:ARG:NH1	1:B:79:TRP:HE1	1.75	0.83
1:B:172:ARG:NH1	1:B:334:ALA:CB	2.42	0.83
1:B:453:THR:HG21	1:B:456:ILE:HB	1.60	0.83
1:A:0:HIS:NE2	1:A:186:ASP:OD2	2.11	0.82
1:B:5:VAL:HG12	1:B:6:GLU:N	1.93	0.82
1:A:199:HIS:CE1	1:A:236:VAL:HG21	2.15	0.82
1:B:143:ILE:HG23	1:B:144:PRO:HD2	1.58	0.82
1:B:376:SER:HB2	2:B:643:HOH:O	1.78	0.82
1:B:327:ARG:NH1	1:B:503:THR:HB	1.93	0.82
1:A:45:ILE:HD12	1:A:55:PHE:CZ	2.15	0.82
1:B:241:LEU:HD23	1:B:241:LEU:H	1.45	0.82
1:B:400:LYS:HA	1:B:439:ARG:HH12	1.43	0.82
1:A:243:GLN:O	1:A:246:GLU:O	1.98	0.82
1:B:511:ALA:O	1:B:523:GLU:OE1	1.97	0.82
1:A:217:ARG:O	1:A:222:GLN:O	1.97	0.82
1:B:502:ILE:HD12	1:B:537:PHE:HE2	0.90	0.82
1:A:228:GLN:HA	1:A:228:GLN:NE2	1.95	0.81
1:B:143:ILE:HD11	1:B:388:HIS:HA	1.59	0.81
1:B:83:ARG:HA	1:B:119:THR:OG1	1.78	0.81
1:A:339:ASP:CB	2:A:722:HOH:O	2.28	0.81
1:A:14:LYS:CB	1:A:14:LYS:NZ	2.42	0.81
1:A:218:ASP:HB2	1:A:221:GLN:HA	1.62	0.81
1:A:297:GLU:O	1:A:304:LYS:HD3	1.81	0.81
1:A:361:LEU:HD23	2:A:717:HOH:O	1.80	0.81
1:B:15:LEU:HB3	1:B:174:VAL:H	1.46	0.81
1:A:332:PRO:HG3	1:A:395:LEU:HD12	1.61	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:566:ASN:HB3	2:A:635:HOH:O	1.80	0.81
1:A:416:THR:H	1:A:448:PHE:HE2	1.28	0.81
1:A:448:PHE:CB	1:A:452:HIS:HA	2.05	0.81
1:A:502:ILE:HD13	1:A:537:PHE:HE2	1.46	0.81
1:B:202:VAL:HG23	1:B:234:LEU:CD2	2.11	0.81
1:A:329:SER:O	1:A:330:HIS:ND1	2.13	0.80
1:B:392:ILE:O	1:B:396:ILE:HG13	1.81	0.80
1:B:272:ARG:HH21	1:B:439:ARG:HH21	1.28	0.80
1:B:21:PHE:CD2	1:B:45:ILE:HD12	2.16	0.80
1:B:465:LEU:N	1:B:465:LEU:HD12	1.97	0.80
1:B:36:GLU:HG2	1:B:37:SER:H	1.47	0.80
1:B:328:THR:HA	1:B:333:TYR:CE2	2.17	0.80
1:B:549:TRP:CZ3	1:B:568:LYS:NZ	2.42	0.79
1:B:341:ALA:HB1	1:B:404:SER:HB3	1.62	0.79
1:B:327:ARG:HH12	1:B:504:GLU:HG3	1.46	0.79
1:B:36:GLU:HG2	1:B:37:SER:N	1.97	0.79
1:B:466:ASN:HB3	1:B:504:GLU:H	1.47	0.79
1:B:375:TYR:CE1	1:B:379:ALA:HB2	2.18	0.79
1:B:470:GLY:N	1:B:529:TRP:HH2	1.80	0.79
1:A:105:MSE:HE1	1:A:115:GLU:HA	1.62	0.79
1:A:513:LEU:HD23	1:A:521:TRP:O	1.82	0.79
1:A:64:VAL:O	1:A:136:ASN:ND2	2.16	0.79
1:B:225:ALA:HB1	1:B:235:GLN:HG3	1.65	0.79
1:A:202:VAL:HG22	1:A:234:LEU:CD2	2.13	0.79
1:B:444:VAL:CG1	1:B:466:ASN:ND2	2.28	0.79
1:A:199:HIS:ND1	1:A:236:VAL:HB	1.98	0.79
1:B:202:VAL:HG23	1:B:234:LEU:HD21	1.64	0.79
1:B:466:ASN:HB3	1:B:504:GLU:N	1.98	0.78
1:A:172:ARG:NE	1:A:334:ALA:HB2	1.98	0.78
1:B:92:THR:CG2	1:B:93:HIS:N	2.47	0.78
1:A:17:GLY:HA2	1:A:47:VAL:CG1	2.01	0.78
1:A:45:ILE:HD12	1:A:55:PHE:HZ	1.46	0.78
1:A:71:ARG:HG2	1:A:71:ARG:HH11	1.49	0.78
1:B:92:THR:HA	2:B:657:HOH:O	1.82	0.78
1:B:466:ASN:HB2	1:B:504:GLU:CB	2.14	0.78
1:B:449:CYS:HB2	1:B:488:GLU:OE1	1.83	0.78
1:B:549:TRP:O	1:B:549:TRP:CD1	2.36	0.78
1:B:590:GLY:O	2:B:641:HOH:O	2.00	0.78
1:B:92:THR:HG23	1:B:93:HIS:N	1.97	0.78
1:A:199:HIS:HE1	1:A:236:VAL:HG21	1.49	0.77
1:A:340:TRP:O	1:A:346:ILE:HD12	1.84	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:392:ILE:HG21	1:A:432:THR:HG22	1.66	0.77
1:B:315:HIS:HE1	1:B:336:GLU:OE1	1.67	0.77
1:B:52:ASN:HD21	1:B:168:ALA:H	1.30	0.77
1:A:238:ASN:CB	1:A:239:PRO:HD3	2.13	0.77
1:A:327:ARG:NH2	1:A:412:ASN:HD21	1.83	0.77
1:B:99:VAL:HG12	1:B:100:ASN:N	1.99	0.77
1:B:452:HIS:O	1:B:453:THR:CG2	2.32	0.77
1:B:508:ASP:OD2	1:B:568:LYS:HG2	1.84	0.77
1:A:15:LEU:HD22	1:A:48:PRO:HD3	1.67	0.76
1:B:122:VAL:CG2	1:B:123:ILE:HD12	2.16	0.76
1:A:392:ILE:HD13	1:A:432:THR:CG2	2.16	0.76
1:B:167:TYR:HB2	1:B:304:LYS:HG3	1.67	0.76
1:B:500:ILE:N	2:B:665:HOH:O	2.10	0.76
1:A:218:ASP:HB2	1:A:220:ASP:O	1.83	0.76
1:A:452:HIS:HD1	1:A:453:THR:N	1.84	0.76
1:A:100:ASN:HA	1:A:129:ARG:HH21	1.51	0.75
1:B:139:ASN:O	1:B:142:THR:HG22	1.85	0.75
1:A:216:LEU:HD21	1:A:250:TYR:HB3	1.68	0.75
1:B:105:MSE:HE2	1:B:116:ALA:HB3	1.67	0.75
1:B:498:GLN:HB2	1:B:499:PRO:HD2	1.66	0.75
1:B:436:ASP:OD2	1:B:438:THR:N	2.19	0.75
1:A:17:GLY:O	1:A:46:ALA:HA	1.87	0.75
1:A:15:LEU:CD2	1:A:173:SER:OG	2.34	0.75
1:B:5:VAL:HG12	1:B:6:GLU:H	1.49	0.75
1:A:373:GLU:OE1	1:A:374:LEU:HD23	1.87	0.75
1:B:202:VAL:CG2	1:B:234:LEU:HD21	2.16	0.75
1:A:203:ASP:OD1	1:A:233:THR:OG1	2.04	0.75
1:A:416:THR:HB	1:A:455:THR:HB	1.69	0.75
1:B:379:ALA:HA	1:B:381:ASN:HD22	1.51	0.74
1:A:433:ARG:NH1	1:A:461:ASP:OD1	2.21	0.74
1:A:242:TRP:CZ2	1:A:345:GLY:HA2	2.23	0.74
1:A:328:THR:HG22	1:A:333:TYR:CD2	2.21	0.74
1:A:340:TRP:C	2:A:695:HOH:O	2.24	0.74
1:B:311:MSE:CE	1:B:336:GLU:HG2	2.18	0.74
1:B:562:ARG:CG	1:B:562:ARG:HH11	2.01	0.74
1:A:198:ASN:O	1:A:237:VAL:O	2.06	0.73
1:B:400:LYS:O	1:B:439:ARG:NH2	2.16	0.73
1:B:559:GLY:H	1:B:562:ARG:NH2	1.83	0.73
1:A:105:MSE:HB3	1:A:116:ALA:HB2	1.70	0.73
1:A:453:THR:CA	2:A:707:HOH:O	2.35	0.73
1:B:272:ARG:HH21	1:B:439:ARG:NH2	1.86	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:328:THR:O	2:A:711:HOH:O	1.94	0.73
1:A:452:HIS:ND1	1:A:453:THR:N	2.37	0.73
1:A:598:GLN:O	1:A:599:GLN:HG2	1.88	0.73
1:B:463:LEU:HD21	1:B:492:TRP:CZ3	2.23	0.73
1:A:311:MSE:SE	2:A:722:HOH:O	2.55	0.73
1:A:378:GLU:O	1:A:378:GLU:CG	2.36	0.73
1:B:292:GLY:O	1:B:547:GLN:HA	1.88	0.72
1:A:470:GLY:HA3	1:A:529:TRP:CH2	2.23	0.72
1:B:417:ARG:NH2	2:B:632:HOH:O	2.22	0.72
1:B:325:SER:OG	2:B:691:HOH:O	2.05	0.72
1:B:465:LEU:O	1:B:502:ILE:HG23	1.89	0.72
1:B:462:VAL:HG13	1:B:499:PRO:O	1.88	0.72
1:B:451:ALA:HA	1:B:495:LYS:HD2	1.69	0.72
1:A:84:ILE:CG2	1:A:176:LEU:HD11	2.19	0.72
1:B:566:ASN:HB3	1:B:568:LYS:CD	2.18	0.72
1:B:547:GLN:CB	2:B:666:HOH:O	2.38	0.72
1:B:466:ASN:OD1	2:B:678:HOH:O	2.08	0.72
1:B:413:GLU:HG2	2:B:678:HOH:O	1.91	0.71
1:B:475:SER:HB2	1:B:520:MSE:HE1	1.73	0.71
1:A:207:VAL:CG1	1:A:210:GLY:H	2.04	0.71
1:A:228:GLN:HA	1:A:228:GLN:HE21	1.53	0.71
1:A:469:TYR:HE2	1:A:485:LEU:HD13	1.56	0.71
1:B:372:LYS:HB2	1:B:372:LYS:HZ3	1.55	0.71
1:B:8:PRO:O	2:B:634:HOH:O	2.07	0.71
1:A:335:GLU:O	1:A:339:ASP:CB	2.39	0.71
1:A:328:THR:OG1	1:A:350:ASP:HA	1.90	0.71
1:B:449:CYS:SG	1:B:450:ASP:N	2.64	0.71
1:B:550:ASN:ND2	1:B:554:PHE:CE2	2.58	0.71
1:A:9:THR:HG23	1:A:178:THR:O	1.91	0.71
1:B:103:GLU:HB2	2:B:647:HOH:O	1.90	0.70
1:B:338:LEU:HB2	2:B:653:HOH:O	1.91	0.70
1:B:38:ALA:HB1	1:B:70:GLN:OE1	1.91	0.70
1:A:172:ARG:CD	1:A:334:ALA:HB2	2.21	0.70
1:A:363:ILE:O	1:A:561:LEU:HG	1.91	0.70
1:B:455:THR:O	1:B:459:LEU:HD12	1.91	0.70
1:A:352:THR:HG22	1:A:395:LEU:HD13	1.72	0.70
1:B:447:MSE:HA	1:B:467:ARG:HD3	1.73	0.70
1:B:172:ARG:HD3	1:B:334:ALA:HB2	1.72	0.70
1:A:30:ILE:HA	1:A:35:TRP:HZ3	1.57	0.70
1:A:450:ASP:OD1	2:A:671:HOH:O	2.08	0.69
1:A:10:ARG:CZ	1:A:10:ARG:HB3	2.23	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:548:VAL:HG21	1:B:584:LEU:HD21	1.74	0.69
1:A:12:ILE:HG22	1:A:79:TRP:HH2	1.57	0.69
1:B:105:MSE:SE	1:B:114:PHE:CB	2.90	0.69
1:B:442:THR:OG1	1:B:443:CYS:N	2.26	0.69
1:A:10:ARG:HD2	1:A:79:TRP:NE1	2.04	0.69
1:A:36:GLU:C	1:A:129:ARG:HH12	1.95	0.69
1:B:43:ARG:HD3	1:B:55:PHE:CE1	2.27	0.69
1:A:151:ASP:OD1	1:A:155:LYS:NZ	2.15	0.69
1:A:144:PRO:HG3	1:A:353:ALA:O	1.91	0.69
1:A:381:ASN:CB	1:A:383:GLU:HB2	2.21	0.69
1:B:15:LEU:HD13	1:B:48:PRO:HD3	1.73	0.69
1:B:584:LEU:O	1:B:588:TRP:HB2	1.93	0.69
1:B:197:CYS:CB	1:B:198:ASN:HB3	2.23	0.69
1:B:359:LEU:CD1	1:B:372:LYS:NZ	2.56	0.69
1:A:336:GLU:HA	2:A:722:HOH:O	1.91	0.69
1:A:232:GLY:O	1:A:233:THR:OG1	2.09	0.69
1:B:15:LEU:O	1:B:15:LEU:HD12	1.92	0.69
1:B:372:LYS:HB2	1:B:372:LYS:NZ	2.07	0.68
1:B:400:LYS:C	1:B:439:ARG:HH22	1.95	0.68
1:B:272:ARG:NH2	1:B:439:ARG:HH21	1.91	0.68
1:A:502:ILE:HD13	1:A:537:PHE:CZ	2.28	0.68
1:B:413:GLU:CG	2:B:678:HOH:O	2.41	0.68
1:B:449:CYS:SG	1:B:488:GLU:CD	2.71	0.68
1:B:45:ILE:HG13	1:B:55:PHE:CZ	2.27	0.68
1:A:330:HIS:N	2:A:711:HOH:O	2.26	0.68
1:A:376:SER:O	1:A:380:VAL:HG23	1.93	0.68
1:A:198:ASN:HB3	1:A:199:HIS:HD2	1.58	0.68
1:B:562:ARG:HA	1:B:566:ASN:CG	2.14	0.68
1:A:199:HIS:CE1	1:A:236:VAL:HG23	2.28	0.68
1:A:207:VAL:HG11	1:A:210:GLY:H	1.58	0.68
1:B:33:ARG:NH1	1:B:36:GLU:HB3	2.09	0.68
1:B:358:ASN:HB3	1:B:360:SER:H	1.59	0.68
1:B:474:GLN:N	2:B:670:HOH:O	2.27	0.68
1:B:5:VAL:CG1	1:B:6:GLU:H	2.06	0.68
1:A:381:ASN:CB	1:A:383:GLU:H	2.05	0.68
1:A:17:GLY:O	1:A:45:ILE:O	2.12	0.68
1:B:216:LEU:H	1:B:226:THR:HG22	1.59	0.68
1:A:295:ARG:O	1:A:329:SER:HB2	1.94	0.68
1:B:99:VAL:O	1:B:100:ASN:C	2.30	0.68
1:A:88:PHE:CE2	1:A:97:VAL:HG21	2.29	0.68
1:B:92:THR:O	1:B:110:GLY:HA2	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:202:VAL:CG1	1:B:204:TRP:HZ3	2.07	0.68
1:B:273:SER:CB	1:B:284:ASN:H	1.97	0.68
1:B:562:ARG:CB	1:B:562:ARG:HH11	2.05	0.68
1:B:195:GLN:CD	1:B:195:GLN:H	1.98	0.67
1:B:212:VAL:HG11	1:B:230:THR:N	2.09	0.67
1:A:329:SER:N	2:A:711:HOH:O	2.19	0.67
1:A:456:ILE:HB	1:A:459:LEU:HD12	1.76	0.67
1:B:341:ALA:HA	1:B:346:ILE:HB	1.75	0.67
1:B:91:VAL:CG1	1:B:134:VAL:CG1	2.72	0.67
1:B:338:LEU:HD12	1:B:339:ASP:N	2.09	0.67
1:B:462:VAL:HG22	1:B:499:PRO:CG	2.24	0.67
1:A:93:HIS:N	2:A:704:HOH:O	2.20	0.67
1:B:197:CYS:CB	1:B:198:ASN:ND2	2.57	0.67
1:B:5:VAL:CG1	1:B:6:GLU:N	2.58	0.67
1:A:83:ARG:HD3	1:A:179:THR:OG1	1.93	0.66
1:A:497:HIS:HD2	2:A:687:HOH:O	1.77	0.66
1:A:315:HIS:O	1:A:319:ASP:HB2	1.95	0.66
1:B:493:GLN:HG3	2:B:644:HOH:O	1.96	0.66
1:A:118:VAL:HG23	1:A:120:PRO:CD	2.22	0.66
1:A:457:SER:HB2	1:A:496:LEU:HD11	1.76	0.66
1:A:94:TYR:HB3	1:A:135:ASN:HB3	1.76	0.66
1:B:202:VAL:HG12	1:B:230:THR:O	1.95	0.66
1:B:296:HIS:HD2	1:B:550:ASN:HD21	1.43	0.66
1:B:302:ARG:CG	1:B:302:ARG:O	2.43	0.66
1:B:337:MSE:CE	1:B:348:VAL:HG21	2.21	0.66
1:B:52:ASN:ND2	1:B:168:ALA:H	1.94	0.66
1:B:190:VAL:HG21	1:B:438:THR:HG21	1.76	0.66
1:A:190:VAL:HG13	1:A:438:THR:HG21	1.76	0.66
1:B:184:VAL:HG12	1:B:185:ASP:N	2.11	0.66
1:B:288:PHE:HZ	1:B:347:VAL:HG21	1.61	0.66
1:B:355:VAL:HA	2:B:683:HOH:O	1.96	0.66
1:B:455:THR:O	1:B:459:LEU:CD1	2.43	0.66
1:B:333:TYR:O	1:B:398:ARG:NH2	2.29	0.65
1:A:187:ILE:HG22	1:A:188:THR:N	2.11	0.65
1:A:456:ILE:HG23	1:A:456:ILE:O	1.95	0.65
1:B:432:THR:OG1	1:B:441:ILE:HD13	1.96	0.65
1:A:187:ILE:HG22	1:A:188:THR:H	1.60	0.65
1:B:327:ARG:HH11	1:B:503:THR:HB	1.60	0.65
1:A:278:GLY:O	1:A:279:GLU:HB3	1.96	0.65
1:B:122:VAL:HG23	1:B:123:ILE:HD12	1.79	0.65
1:B:12:ILE:HG23	1:B:12:ILE:O	1.95	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:20:ALA:HB3	1:A:70:GLN:HB3	1.79	0.65
1:A:381:ASN:HB2	1:A:383:GLU:HB2	1.77	0.65
1:A:17:GLY:HA3	1:A:47:VAL:O	1.96	0.65
1:B:115:GLU:HA	1:B:115:GLU:OE1	1.96	0.65
1:B:448:PHE:O	1:B:448:PHE:HD1	1.79	0.65
1:B:547:GLN:HB3	2:B:666:HOH:O	1.97	0.65
1:B:559:GLY:N	1:B:562:ARG:HH22	1.87	0.65
1:B:191:THR:HG22	1:B:200:ALA:CB	2.27	0.65
1:B:359:LEU:CD1	1:B:372:LYS:HZ3	2.10	0.65
1:A:195:GLN:HG3	1:A:195:GLN:O	1.97	0.64
1:A:107:HIS:HE1	1:A:394:GLU:OE1	1.81	0.64
1:A:238:ASN:OD1	1:A:239:PRO:HD3	1.98	0.64
1:A:436:ASP:OD1	1:A:439:ARG:NH1	2.30	0.64
1:A:546:GLU:OE2	1:A:587:ARG:NH1	2.30	0.64
1:B:150:THR:O	2:B:642:HOH:O	2.14	0.64
1:B:359:LEU:HD11	1:B:372:LYS:HZ3	1.63	0.64
1:B:414:PRO:HA	2:B:679:HOH:O	1.97	0.64
1:A:5:VAL:HG11	1:A:266:PRO:CD	2.26	0.64
1:A:82:GLN:HA	1:A:82:GLN:NE2	2.11	0.64
1:B:241:LEU:CD2	1:B:241:LEU:H	2.11	0.64
1:B:542:ALA:O	2:B:665:HOH:O	2.15	0.64
1:A:470:GLY:O	1:A:471:TRP:C	2.36	0.64
1:B:14:LYS:CD	1:B:174:VAL:O	2.42	0.64
1:B:351:GLU:HG2	1:B:409:SER:HB3	1.80	0.64
1:A:238:ASN:CB	1:A:239:PRO:CD	2.76	0.64
1:A:455:THR:C	1:A:456:ILE:HG22	2.19	0.64
1:A:497:HIS:CD2	2:A:687:HOH:O	2.50	0.64
1:B:292:GLY:HA2	1:B:323:ALA:HB1	1.80	0.64
1:B:560:ILE:O	1:B:562:ARG:N	2.31	0.64
1:B:466:ASN:CB	1:B:504:GLU:H	2.11	0.63
1:A:14:LYS:HE2	1:A:73:VAL:HG21	1.80	0.63
1:A:172:ARG:HD3	1:A:334:ALA:HB2	1.81	0.63
1:B:33:ARG:HA	1:B:35:TRP:CZ3	2.34	0.63
1:B:359:LEU:HD12	1:B:372:LYS:NZ	2.13	0.63
1:A:340:TRP:HD1	1:A:340:TRP:O	1.82	0.63
1:B:517:TYR:O	1:B:519:ASP:N	2.32	0.63
1:B:526:GLN:O	1:B:530:LEU:HB2	1.98	0.63
1:B:535:ARG:O	1:B:539:ARG:HB2	1.99	0.63
1:B:482:GLU:HG3	1:B:536:VAL:HG21	1.80	0.63
1:A:102:GLN:HG3	1:A:121:TYR:CD1	2.34	0.63
1:B:355:VAL:HG23	1:B:412:ASN:HD22	1.63	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:562:ARG:HG3	1:B:562:ARG:HH11	1.62	0.63
1:A:186:ASP:HB3	1:A:206:VAL:HG11	1.80	0.63
1:A:30:ILE:HB	2:A:694:HOH:O	1.98	0.63
1:A:455:THR:O	1:A:456:ILE:HG22	1.98	0.63
1:A:247:GLY:C	2:A:693:HOH:O	2.37	0.63
1:A:455:THR:HG23	1:A:456:ILE:HG21	1.80	0.63
1:B:321:ILE:HG12	1:B:321:ILE:O	1.99	0.63
1:B:468:TYR:CD2	1:B:468:TYR:N	2.67	0.63
1:B:501:ILE:HG12	1:B:545:GLY:HA3	1.81	0.63
1:A:9:THR:CG2	1:A:178:THR:O	2.47	0.63
1:A:485:LEU:HD23	1:A:536:VAL:HG11	1.80	0.63
1:B:549:TRP:C	1:B:549:TRP:CD1	2.66	0.63
1:B:69:TYR:CD1	1:B:170:ILE:CD1	2.75	0.63
1:A:186:ASP:HB3	1:A:206:VAL:HG13	1.81	0.62
1:B:392:ILE:HD13	1:B:410:ILE:HG23	1.80	0.62
1:B:61:ARG:NH1	2:B:624:HOH:O	2.32	0.62
1:A:279:GLU:HG2	1:A:279:GLU:O	1.99	0.62
1:B:31:ASP:HB2	2:B:675:HOH:O	1.99	0.62
1:B:402:HIS:CE1	2:B:638:HOH:O	2.52	0.62
1:A:476:GLY:N	1:A:520:MSE:HE2	2.14	0.62
1:B:465:LEU:HD11	1:B:500:ILE:HG12	1.81	0.62
1:A:447:MSE:O	1:A:448:PHE:HD1	1.82	0.62
1:A:73:VAL:HG22	1:A:74:PHE:H	1.64	0.62
1:A:7:THR:O	1:A:9:THR:O	2.17	0.62
1:B:99:VAL:CG1	1:B:100:ASN:N	2.62	0.62
1:B:591:MSE:HE2	1:B:597:PRO:HD3	1.81	0.62
1:A:351:GLU:HG2	1:A:409:SER:OG	2.00	0.62
1:A:455:THR:O	1:A:455:THR:HG22	1.98	0.62
1:B:151:ASP:OD1	1:B:152:GLU:N	2.31	0.62
1:B:241:LEU:O	1:B:243:GLN:HG3	1.99	0.62
1:A:217:ARG:HG3	1:A:218:ASP:HB3	1.80	0.62
1:B:36:GLU:HA	1:B:129:ARG:NH1	2.15	0.62
2:A:662:HOH:O	1:B:12:ILE:HD11	1.99	0.62
1:B:36:GLU:CG	1:B:37:SER:H	2.13	0.62
1:A:520:MSE:O	1:A:521:TRP:HB2	1.99	0.62
1:B:119:THR:N	1:B:120:PRO:HD3	2.15	0.62
1:B:119:THR:HG21	2:B:693:HOH:O	2.00	0.61
1:B:182:THR:HG21	1:B:258:SER:HB2	1.81	0.61
1:B:372:LYS:N	1:B:373:GLU:HA	2.15	0.61
1:B:570:ILE:HD13	1:B:584:LEU:HD22	1.81	0.61
1:A:207:VAL:HG11	1:A:210:GLY:O	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:340:TRP:CD1	1:A:340:TRP:O	2.53	0.61
1:A:372:LYS:HB2	1:A:373:GLU:OE2	2.00	0.61
1:A:452:HIS:CD2	1:A:492:TRP:HH2	2.18	0.61
1:A:525:TYR:HB3	2:A:708:HOH:O	1.98	0.61
1:B:94:TYR:HB2	1:B:108:GLN:OE1	2.00	0.61
1:A:218:ASP:CB	1:A:221:GLN:HA	2.29	0.61
1:B:139:ASN:HA	1:B:146:GLY:O	2.00	0.61
1:B:212:VAL:HG22	1:B:230:THR:HG22	1.83	0.61
1:B:172:ARG:NH1	1:B:334:ALA:N	2.48	0.61
1:B:375:TYR:CD1	1:B:379:ALA:HB2	2.35	0.61
1:B:21:PHE:CE2	1:B:45:ILE:HD12	2.35	0.61
1:B:509:THR:HG21	1:B:526:GLN:HB2	1.83	0.61
1:A:228:GLN:CA	1:A:228:GLN:NE2	2.63	0.61
1:A:452:HIS:CE1	1:A:453:THR:O	2.54	0.61
1:B:212:VAL:CG2	1:B:230:THR:HG22	2.31	0.61
1:A:214:VAL:HG12	1:A:227:GLY:HA3	1.83	0.61
1:B:388:HIS:HD2	1:B:392:ILE:HD11	1.65	0.61
1:B:519:ASP:O	1:B:525:TYR:HB2	2.01	0.61
1:B:386:GLN:O	1:B:389:LEU:HB3	2.01	0.60
1:A:562:ARG:NH1	1:A:566:ASN:HD22	1.99	0.60
1:B:187:ILE:HA	1:B:204:TRP:HB2	1.83	0.60
1:B:293:PHE:HZ	1:B:321:ILE:HD13	1.66	0.60
1:B:92:THR:CG2	1:B:93:HIS:H	2.14	0.60
1:A:136:ASN:HD22	1:A:136:ASN:C	2.05	0.60
1:A:422:ARG:HB2	1:A:454:ASP:HB2	1.83	0.60
1:A:468:TYR:OH	1:A:568:LYS:HD3	2.02	0.60
1:A:476:GLY:N	1:A:520:MSE:CE	2.64	0.60
1:A:550:ASN:ND2	1:A:554:PHE:CE2	2.70	0.60
1:A:93:HIS:C	2:A:705:HOH:O	2.39	0.60
1:B:402:HIS:CG	2:B:654:HOH:O	2.54	0.60
1:A:12:ILE:HD12	2:A:698:HOH:O	2.01	0.60
1:B:105:MSE:HE2	1:B:116:ALA:CB	2.31	0.60
1:A:11:GLU:HG2	1:A:11:GLU:O	2.01	0.60
1:A:376:SER:O	1:A:380:VAL:CG2	2.49	0.60
1:A:10:ARG:CD	1:A:79:TRP:HE1	2.08	0.60
1:B:449:CYS:C	1:B:452:HIS:HB2	2.21	0.60
1:B:467:ARG:HB2	1:B:469:TYR:CZ	2.37	0.60
1:A:-1:SER:O	1:A:0:HIS:CB	2.48	0.60
1:A:450:ASP:O	1:A:452:HIS:O	2.19	0.60
1:A:14:LYS:CB	1:A:14:LYS:HZ2	2.14	0.60
1:B:143:ILE:CG2	1:B:144:PRO:HD2	2.30	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:379:ALA:HA	1:B:381:ASN:ND2	2.17	0.59
1:B:184:VAL:HG12	1:B:185:ASP:H	1.67	0.59
1:B:341:ALA:HB1	1:B:404:SER:CB	2.30	0.59
1:B:33:ARG:HA	1:B:35:TRP:CH2	2.37	0.59
1:B:444:VAL:HA	1:B:464:CYS:O	2.02	0.59
1:A:33:ARG:HB3	1:A:36:GLU:CD	2.22	0.59
1:A:172:ARG:HD3	1:A:334:ALA:CB	2.32	0.59
1:A:469:TYR:CE2	1:A:485:LEU:HD13	2.35	0.59
1:B:143:ILE:HD13	1:B:391:ALA:HB2	1.85	0.59
1:B:417:ARG:CG	1:B:418:PRO:HD3	2.30	0.59
1:B:547:GLN:HB2	2:B:666:HOH:O	1.99	0.59
1:B:562:ARG:HG2	1:B:566:ASN:ND2	2.16	0.59
1:A:105:MSE:CE	1:A:114:PHE:O	2.50	0.59
1:B:184:VAL:HG21	1:B:254:VAL:CG1	2.29	0.59
1:B:455:THR:CG2	1:B:456:ILE:HG13	2.33	0.59
1:B:99:VAL:HG23	1:B:104:VAL:HG21	1.84	0.59
1:A:202:VAL:HG22	1:A:234:LEU:HD22	1.85	0.59
1:A:202:VAL:HG22	1:A:234:LEU:HD21	1.81	0.59
1:B:91:VAL:HG22	1:B:170:ILE:HG12	1.84	0.59
1:B:562:ARG:HB2	1:B:562:ARG:HH11	1.67	0.59
1:A:321:ILE:HG23	1:A:321:ILE:O	2.02	0.59
1:B:470:GLY:N	1:B:529:TRP:CH2	2.66	0.59
1:B:359:LEU:HD11	1:B:372:LYS:NZ	2.17	0.59
1:B:68:TRP:CZ3	1:B:133:CYS:HB2	2.37	0.59
1:A:216:LEU:HD21	1:A:250:TYR:CB	2.33	0.59
1:B:520:MSE:HB3	1:B:521:TRP:HD1	1.66	0.59
1:B:99:VAL:HG12	1:B:100:ASN:H	1.67	0.58
1:A:456:ILE:O	1:A:460:PHE:HD2	1.86	0.58
1:B:211:ASP:O	1:B:256:ALA:HA	2.04	0.58
1:B:273:SER:HB3	1:B:284:ASN:CA	2.33	0.58
1:B:295:ARG:HH12	1:B:314:ASP:HB3	1.69	0.58
1:B:299:ALA:CB	1:B:310:LEU:HD11	2.28	0.58
1:B:183:TRP:CE3	1:B:184:VAL:O	2.56	0.58
1:B:184:VAL:CG1	1:B:185:ASP:H	2.15	0.58
1:B:416:THR:HG23	1:B:453:THR:HA	1.83	0.58
1:A:36:GLU:HB2	2:A:714:HOH:O	2.04	0.58
1:B:102:GLN:HB2	2:B:668:HOH:O	2.02	0.58
1:A:249:LEU:HG	2:A:693:HOH:O	2.01	0.58
1:B:0:HIS:N	1:B:0:HIS:ND1	2.52	0.58
1:B:510:LEU:HD23	1:B:513:LEU:HD12	1.85	0.58
1:B:465:LEU:O	1:B:502:ILE:HA	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:143:ILE:HG22	1:A:353:ALA:HB3	1.84	0.58
1:B:206:VAL:HG13	1:B:206:VAL:O	2.03	0.58
1:A:338:LEU:O	1:A:342:ASP:HB2	2.04	0.58
1:A:486:GLU:OE2	1:A:539:ARG:HD2	2.04	0.58
1:B:453:THR:CG2	1:B:456:ILE:HB	2.30	0.58
1:B:91:VAL:O	1:B:110:GLY:HA2	2.03	0.58
1:A:104:VAL:O	2:A:655:HOH:O	2.16	0.57
1:B:298:ASP:OD2	1:B:554:PHE:HA	2.03	0.57
1:A:278:GLY:HA2	2:A:709:HOH:O	2.04	0.57
1:A:441:ILE:HD12	1:A:460:PHE:CE1	2.38	0.57
1:B:302:ARG:CD	2:B:645:HOH:O	2.44	0.57
1:B:412:ASN:O	2:B:683:HOH:O	2.17	0.57
1:B:43:ARG:HD3	1:B:55:PHE:CD1	2.40	0.57
1:B:36:GLU:CG	1:B:37:SER:N	2.66	0.57
1:A:195:GLN:O	1:A:195:GLN:CG	2.52	0.57
1:A:469:TYR:CD2	1:A:533:TYR:OH	2.57	0.57
1:B:466:ASN:CB	1:B:504:GLU:N	2.67	0.57
1:A:219:ALA:N	2:A:686:HOH:O	2.30	0.57
1:A:279:GLU:CG	1:A:279:GLU:O	2.52	0.57
1:B:292:GLY:HA3	1:B:325:SER:O	2.04	0.57
1:B:328:THR:OG1	1:B:331:TYR:O	2.20	0.57
1:A:94:TYR:O	1:A:134:VAL:HA	2.05	0.57
1:A:205:GLN:HB2	1:A:231:SER:H	1.69	0.57
1:A:304:LYS:NZ	2:A:656:HOH:O	2.34	0.57
1:A:343:GLU:N	2:A:695:HOH:O	2.36	0.57
1:A:453:THR:C	2:A:707:HOH:O	2.42	0.57
1:A:187:ILE:HG12	1:A:205:GLN:NE2	2.19	0.57
1:A:468:TYR:CE2	1:A:549:TRP:HD1	2.23	0.57
1:B:-1:SER:C	1:B:0:HIS:ND1	2.57	0.57
1:B:208:ALA:O	1:B:210:GLY:N	2.35	0.57
1:B:216:LEU:HA	1:B:252:LEU:HA	1.87	0.57
1:B:272:ARG:HE	1:B:439:ARG:HE	1.52	0.57
1:B:83:ARG:NE	1:B:179:THR:HG23	2.20	0.57
1:A:138:LEU:HD22	1:A:144:PRO:O	2.05	0.57
1:A:525:TYR:O	1:A:526:GLN:C	2.40	0.57
1:A:470:GLY:CA	1:A:529:TRP:CH2	2.88	0.57
1:B:388:HIS:CD2	1:B:392:ILE:HD11	2.40	0.57
1:A:136:ASN:ND2	1:A:136:ASN:C	2.57	0.57
1:A:51:PHE:C	1:A:51:PHE:CD1	2.78	0.57
1:A:563:VAL:HG23	1:A:566:ASN:OD1	2.04	0.57
1:B:243:GLN:OE1	1:B:246:GLU:HB2	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:608:HOH:O	1:B:340:TRP:HH2	1.88	0.57
1:A:313:HIS:CD2	1:B:301:LEU:HD22	2.40	0.56
1:A:328:THR:HG22	1:A:333:TYR:CD1	2.39	0.56
1:A:0:HIS:CE1	1:A:206:VAL:HG11	2.40	0.56
1:B:385:GLN:HB2	1:B:424:TYR:CE1	2.41	0.56
1:A:475:SER:OG	1:A:520:MSE:HE1	2.05	0.56
1:B:465:LEU:CD1	1:B:500:ILE:HG23	2.35	0.56
1:A:14:LYS:CD	1:A:176:LEU:HB2	2.29	0.56
1:A:221:GLN:HG3	2:A:648:HOH:O	2.05	0.56
1:A:447:MSE:O	1:A:448:PHE:CD1	2.58	0.56
1:A:-1:SER:O	1:A:0:HIS:HB2	2.06	0.56
1:B:15:LEU:HD23	1:B:173:SER:HB3	1.82	0.56
1:A:335:GLU:CG	1:A:335:GLU:O	2.52	0.56
1:A:381:ASN:HB3	1:A:383:GLU:H	1.69	0.56
1:B:466:ASN:CB	1:B:504:GLU:HB2	2.21	0.56
1:B:288:PHE:HA	1:B:594:GLY:O	2.05	0.56
1:B:195:GLN:CD	1:B:195:GLN:N	2.58	0.56
1:B:196:ASP:OD2	1:B:196:ASP:N	2.37	0.56
1:B:357:PHE:C	1:B:358:ASN:OD1	2.44	0.56
1:B:36:GLU:HA	1:B:129:ARG:CZ	2.36	0.56
1:B:218:ASP:HB2	1:B:248:TYR:OH	2.05	0.55
1:A:309:VAL:HG21	1:B:302:ARG:HE	1.70	0.55
1:B:315:HIS:CE1	1:B:336:GLU:OE1	2.54	0.55
1:B:359:LEU:HD12	1:B:372:LYS:HZ1	1.70	0.55
1:B:388:HIS:O	1:B:392:ILE:HG13	2.06	0.55
1:B:402:HIS:CB	2:B:654:HOH:O	2.53	0.55
1:B:415:ASP:N	2:B:679:HOH:O	1.92	0.55
1:B:445:ASN:C	1:B:445:ASN:OD1	2.44	0.55
1:B:94:TYR:HD2	1:B:135:ASN:HB2	1.72	0.55
1:B:41:GLU:HA	2:B:623:HOH:O	2.04	0.55
1:A:337:MSE:O	1:A:341:ALA:HB3	2.06	0.55
1:B:282:LEU:HA	1:B:286:LYS:O	2.07	0.55
1:B:566:ASN:CB	1:B:568:LYS:HD2	2.24	0.55
1:B:570:ILE:CD1	1:B:584:LEU:HD22	2.37	0.55
1:A:456:ILE:CB	1:A:459:LEU:HD12	2.36	0.55
1:B:377:GLU:HA	1:B:380:VAL:HG13	1.89	0.55
1:A:101:ASN:N	1:A:101:ASN:OD1	2.39	0.55
1:A:107:HIS:CD2	1:A:109:GLY:O	2.59	0.55
1:A:454:ASP:N	1:A:454:ASP:OD1	2.38	0.55
1:B:299:ALA:HB2	1:B:310:LEU:CD1	2.31	0.55
1:A:102:GLN:CG	1:A:121:TYR:CD1	2.90	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:321:ILE:CG2	1:A:321:ILE:O	2.55	0.55
1:B:187:ILE:HA	1:B:204:TRP:CB	2.37	0.55
1:B:402:HIS:HB3	2:B:654:HOH:O	2.06	0.55
1:A:73:VAL:O	1:A:127:SER:HA	2.07	0.55
1:A:475:SER:OG	1:A:520:MSE:CE	2.55	0.55
1:B:99:VAL:CG1	1:B:100:ASN:H	2.20	0.55
1:B:94:TYR:HD2	1:B:135:ASN:CB	2.20	0.55
1:B:249:LEU:HD21	1:B:268:ARG:HH11	1.71	0.55
1:B:455:THR:HG23	1:B:456:ILE:HG13	1.89	0.55
1:B:174:VAL:O	1:B:174:VAL:HG13	2.08	0.54
1:B:447:MSE:CE	1:B:467:ARG:HB3	2.23	0.54
1:A:12:ILE:CG2	1:A:79:TRP:HH2	2.20	0.54
1:A:315:HIS:CD2	1:A:318:MSE:HE3	2.42	0.54
1:A:562:ARG:HH11	1:A:566:ASN:HD22	1.53	0.54
1:B:18:LEU:H	1:B:46:ALA:HA	1.72	0.54
1:B:156:LYS:HD2	2:B:604:HOH:O	2.07	0.54
1:B:351:GLU:HG2	1:B:409:SER:CB	2.37	0.54
1:A:216:LEU:CD2	1:A:250:TYR:HB3	2.37	0.54
1:B:562:ARG:HB2	1:B:562:ARG:NH1	2.23	0.54
1:A:311:MSE:HE3	1:A:340:TRP:CE3	2.43	0.54
1:A:377:GLU:OE2	1:A:377:GLU:CA	2.55	0.54
1:A:417:ARG:NH2	2:A:625:HOH:O	2.40	0.54
1:B:494:GLU:O	1:B:495:LYS:C	2.45	0.54
1:A:456:ILE:CG1	1:A:459:LEU:CB	2.59	0.54
1:A:17:GLY:CA	1:A:47:VAL:H	2.17	0.54
1:B:407:MSE:SE	1:B:442:THR:HG21	2.58	0.54
1:A:202:VAL:CG2	1:A:234:LEU:HD22	2.38	0.54
1:A:20:ALA:HB1	1:A:42:SER:HB2	1.90	0.54
1:A:308:ASN:O	1:A:312:VAL:HG23	2.07	0.54
1:B:114:PHE:CD2	1:B:114:PHE:N	2.76	0.54
1:B:184:VAL:CG1	1:B:185:ASP:N	2.70	0.54
1:B:295:ARG:HG3	1:B:326:TYR:CD1	2.42	0.54
1:A:12:ILE:CG2	1:A:176:LEU:HB3	2.38	0.54
1:A:469:TYR:HD2	1:A:533:TYR:OH	1.91	0.54
1:A:535:ARG:HA	2:A:650:HOH:O	2.07	0.54
1:B:51:PHE:CE2	1:B:168:ALA:HB3	2.43	0.54
1:A:0:HIS:CD2	1:A:186:ASP:OD2	2.60	0.53
1:B:144:PRO:HD3	1:B:353:ALA:O	2.04	0.53
1:A:12:ILE:HG23	1:A:12:ILE:O	2.09	0.53
1:A:242:TRP:HZ2	1:A:345:GLY:HA2	1.74	0.53
1:A:548:VAL:CG1	1:A:570:ILE:CD1	2.84	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:52:ASN:ND2	1:B:167:TYR:HA	2.23	0.53
1:B:122:VAL:HG23	1:B:123:ILE:CD1	2.37	0.53
1:B:138:LEU:HD13	1:B:144:PRO:O	2.08	0.53
1:B:15:LEU:CD2	1:B:173:SER:CA	2.80	0.53
1:B:293:PHE:CE1	1:B:570:ILE:HD12	2.43	0.53
1:A:36:GLU:C	1:A:129:ARG:NH1	2.62	0.53
1:A:147:MSE:HE3	1:A:161:PHE:HZ	1.74	0.53
1:A:39:LEU:HB2	1:A:70:GLN:HE21	1.73	0.53
1:A:479:GLU:OE1	1:A:479:GLU:N	2.30	0.53
1:B:217:ARG:NH1	1:B:223:VAL:HG22	2.24	0.53
1:B:398:ARG:HG2	1:B:399:ASP:OD1	2.08	0.53
1:B:469:TYR:CD2	1:B:485:LEU:HD13	2.43	0.53
1:B:407:MSE:SE	1:B:442:THR:CG2	3.06	0.53
1:B:450:ASP:N	1:B:452:HIS:HB2	2.23	0.53
1:B:445:ASN:ND2	1:B:465:LEU:HB3	2.24	0.53
1:A:0:HIS:CD2	1:A:186:ASP:CG	2.82	0.53
1:A:224:VAL:HG22	1:A:237:VAL:HG21	1.91	0.53
1:A:86:LEU:HB2	1:A:176:LEU:HD22	1.89	0.53
1:B:96:LYS:CE	1:B:103:GLU:OE2	2.50	0.53
1:A:205:GLN:HG3	1:A:212:VAL:HG21	1.89	0.53
1:A:297:GLU:O	1:A:304:LYS:HA	2.08	0.53
1:B:183:TRP:HE3	1:B:184:VAL:O	1.92	0.53
1:B:241:LEU:O	1:B:243:GLN:NE2	2.41	0.53
1:B:276:VAL:HG21	1:B:461:ASP:HB3	1.90	0.53
1:B:375:TYR:CD1	1:B:379:ALA:CB	2.92	0.53
1:B:467:ARG:HH21	1:B:492:TRP:HE1	1.55	0.53
1:A:212:VAL:HA	1:A:255:THR:O	2.09	0.53
1:B:202:VAL:HG23	1:B:234:LEU:HD22	1.90	0.53
1:B:193:VAL:HG11	1:B:271:ILE:CG2	2.39	0.53
1:B:495:LYS:HG2	1:B:496:LEU:HG	1.91	0.53
1:B:562:ARG:HA	1:B:566:ASN:OD1	2.09	0.53
1:A:292:GLY:HA3	1:A:325:SER:O	2.09	0.53
1:A:140:TRP:HB3	1:A:379:ALA:O	2.09	0.53
1:B:114:PHE:HD2	1:B:114:PHE:N	2.07	0.53
1:A:494:GLU:O	1:A:497:HIS:CE1	2.62	0.52
1:B:339:ASP:O	1:B:343:GLU:HG3	2.09	0.52
1:A:73:VAL:HG22	1:A:74:PHE:N	2.24	0.52
1:B:82:GLN:CD	1:B:82:GLN:N	2.63	0.52
1:A:180:PRO:HB2	1:A:261:GLU:HG2	1.91	0.52
1:A:139:ASN:H	1:A:142:THR:CG2	2.22	0.52
1:A:33:ARG:NH1	1:A:36:GLU:OE2	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:377:GLU:OE2	1:A:377:GLU:HA	2.10	0.52
1:B:217:ARG:HD3	1:B:222:GLN:C	2.30	0.52
1:B:396:ILE:HG23	1:B:408:TRP:CZ2	2.44	0.52
1:A:515:SER:HB3	1:A:517:TYR:O	2.08	0.52
1:A:39:LEU:HD13	1:A:70:GLN:NE2	2.24	0.52
1:B:151:ASP:HB3	1:B:155:LYS:HB2	1.91	0.52
1:B:288:PHE:C	1:B:288:PHE:CD2	2.82	0.52
1:B:465:LEU:HD13	1:B:500:ILE:HG23	1.91	0.52
1:B:6:GLU:O	1:B:7:THR:HB	2.10	0.52
1:A:21:PHE:CE2	1:A:23:LEU:HD23	2.44	0.52
1:A:344:HIS:ND1	1:A:344:HIS:N	2.57	0.52
1:B:107:HIS:HE1	1:B:394:GLU:OE1	1.92	0.52
1:B:19:TRP:CE3	1:B:71:ARG:HB3	2.44	0.52
1:A:340:TRP:CA	2:A:695:HOH:O	2.56	0.52
1:A:289:TYR:OH	1:A:546:GLU:OE1	2.19	0.52
1:A:482:GLU:OE2	1:A:539:ARG:NH2	2.42	0.52
1:A:504:GLU:HG2	1:A:549:TRP:HB2	1.92	0.52
1:A:71:ARG:NH1	1:A:72:GLU:O	2.43	0.52
1:B:92:THR:HG22	1:B:93:HIS:H	1.75	0.52
1:A:16:ASP:OD2	1:A:18:LEU:HD12	2.10	0.52
1:A:456:ILE:HG13	1:A:459:LEU:CD1	2.39	0.52
1:A:259:GLN:HA	1:A:259:GLN:HE21	1.75	0.51
1:A:469:TYR:HB2	1:A:533:TYR:OH	2.10	0.51
1:A:563:VAL:O	1:A:564:GLY:C	2.48	0.51
1:B:379:ALA:HB3	2:B:684:HOH:O	2.09	0.51
1:A:311:MSE:HE3	1:A:340:TRP:HE3	1.75	0.51
1:A:453:THR:HA	2:A:707:HOH:O	2.07	0.51
1:A:550:ASN:OD1	1:A:551:PHE:N	2.43	0.51
1:B:82:GLN:HB3	1:B:179:THR:O	2.10	0.51
1:B:338:LEU:O	1:B:342:ASP:HB2	2.10	0.51
1:B:414:PRO:HD3	1:B:444:VAL:O	2.10	0.51
1:A:205:GLN:OE1	1:A:206:VAL:N	2.41	0.51
1:A:297:GLU:HG3	1:A:331:TYR:HE1	1.76	0.51
1:B:33:ARG:HG3	1:B:35:TRP:CZ2	2.45	0.51
1:B:438:THR:HG23	1:B:439:ARG:HG3	1.91	0.51
1:B:99:VAL:O	1:B:101:ASN:N	2.43	0.51
1:A:180:PRO:HG3	1:A:262:CYS:O	2.09	0.51
1:B:110:GLY:N	2:B:688:HOH:O	2.42	0.51
1:B:380:VAL:HG12	2:B:684:HOH:O	2.09	0.51
1:B:482:GLU:HG3	1:B:536:VAL:CG2	2.40	0.51
1:A:381:ASN:HB2	1:A:384:THR:H	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:98:TRP:CZ3	1:A:103:GLU:HB3	2.46	0.51
1:B:396:ILE:HA	1:B:408:TRP:CH2	2.45	0.51
1:B:548:VAL:HG21	1:B:584:LEU:CD2	2.40	0.51
1:A:229:GLY:O	1:A:230:THR:C	2.49	0.51
1:B:-1:SER:H2	1:B:0:HIS:CE1	2.28	0.51
1:B:141:GLN:HA	1:B:384:THR:HG22	1.93	0.51
1:B:538:ASP:HB2	1:B:597:PRO:HG2	1.93	0.51
1:B:202:VAL:O	1:B:231:SER:HA	2.10	0.51
1:B:302:ARG:O	1:B:302:ARG:HG2	2.10	0.51
1:B:352:THR:HG22	1:B:353:ALA:N	2.26	0.51
1:B:82:GLN:CD	1:B:82:GLN:H	2.14	0.51
1:A:337:MSE:HE1	1:A:348:VAL:HG11	1.92	0.51
1:A:198:ASN:O	1:A:199:HIS:CD2	2.64	0.51
1:B:187:ILE:CG2	1:B:188:THR:N	2.74	0.51
1:A:20:ALA:HB1	1:A:42:SER:CB	2.41	0.50
1:A:216:LEU:HD13	1:A:216:LEU:O	2.12	0.50
1:B:83:ARG:NH2	1:B:183:TRP:CE3	2.79	0.50
1:A:450:ASP:CG	2:A:671:HOH:O	2.48	0.50
1:B:467:ARG:C	1:B:468:TYR:CD2	2.84	0.50
1:B:493:GLN:HG2	1:B:494:GLU:N	2.26	0.50
1:B:91:VAL:HG11	1:B:134:VAL:HG13	1.94	0.50
1:B:216:LEU:HD12	1:B:216:LEU:C	2.32	0.50
1:B:171:HIS:CG	1:B:304:LYS:O	2.64	0.50
1:B:553:ASP:OD1	1:B:578:LYS:NZ	2.43	0.50
1:B:76:PRO:O	1:B:79:TRP:HB2	2.12	0.50
1:A:198:ASN:HB3	1:A:199:HIS:CD2	2.42	0.50
1:A:340:TRP:CH2	1:B:44:ALA:HB3	2.46	0.50
1:A:453:THR:O	2:A:707:HOH:O	2.19	0.50
1:B:244:PRO:HG2	1:B:593:PHE:CE1	2.46	0.50
1:B:469:TYR:HD2	1:B:533:TYR:HH	1.60	0.50
1:A:372:LYS:C	1:A:373:GLU:HG3	2.31	0.50
1:B:101:ASN:N	1:B:101:ASN:ND2	2.45	0.50
1:B:476:GLY:HA2	1:B:525:TYR:OH	2.11	0.50
1:B:499:PRO:HA	2:B:665:HOH:O	2.11	0.50
1:A:116:ALA:HB1	2:A:655:HOH:O	2.11	0.50
1:A:565:GLY:O	1:A:567:LYS:HD3	2.11	0.50
1:A:92:THR:HA	1:A:110:GLY:O	2.12	0.50
1:B:549:TRP:HZ3	1:B:568:LYS:HZ3	0.75	0.50
1:A:392:ILE:HD13	1:A:432:THR:HG22	1.91	0.50
1:A:452:HIS:ND1	1:A:453:THR:O	2.45	0.50
1:A:453:THR:N	2:A:707:HOH:O	2.43	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:552:ALA:HA	1:A:571:PHE:O	2.11	0.50
1:B:102:GLN:NE2	1:B:102:GLN:O	2.45	0.50
1:B:242:TRP:CE2	1:B:403:PRO:HB2	2.47	0.50
1:B:337:MSE:HE1	1:B:348:VAL:CG2	2.29	0.50
1:A:21:PHE:HE2	1:A:23:LEU:CD2	2.25	0.50
1:A:248:TYR:HB3	2:A:689:HOH:O	2.10	0.50
1:A:381:ASN:HB2	1:A:383:GLU:H	1.77	0.50
1:B:267:LEU:CD1	1:B:269:VAL:HG13	2.42	0.50
1:A:83:ARG:CB	1:A:179:THR:O	2.44	0.49
1:A:214:VAL:O	1:A:227:GLY:N	2.45	0.49
1:B:469:TYR:HD2	1:B:533:TYR:OH	1.95	0.49
1:B:566:ASN:N	2:B:682:HOH:O	2.18	0.49
1:A:337:MSE:HB2	2:A:614:HOH:O	2.13	0.49
1:A:15:LEU:CD2	1:A:48:PRO:HD3	2.40	0.49
1:B:92:THR:HG21	1:B:168:ALA:CB	2.42	0.49
1:B:51:PHE:HE2	1:B:168:ALA:HB3	1.76	0.49
1:A:312:VAL:HG11	1:B:54:GLN:NE2	2.27	0.49
1:B:558:GLN:OE1	1:B:559:GLY:N	2.46	0.49
1:B:96:LYS:HE3	1:B:106:GLU:OE2	2.12	0.49
1:A:242:TRP:HA	2:A:689:HOH:O	2.10	0.49
1:B:25:ARG:C	1:B:27:ASN:N	2.63	0.49
1:B:433:ARG:HA	2:B:627:HOH:O	2.11	0.49
1:B:490:LEU:O	1:B:493:GLN:HB3	2.11	0.49
1:A:69:TYR:CE2	1:A:170:ILE:HG13	2.47	0.49
1:A:197:CYS:CB	1:A:198:ASN:OD1	2.53	0.49
1:A:230:THR:C	1:A:231:SER:OG	2.50	0.49
1:A:238:ASN:HB3	1:A:239:PRO:CD	2.43	0.49
1:B:122:VAL:HG22	1:B:123:ILE:HD12	1.93	0.49
2:A:662:HOH:O	1:B:12:ILE:CD1	2.56	0.49
1:A:83:ARG:NH2	1:A:183:TRP:CH2	2.80	0.49
1:A:222:GLN:HG2	2:A:645:HOH:O	2.12	0.49
1:A:422:ARG:NH1	1:A:454:ASP:O	2.46	0.49
1:B:11:GLU:OE1	1:B:11:GLU:N	2.45	0.49
1:B:295:ARG:HB2	1:B:333:TYR:OH	2.12	0.49
1:B:556:THR:HG23	1:B:565:GLY:HA2	1.95	0.49
1:A:254:VAL:O	1:A:264:ILE:HA	2.13	0.49
1:B:171:HIS:HB3	1:B:304:LYS:O	2.13	0.49
1:B:392:ILE:HG21	1:B:432:THR:CG2	2.43	0.49
1:B:93:HIS:CD2	1:B:138:LEU:HD21	2.48	0.49
1:A:216:LEU:C	1:A:216:LEU:HD22	2.33	0.49
1:A:288:PHE:CZ	1:A:347:VAL:HG11	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:456:ILE:HA	1:A:459:LEU:H	1.77	0.49
1:A:314:ASP:OD1	1:A:551:PHE:HE2	1.95	0.49
1:A:392:ILE:CG2	1:A:432:THR:HG22	2.42	0.49
1:A:470:GLY:N	1:A:529:TRP:CH2	2.80	0.49
1:A:555:ALA:HA	1:A:565:GLY:HA2	1.94	0.49
1:B:410:ILE:HD12	1:B:460:PHE:HE1	1.78	0.49
1:B:488:GLU:HG3	1:B:488:GLU:O	2.13	0.49
1:A:16:ASP:OD2	1:A:18:LEU:CD1	2.61	0.49
1:A:10:ARG:NH1	1:A:10:ARG:CB	2.76	0.48
1:A:273:SER:O	1:A:283:ILE:HA	2.14	0.48
1:A:32:GLN:HB2	1:A:34:TRP:HE1	1.78	0.48
1:A:35:TRP:CE2	1:A:36:GLU:OE2	2.66	0.48
1:A:373:GLU:N	1:A:373:GLU:OE2	2.46	0.48
1:A:407:MSE:SE	1:A:462:VAL:CG1	3.11	0.48
1:A:81:GLY:C	1:A:82:GLN:HE21	2.15	0.48
1:B:341:ALA:HB1	1:B:346:ILE:O	2.13	0.48
1:B:328:THR:O	1:B:351:GLU:HB2	2.13	0.48
1:A:21:PHE:CE2	1:A:23:LEU:CD2	2.96	0.48
1:B:102:GLN:HE21	1:B:102:GLN:N	2.11	0.48
1:B:83:ARG:CG	1:B:179:THR:HG23	2.43	0.48
1:B:35:TRP:CE2	1:B:98:TRP:CZ3	3.00	0.48
1:B:392:ILE:HG21	1:B:432:THR:HG22	1.95	0.48
1:B:467:ARG:NH2	1:B:492:TRP:HE1	2.11	0.48
1:A:100:ASN:C	1:A:101:ASN:OD1	2.51	0.48
1:A:337:MSE:HE2	1:A:337:MSE:HA	1.95	0.48
1:A:376:SER:O	1:A:377:GLU:OE2	2.31	0.48
1:A:401:ASN:HB2	2:A:676:HOH:O	2.12	0.48
1:A:20:ALA:HB1	1:A:42:SER:OG	2.12	0.48
1:A:504:GLU:HG2	1:A:549:TRP:CG	2.47	0.48
1:B:138:LEU:HB2	1:B:158:GLN:HE22	1.78	0.48
1:B:12:ILE:HG22	1:B:176:LEU:HG	1.95	0.48
1:A:183:TRP:CE2	1:A:208:ALA:CB	2.96	0.48
1:A:362:GLY:O	1:A:363:ILE:CB	2.62	0.48
1:A:529:TRP:CE2	1:A:533:TYR:HE1	2.32	0.48
1:B:199:HIS:CD2	1:B:199:HIS:O	2.66	0.48
1:A:187:ILE:CG2	1:A:188:THR:H	2.26	0.48
1:A:249:LEU:HD22	1:A:268:ARG:HB3	1.96	0.48
1:A:330:HIS:O	2:A:701:HOH:O	2.20	0.48
1:B:213:SER:HB3	1:B:255:THR:CB	2.23	0.48
1:B:76:PRO:HD2	1:B:79:TRP:CE3	2.48	0.48
1:A:456:ILE:HG13	1:A:459:LEU:HD12	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:183:TRP:CE3	1:B:185:ASP:HB2	2.48	0.48
1:B:27:ASN:O	1:B:28:CYS:SG	2.72	0.48
1:B:286:LYS:HE3	1:B:286:LYS:HB2	1.77	0.48
1:B:162:HIS:CD2	1:B:164:PHE:CZ	3.01	0.48
1:B:375:TYR:CE2	1:B:379:ALA:N	2.81	0.48
1:A:327:ARG:HA	1:A:349:ILE:O	2.14	0.48
1:A:107:HIS:CE1	1:A:394:GLU:OE1	2.65	0.48
1:B:424:TYR:HB2	2:B:626:HOH:O	2.14	0.48
1:A:230:THR:HG22	1:A:231:SER:OG	2.14	0.48
1:A:449:CYS:HA	1:A:452:HIS:HB2	1.96	0.48
1:B:481:ALA:O	1:B:485:LEU:HB2	2.14	0.48
1:A:119:THR:N	1:A:120:PRO:CD	2.77	0.47
1:A:255:THR:HG23	1:A:264:ILE:HG23	1.95	0.47
1:B:142:THR:HG22	1:B:145:PRO:HA	1.96	0.47
1:B:471:TRP:CZ3	1:B:520:MSE:HG2	2.35	0.47
1:A:116:ALA:CB	2:A:655:HOH:O	2.62	0.47
1:A:140:TRP:HE1	1:A:147:MSE:HE2	1.78	0.47
1:A:335:GLU:N	2:A:614:HOH:O	2.25	0.47
1:B:194:ALA:HB3	1:B:196:ASP:OD2	2.14	0.47
1:B:248:TYR:CD1	1:B:248:TYR:C	2.87	0.47
1:B:48:PRO:O	2:B:645:HOH:O	2.20	0.47
1:A:17:GLY:HA3	1:A:47:VAL:N	2.21	0.47
1:A:183:TRP:HZ3	1:A:185:ASP:OD1	1.97	0.47
1:A:237:VAL:CG1	1:A:238:ASN:N	2.37	0.47
1:A:273:SER:HB3	1:A:284:ASN:HA	1.96	0.47
1:A:341:ALA:HA	1:A:346:ILE:HB	1.96	0.47
1:A:10:ARG:NH1	1:A:10:ARG:HB3	2.30	0.47
1:A:19:TRP:CZ2	1:A:71:ARG:HD2	2.49	0.47
1:A:162:HIS:HB3	1:A:355:VAL:HB	1.97	0.47
1:A:540:VAL:O	1:A:596:LYS:NZ	2.47	0.47
1:B:189:VAL:O	1:B:190:VAL:HB	2.13	0.47
1:B:1:MSE:SE	1:B:113:PRO:HB2	2.64	0.47
1:B:293:PHE:CD2	1:B:551:PHE:HD1	2.32	0.47
1:A:52:ASN:HD21	1:A:168:ALA:H	1.63	0.47
1:A:205:GLN:HB2	1:A:231:SER:HA	1.96	0.47
1:A:327:ARG:HB2	1:A:349:ILE:HB	1.96	0.47
1:B:67:VAL:O	1:B:134:VAL:HG23	2.14	0.47
1:A:19:TRP:CE3	1:A:69:TYR:HB3	2.49	0.47
1:A:397:ALA:O	1:A:400:LYS:HD2	2.14	0.47
1:A:321:ILE:CG2	1:A:588:TRP:CE3	2.97	0.47
1:B:212:VAL:HG21	1:B:230:THR:CG2	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:399:ASP:HB3	1:B:405:VAL:HG21	1.95	0.47
1:B:83:ARG:HA	1:B:119:THR:HG1	1.77	0.47
1:A:241:LEU:O	1:A:248:TYR:HB3	2.15	0.47
1:A:320:TRP:CZ3	1:A:321:ILE:HG13	2.49	0.47
1:A:452:HIS:C	1:A:453:THR:OG1	2.53	0.47
1:B:189:VAL:HG12	1:B:190:VAL:N	2.29	0.47
1:B:295:ARG:HB3	1:B:295:ARG:HE	1.48	0.47
1:B:449:CYS:HG	1:B:488:GLU:CD	2.16	0.47
1:B:73:VAL:O	1:B:127:SER:HA	2.15	0.47
1:A:29:GLY:HA2	1:A:34:TRP:CD2	2.50	0.47
1:B:280:GLN:NE2	2:B:633:HOH:O	2.45	0.47
1:B:2:LEU:HD11	1:B:187:ILE:H	1.80	0.47
1:B:33:ARG:HH11	1:B:36:GLU:HB3	1.80	0.47
1:A:15:LEU:HD21	1:A:173:SER:OG	2.14	0.47
1:A:507:VAL:CG1	1:A:529:TRP:CD1	2.98	0.47
1:B:268:ARG:O	1:B:269:VAL:HG13	2.14	0.47
1:A:309:VAL:HG21	1:B:302:ARG:HB3	1.96	0.47
1:B:357:PHE:HB2	2:B:679:HOH:O	2.14	0.47
1:A:10:ARG:CZ	1:A:10:ARG:CB	2.92	0.47
1:A:295:ARG:N	1:A:329:SER:OG	2.47	0.47
1:A:547:GLN:NE2	2:A:663:HOH:O	2.48	0.47
1:B:191:THR:OG1	1:B:271:ILE:HA	2.15	0.47
1:B:468:TYR:OH	1:B:504:GLU:HB3	2.14	0.47
1:A:468:TYR:O	1:A:472:TYR:CD2	2.68	0.47
1:A:4:PRO:HD3	1:A:87:ARG:NH1	2.30	0.47
1:A:513:LEU:O	1:A:522:SER:HA	2.15	0.47
1:B:252:LEU:HD22	1:B:269:VAL:HG21	1.97	0.47
1:B:315:HIS:HB3	1:B:340:TRP:CZ3	2.50	0.47
1:B:570:ILE:CD1	1:B:584:LEU:CD2	2.93	0.47
1:A:119:THR:N	1:A:120:PRO:HD2	2.30	0.46
1:A:24:ASP:OD2	1:A:29:GLY:HA3	2.15	0.46
1:A:340:TRP:HA	1:A:344:HIS:CE1	2.49	0.46
1:A:35:TRP:CD2	1:A:36:GLU:OE1	2.68	0.46
1:B:18:LEU:HA	1:B:45:ILE:O	2.16	0.46
1:A:302:ARG:HH22	1:B:307:ASP:CG	2.18	0.46
1:B:375:TYR:CG	1:B:379:ALA:HB3	2.50	0.46
1:A:141:GLN:NE2	1:A:381:ASN:OD1	2.47	0.46
1:A:471:TRP:HZ2	1:A:521:TRP:CZ2	2.34	0.46
1:A:474:GLN:HE21	1:A:480:THR:HG22	1.80	0.46
1:B:155:LYS:HD2	1:B:155:LYS:HA	1.82	0.46
1:A:74:PHE:CE1	1:B:7:THR:HA	2.47	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:218:ASP:HA	2:A:686:HOH:O	2.15	0.46
1:B:217:ARG:N	1:B:251:GLU:O	2.44	0.46
1:A:207:VAL:HG13	1:A:210:GLY:H	1.79	0.46
1:A:381:ASN:HB2	1:A:383:GLU:N	2.31	0.46
1:A:480:THR:O	1:A:484:VAL:HG13	2.15	0.46
1:B:273:SER:CB	1:B:284:ASN:N	2.65	0.46
1:B:533:TYR:HB3	1:B:537:PHE:CE1	2.50	0.46
1:B:562:ARG:HG3	1:B:562:ARG:NH1	2.29	0.46
1:B:272:ARG:HD2	1:B:274:VAL:HG21	1.97	0.46
1:B:293:PHE:CZ	1:B:321:ILE:HD13	2.48	0.46
1:B:172:ARG:HH12	1:B:334:ALA:N	2.13	0.46
1:B:43:ARG:HG2	1:B:44:ALA:N	2.27	0.46
1:B:531:ASP:HA	1:B:534:HIS:ND1	2.31	0.46
1:A:468:TYR:O	1:A:472:TYR:HD2	1.99	0.46
1:B:47:VAL:HG13	1:B:170:ILE:HG22	1.97	0.46
1:A:33:ARG:C	1:A:36:GLU:OE1	2.54	0.46
1:B:219:ALA:O	1:B:220:ASP:OD2	2.34	0.46
1:B:242:TRP:CD1	1:B:270:GLY:HA3	2.51	0.46
1:B:304:LYS:HE3	1:B:331:TYR:CE2	2.50	0.46
1:B:470:GLY:HA2	1:B:474:GLN:HB2	1.98	0.46
1:B:83:ARG:HH11	1:B:118:VAL:CG1	2.28	0.46
1:A:187:ILE:CG2	1:A:188:THR:N	2.79	0.46
1:A:329:SER:HB2	2:A:678:HOH:O	2.15	0.46
1:A:33:ARG:O	1:A:36:GLU:OE1	2.34	0.46
1:A:588:TRP:HA	1:A:591:MSE:HE3	1.98	0.46
1:A:29:GLY:HA3	1:A:68:TRP:CZ2	2.51	0.46
1:B:15:LEU:HD13	1:B:48:PRO:CD	2.44	0.46
1:B:293:PHE:HA	1:B:548:VAL:O	2.15	0.46
1:B:306:PHE:HE1	1:B:311:MSE:HE3	1.81	0.46
1:B:341:ALA:CB	1:B:404:SER:CB	2.93	0.46
1:B:432:THR:HB	1:B:441:ILE:HD11	1.98	0.46
1:A:514:HIS:HA	1:A:524:GLU:OE2	2.16	0.45
1:A:309:VAL:HG21	1:B:302:ARG:NE	2.31	0.45
1:B:318:MSE:HA	1:B:321:ILE:HG22	1.98	0.45
1:B:291:THR:OG1	1:B:324:ASN:CG	2.55	0.45
1:B:560:ILE:O	1:B:561:LEU:C	2.54	0.45
1:A:139:ASN:N	1:A:142:THR:HG21	2.31	0.45
1:A:342:ASP:CG	2:A:673:HOH:O	2.48	0.45
1:A:560:ILE:C	1:A:562:ARG:N	2.69	0.45
1:B:138:LEU:HB3	1:B:142:THR:HG21	1.97	0.45
1:B:570:ILE:HD11	1:B:584:LEU:CD2	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:66:ASN:HA	1:B:134:VAL:O	2.16	0.45
1:A:295:ARG:O	1:A:329:SER:CB	2.62	0.45
1:A:381:ASN:HB2	1:A:383:GLU:CB	2.45	0.45
1:A:550:ASN:HD22	1:A:554:PHE:HE2	1.62	0.45
1:B:94:TYR:O	1:B:134:VAL:HA	2.16	0.45
1:B:213:SER:OG	1:B:228:GLN:NE2	2.48	0.45
1:B:184:VAL:CG2	1:B:254:VAL:HG12	2.41	0.45
1:B:469:TYR:CD2	1:B:533:TYR:OH	2.68	0.45
1:B:504:GLU:HG2	1:B:549:TRP:CD1	2.51	0.45
1:A:225:ALA:HB1	1:A:235:GLN:HG2	1.99	0.45
1:A:455:THR:C	1:A:456:ILE:CG2	2.83	0.45
1:A:442:THR:CA	1:A:460:PHE:CD1	2.99	0.45
1:A:457:SER:CB	1:A:496:LEU:HD11	2.46	0.45
1:B:176:LEU:C	1:B:176:LEU:HD12	2.36	0.45
1:B:197:CYS:CB	1:B:198:ASN:HD22	2.28	0.45
1:B:465:LEU:N	1:B:465:LEU:CD1	2.69	0.45
1:A:139:ASN:H	1:A:142:THR:HG21	1.81	0.45
1:A:442:THR:HA	1:A:460:PHE:CD1	2.51	0.45
1:A:453:THR:O	1:A:455:THR:N	2.49	0.45
1:A:39:LEU:HD13	1:A:70:GLN:HE21	1.81	0.45
1:B:151:ASP:HB3	1:B:155:LYS:CB	2.46	0.45
1:B:217:ARG:HG2	2:B:628:HOH:O	2.17	0.45
1:B:257:LYS:HA	1:B:262:CYS:HB3	1.97	0.45
1:B:311:MSE:HE2	1:B:336:GLU:CG	2.38	0.45
1:B:358:ASN:OD1	1:B:358:ASN:N	2.48	0.45
1:A:248:TYR:CB	2:A:689:HOH:O	2.64	0.45
1:B:197:CYS:HB3	1:B:198:ASN:HD22	1.76	0.45
1:B:377:GLU:HB2	1:B:419:GLN:OE1	2.16	0.45
1:B:422:ARG:HB3	1:B:454:ASP:OD2	2.17	0.45
1:B:453:THR:CB	1:B:456:ILE:HB	2.46	0.45
1:B:47:VAL:CG1	1:B:170:ILE:HG22	2.47	0.45
1:A:385:GLN:HE22	1:A:427:PRO:HG2	1.80	0.45
1:A:51:PHE:CD2	1:A:168:ALA:O	2.69	0.45
1:B:379:ALA:C	2:B:684:HOH:O	2.54	0.45
1:A:295:ARG:HB3	1:A:295:ARG:HH11	1.82	0.45
1:A:398:ARG:HH11	1:A:398:ARG:HG2	1.81	0.45
1:A:420:GLY:N	2:A:697:HOH:O	2.49	0.45
1:A:474:GLN:HE22	1:A:484:VAL:HG13	1.82	0.45
1:B:36:GLU:CB	1:B:101:ASN:HD21	2.15	0.45
1:B:14:LYS:C	1:B:16:ASP:N	2.69	0.45
1:B:14:LYS:O	1:B:16:ASP:N	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:259:GLN:HA	1:A:259:GLN:NE2	2.32	0.45
1:A:381:ASN:C	1:A:383:GLU:N	2.68	0.45
1:B:83:ARG:HG2	1:B:179:THR:HG23	1.98	0.45
1:B:463:LEU:CD2	1:B:492:TRP:CZ3	2.99	0.45
1:A:312:VAL:HG11	1:B:54:GLN:HE21	1.81	0.45
1:B:564:GLY:O	1:B:567:LYS:HE3	2.17	0.45
1:A:205:GLN:HB2	1:A:231:SER:N	2.30	0.44
1:A:293:PHE:HE1	1:A:570:ILE:HD13	1.81	0.44
1:B:24:ASP:OD1	1:B:27:ASN:O	2.35	0.44
1:A:87:ARG:HB3	1:A:115:GLU:CB	2.48	0.44
1:A:377:GLU:OE1	2:A:691:HOH:O	2.21	0.44
1:A:400:LYS:O	1:A:439:ARG:NH2	2.46	0.44
1:A:532:MSE:O	1:A:533:TYR:C	2.54	0.44
1:B:101:ASN:HD21	1:B:129:ARG:HH12	1.65	0.44
1:B:23:LEU:HD13	1:B:63:TYR:CD1	2.52	0.44
1:B:241:LEU:N	1:B:241:LEU:CD2	2.79	0.44
1:A:138:LEU:CA	1:A:142:THR:HG21	2.46	0.44
1:A:151:ASP:HB3	1:A:155:LYS:HB3	1.87	0.44
1:A:7:THR:HB	1:A:8:PRO:HD2	1.98	0.44
1:A:82:GLN:CA	1:A:82:GLN:NE2	2.80	0.44
1:B:10:ARG:NH1	1:B:10:ARG:CB	2.69	0.44
1:B:47:VAL:CG1	1:B:170:ILE:CG2	2.96	0.44
1:B:183:TRP:CZ3	1:B:185:ASP:HB2	2.53	0.44
1:B:242:TRP:NE1	1:B:403:PRO:HB2	2.32	0.44
1:B:83:ARG:NH2	1:B:183:TRP:CD2	2.85	0.44
1:A:462:VAL:HG23	1:A:499:PRO:HB2	1.99	0.44
1:B:5:VAL:HG11	1:B:266:PRO:HG2	2.00	0.44
1:B:33:ARG:HG2	1:B:33:ARG:HH11	1.82	0.44
1:B:498:GLN:HB2	1:B:499:PRO:CD	2.40	0.44
1:A:15:LEU:C	1:A:17:GLY:N	2.68	0.44
1:A:455:THR:O	1:A:456:ILE:CG2	2.66	0.44
1:A:469:TYR:O	1:A:473:VAL:HG23	2.18	0.44
1:A:511:ALA:O	1:A:523:GLU:OE2	2.35	0.44
1:B:21:PHE:HE2	1:B:69:TYR:HE2	1.66	0.44
1:A:268:ARG:NH2	1:A:343:GLU:HG3	2.33	0.44
1:A:313:HIS:CG	1:B:301:LEU:HD22	2.52	0.44
1:B:390:GLN:O	1:B:394:GLU:HG3	2.17	0.44
1:B:467:ARG:HG3	1:B:469:TYR:OH	2.17	0.44
1:B:592:ASN:HB2	1:B:595:GLU:HG2	2.00	0.44
1:A:2:LEU:HD11	1:A:187:ILE:HG13	2.00	0.44
1:A:197:CYS:C	1:A:198:ASN:OD1	2.56	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:314:ASP:OD1	1:A:551:PHE:CE2	2.71	0.44
1:A:35:TRP:CE2	1:A:36:GLU:CD	2.91	0.44
1:B:448:PHE:O	1:B:448:PHE:CD1	2.65	0.44
1:B:532:MSE:C	1:B:532:MSE:SE	3.06	0.44
1:A:23:LEU:HD22	1:A:67:VAL:HG12	2.00	0.44
1:B:10:ARG:H	1:B:178:THR:CG2	2.15	0.44
1:B:183:TRP:O	1:B:206:VAL:HG23	2.17	0.44
1:B:236:VAL:O	1:B:236:VAL:HG23	2.17	0.44
1:B:379:ALA:O	1:B:380:VAL:CG1	2.66	0.44
1:B:556:THR:HB	1:B:562:ARG:HD2	1.99	0.44
1:A:92:THR:OG1	1:A:168:ALA:HA	2.18	0.43
1:A:230:THR:C	1:A:231:SER:HG	2.22	0.43
1:A:183:TRP:CD1	1:A:183:TRP:N	2.86	0.43
1:A:202:VAL:CG2	1:A:234:LEU:CD2	2.90	0.43
1:A:32:GLN:HB2	1:A:34:TRP:NE1	2.33	0.43
1:A:4:PRO:HG2	1:A:87:ARG:HD3	2.00	0.43
1:A:476:GLY:CA	1:A:520:MSE:HE2	2.49	0.43
1:A:534:HIS:CE1	1:A:587:ARG:HD2	2.54	0.43
1:B:184:VAL:O	1:B:185:ASP:HB2	2.17	0.43
1:B:248:TYR:C	1:B:248:TYR:HD1	2.20	0.43
1:B:562:ARG:CG	1:B:562:ARG:NH1	2.70	0.43
1:A:92:THR:C	1:A:110:GLY:HA2	2.35	0.43
1:A:407:MSE:SE	1:A:462:VAL:HG11	2.68	0.43
1:B:47:VAL:HG11	1:B:170:ILE:HG21	2.00	0.43
1:B:33:ARG:HG3	1:B:35:TRP:CE2	2.52	0.43
1:B:7:THR:OG1	2:B:690:HOH:O	2.21	0.43
1:A:202:VAL:HG13	1:A:204:TRP:CZ3	2.53	0.43
1:B:110:GLY:CA	2:B:688:HOH:O	2.67	0.43
1:B:214:VAL:O	1:B:214:VAL:HG12	2.18	0.43
1:B:21:PHE:HB2	1:B:45:ILE:HB	2.01	0.43
1:B:349:ILE:O	1:B:349:ILE:HG22	2.17	0.43
1:B:375:TYR:CZ	1:B:379:ALA:HB2	2.54	0.43
1:B:244:PRO:HG2	1:B:593:PHE:HE1	1.83	0.43
1:B:75:ILE:HD11	1:B:128:VAL:CG2	2.48	0.43
1:B:240:HIS:CD2	1:B:250:TYR:OH	2.71	0.43
1:B:186:ASP:HB3	1:B:205:GLN:HB3	2.00	0.43
1:B:21:PHE:CZ	1:B:51:PHE:HB2	2.54	0.43
1:A:144:PRO:HD3	1:A:353:ALA:HB1	2.01	0.43
1:A:183:TRP:CZ3	1:A:185:ASP:CG	2.92	0.43
1:A:295:ARG:HB3	1:A:295:ARG:NH1	2.33	0.43
1:B:203:ASP:O	1:B:204:TRP:HB3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:531:ASP:C	1:B:531:ASP:OD1	2.57	0.43
1:B:583:LEU:O	1:B:585:GLN:N	2.52	0.43
1:A:105:MSE:HE1	1:A:115:GLU:CA	2.42	0.43
1:A:238:ASN:CG	1:A:239:PRO:CD	2.57	0.43
1:A:351:GLU:O	1:A:395:LEU:HD11	2.19	0.43
1:A:187:ILE:O	1:A:400:LYS:HE2	2.19	0.43
1:B:315:HIS:CD2	1:B:340:TRP:CE3	3.07	0.43
1:A:160:TYR:CD2	1:A:160:TYR:N	2.86	0.43
1:A:24:ASP:OD1	1:A:26:GLU:O	2.37	0.43
1:A:451:ALA:O	1:A:453:THR:OG1	2.37	0.43
1:A:550:ASN:O	1:A:551:PHE:C	2.54	0.43
1:B:193:VAL:HG23	1:B:194:ALA:O	2.19	0.43
1:B:489:LEU:O	1:B:493:GLN:N	2.49	0.43
1:A:193:VAL:CG2	1:A:285:HIS:NE2	2.82	0.43
1:A:469:TYR:HB2	1:A:529:TRP:HZ2	1.83	0.43
1:B:105:MSE:SE	1:B:114:PHE:HB2	2.68	0.43
1:B:358:ASN:HB3	1:B:360:SER:HB3	2.01	0.43
1:B:453:THR:OG1	1:B:457:SER:N	2.39	0.43
1:A:150:THR:HA	1:A:155:LYS:O	2.19	0.42
1:A:186:ASP:OD1	1:A:400:LYS:NZ	2.40	0.42
1:A:561:LEU:O	1:A:566:ASN:ND2	2.51	0.42
1:B:265:TYR:HD2	2:B:655:HOH:O	2.01	0.42
1:B:486:GLU:O	1:B:489:LEU:N	2.52	0.42
1:A:398:ARG:NH1	1:A:398:ARG:HG2	2.34	0.42
1:A:525:TYR:HD2	2:A:708:HOH:O	2.02	0.42
1:A:413:GLU:HG3	1:A:466:ASN:HD22	1.84	0.42
1:B:187:ILE:HG22	1:B:188:THR:N	2.33	0.42
1:B:414:PRO:CD	1:B:444:VAL:O	2.67	0.42
1:B:293:PHE:HE1	1:B:570:ILE:HD12	1.83	0.42
1:A:102:GLN:OE1	1:A:102:GLN:CA	2.54	0.42
1:A:171:HIS:NE2	1:A:304:LYS:HB2	2.35	0.42
1:B:101:ASN:ND2	1:B:129:ARG:HH12	2.17	0.42
1:A:12:ILE:CD1	2:A:698:HOH:O	2.63	0.42
1:A:426:ALA:HA	1:A:459:LEU:HD13	2.01	0.42
1:A:477:ASP:OD1	1:A:480:THR:HB	2.20	0.42
1:A:507:VAL:HG13	1:A:529:TRP:CD1	2.55	0.42
1:B:243:GLN:O	1:B:247:GLY:N	2.42	0.42
1:B:359:LEU:O	1:B:359:LEU:HG	2.20	0.42
1:B:291:THR:O	1:B:588:TRP:CH2	2.72	0.42
1:A:160:TYR:CD1	1:A:162:HIS:CD2	3.07	0.42
1:A:19:TRP:HE3	1:A:69:TYR:HB3	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:12:ILE:O	1:B:12:ILE:CG2	2.65	0.42
1:B:94:TYR:CD2	1:B:135:ASN:HB2	2.53	0.42
1:B:1:MSE:HB3	1:B:1:MSE:HE3	1.72	0.42
1:B:189:VAL:HG11	1:B:269:VAL:HG11	2.01	0.42
1:B:39:LEU:HA	1:B:39:LEU:HD12	1.71	0.42
1:B:549:TRP:HZ3	1:B:568:LYS:CE	2.28	0.42
1:B:88:PHE:N	1:B:88:PHE:CD2	2.87	0.42
1:A:192:HIS:HB2	1:A:200:ALA:HB3	2.00	0.42
1:A:330:HIS:N	2:A:678:HOH:O	2.31	0.42
1:A:426:ALA:O	1:A:429:ALA:HB3	2.19	0.42
1:A:502:ILE:HD12	1:A:537:PHE:CE2	2.48	0.42
1:B:400:LYS:HA	1:B:439:ARG:NH1	2.23	0.42
1:B:354:ALA:HB3	1:B:411:ALA:HA	2.02	0.42
1:A:15:LEU:HD23	1:A:173:SER:HG	1.78	0.42
1:A:344:HIS:O	1:A:345:GLY:C	2.57	0.42
1:A:396:ILE:O	1:A:400:LYS:HB3	2.20	0.42
1:A:426:ALA:HB3	1:A:427:PRO:HD3	2.02	0.42
1:A:498:GLN:HB2	1:A:499:PRO:CD	2.49	0.42
1:A:138:LEU:HA	1:A:142:THR:HG21	2.01	0.42
1:A:351:GLU:CG	1:A:409:SER:OG	2.68	0.42
1:B:143:ILE:HD11	1:B:388:HIS:CA	2.41	0.42
1:B:175:MSE:HE2	1:B:175:MSE:H	1.85	0.42
1:B:292:GLY:N	2:B:691:HOH:O	2.52	0.42
1:A:248:TYR:N	2:A:689:HOH:O	2.53	0.42
1:B:213:SER:CB	1:B:255:THR:HB	2.23	0.42
1:B:449:CYS:SG	1:B:488:GLU:OE2	2.78	0.42
1:A:315:HIS:CD2	1:A:318:MSE:CE	3.03	0.41
1:B:137:GLU:HG2	1:B:148:VAL:HG11	2.01	0.41
1:B:92:THR:HG21	1:B:168:ALA:HB1	2.01	0.41
1:B:272:ARG:HG3	1:B:274:VAL:CG2	2.36	0.41
1:B:6:GLU:HA	1:B:9:THR:O	2.19	0.41
1:B:83:ARG:HE	1:B:179:THR:HG23	1.85	0.41
1:B:194:ALA:CB	1:B:196:ASP:OD2	2.69	0.41
1:A:507:VAL:HG22	1:A:526:GLN:HG3	2.02	0.41
1:A:505:TYR:CZ	1:A:548:VAL:HG22	2.55	0.41
1:B:142:THR:CG2	1:B:142:THR:O	2.66	0.41
1:B:372:LYS:CB	1:B:372:LYS:HZ3	2.29	0.41
1:B:432:THR:OG1	1:B:441:ILE:CD1	2.65	0.41
1:B:276:VAL:CG1	1:B:499:PRO:HG3	2.50	0.41
1:A:18:LEU:C	1:A:19:TRP:HD1	2.23	0.41
1:A:199:HIS:CE1	1:A:236:VAL:HB	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:104:VAL:HG12	1:B:105:MSE:HG2	2.02	0.41
1:B:388:HIS:O	1:B:392:ILE:CG1	2.68	0.41
1:A:417:ARG:HE	1:A:417:ARG:HB2	1.57	0.41
1:B:425:PHE:CD2	1:B:455:THR:HG21	2.55	0.41
1:B:474:GLN:HE22	1:B:484:VAL:HG21	1.86	0.41
1:A:348:VAL:HG12	1:A:349:ILE:N	2.35	0.41
1:B:212:VAL:CG2	1:B:230:THR:CG2	2.99	0.41
1:A:118:VAL:C	1:A:120:PRO:HD2	2.41	0.41
1:A:199:HIS:CE1	1:A:236:VAL:CB	3.04	0.41
1:A:463:LEU:HD21	1:A:492:TRP:CE3	2.56	0.41
1:B:172:ARG:HH22	1:B:333:TYR:HA	1.85	0.41
1:B:47:VAL:CG1	1:B:48:PRO:HA	2.50	0.41
1:B:538:ASP:HA	1:B:596:LYS:NZ	2.36	0.41
1:A:333:TYR:O	1:A:398:ARG:NH2	2.54	0.41
1:A:375:TYR:O	1:A:377:GLU:N	2.53	0.41
1:B:531:ASP:HA	1:B:534:HIS:HB2	2.02	0.41
1:B:562:ARG:HG2	1:B:566:ASN:HD22	1.83	0.41
1:A:11:GLU:HB2	1:A:177:TYR:HB2	2.03	0.41
1:A:193:VAL:HG22	1:A:273:SER:HB2	2.03	0.41
1:A:421:ALA:HB1	1:A:455:THR:OG1	2.21	0.41
1:A:163:ASP:HB3	2:A:706:HOH:O	2.20	0.41
1:A:358:ASN:O	1:A:359:LEU:HD13	2.21	0.41
1:A:397:ALA:O	1:A:400:LYS:CD	2.68	0.41
1:A:531:ASP:OD1	1:A:583:LEU:HD21	2.20	0.41
1:B:180:PRO:HB2	1:B:261:GLU:HG3	2.03	0.41
1:B:273:SER:HB3	1:B:284:ASN:HA	2.03	0.41
1:B:342:ASP:OD1	1:B:404:SER:OG	2.38	0.41
1:B:459:LEU:HG	1:B:459:LEU:H	1.52	0.41
1:B:538:ASP:CB	1:B:597:PRO:HG2	2.51	0.41
1:A:160:TYR:HD1	1:A:162:HIS:CD2	2.39	0.41
1:A:233:THR:O	1:A:234:LEU:CD2	2.52	0.41
1:A:413:GLU:CG	1:A:466:ASN:HD22	2.34	0.41
1:A:508:ASP:OD2	1:A:568:LYS:HD3	2.20	0.41
1:A:95:GLY:O	1:A:106:GLU:HA	2.21	0.41
1:B:15:LEU:CD1	1:B:15:LEU:O	2.64	0.41
1:B:275:ALA:O	1:B:282:LEU:HD13	2.20	0.41
1:B:380:VAL:O	1:B:380:VAL:HG22	2.20	0.41
1:B:35:TRP:CD1	1:B:98:TRP:CE3	3.09	0.41
1:A:176:LEU:HD13	1:A:177:TYR:N	2.36	0.40
1:A:179:THR:CB	2:A:715:HOH:O	2.38	0.40
1:B:328:THR:CA	1:B:333:TYR:CZ	2.97	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:358:ASN:OD1	1:B:415:ASP:HB2	2.21	0.40
1:B:437:PRO:HA	2:B:627:HOH:O	2.19	0.40
1:B:83:ARG:HH11	1:B:118:VAL:HG12	1.87	0.40
1:A:238:ASN:ND2	1:A:239:PRO:HD3	2.25	0.40
1:B:217:ARG:HD2	1:B:221:GLN:HA	2.02	0.40
1:B:335:GLU:O	1:B:335:GLU:CG	2.67	0.40
1:B:242:TRP:NE1	1:B:403:PRO:CB	2.84	0.40
1:B:538:ASP:O	1:B:596:LYS:NZ	2.54	0.40
1:A:97:VAL:HG22	1:A:132:VAL:HG22	2.03	0.40
1:A:218:ASP:HB2	1:A:221:GLN:CA	2.42	0.40
1:A:230:THR:O	1:A:231:SER:OG	2.34	0.40
1:A:342:ASP:OD1	1:A:404:SER:OG	2.33	0.40
1:B:524:GLU:N	1:B:524:GLU:OE1	2.49	0.40
1:A:13:LYS:HE3	1:A:175:MSE:HE2	2.02	0.40
1:A:384:THR:O	1:A:385:GLN:C	2.60	0.40
1:A:321:ILE:CG2	1:A:588:TRP:HE3	2.33	0.40
1:B:119:THR:N	1:B:120:PRO:CD	2.83	0.40
1:A:456:ILE:O	1:A:456:ILE:CG2	2.60	0.40
1:A:85:VAL:HA	1:A:117:ASP:O	2.21	0.40
1:B:75:ILE:HD11	1:B:128:VAL:HG21	2.04	0.40
1:B:139:ASN:O	1:B:145:PRO:HA	2.22	0.40
1:B:183:TRP:CZ3	1:B:185:ASP:CG	2.94	0.40
1:B:297:GLU:O	1:B:304:LYS:HA	2.21	0.40
1:B:392:ILE:CD1	1:B:410:ILE:HG23	2.48	0.40
1:B:420:GLY:HA3	2:B:671:HOH:O	2.21	0.40
1:B:463:LEU:HB3	1:B:500:ILE:HG12	2.02	0.40

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:152:GLU:OE2	2:A:685:HOH:O 2_554	1.03	1.17
1:B:152:GLU:CD	2:A:685:HOH:O 2_554	1.50	0.70
1:B:152:GLU:OE1	2:A:685:HOH:O 2_554	1.83	0.37
1:A:599:GLN:O	1:B:603:GLN:C 2_564	2.17	0.03

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	593/605 (98%)	522 (88%)	58 (10%)	13 (2%)	6	24
1	B	593/605 (98%)	494 (83%)	76 (13%)	23 (4%)	3	12
All	All	1186/1210 (98%)	1016 (86%)	134 (11%)	36 (3%)	4	17

All (36) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	228	GLN
1	B	7	THR
1	B	119	THR
1	B	123	ILE
1	B	144	PRO
1	B	209	ASN
1	B	561	LEU
1	A	237	VAL
1	B	137	GLU
1	B	198	ASN
1	B	335	GLU
1	B	560	ILE
1	A	0	HIS
1	A	378	GLU
1	B	337	MSE
1	B	339	ASP
1	B	453	THR
1	B	518	THR
1	A	7	THR
1	A	199	HIS
1	A	550	ASN
1	B	109	GLY
1	B	239	PRO
1	B	541	SER
1	A	230	THR

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Mol	Chain	Res	Type
1	B	27	ASN
1	B	100	ASN
1	B	230	THR
1	A	152	GLU
1	A	65	GLY
1	A	154	GLY
1	A	266	PRO
1	B	190	VAL
1	B	266	PRO
1	B	446	VAL
1	A	224	VAL

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	505/501 (101%)	417 (83%)	88 (17%)	2	6
1	B	502/501 (100%)	387 (77%)	115 (23%)	1	2
All	All	1007/1002 (100%)	804 (80%)	203 (20%)	1	4

All (203) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	0	HIS
1	A	1	MSE
1	A	10	ARG
1	A	11	GLU
1	A	12	ILE
1	A	15	LEU
1	A	33	ARG
1	A	47	VAL
1	A	51	PHE
1	A	71	ARG
1	A	74	PHE
1	A	75	ILE

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Mol	Chain	Res	Type
1	A	76	PRO
1	A	82	GLN
1	A	85	VAL
1	A	96	LYS
1	A	101	ASN
1	A	102	GLN
1	A	103	GLU
1	A	112	THR
1	A	128	VAL
1	A	136	ASN
1	A	148	VAL
1	A	151	ASP
1	A	153	ASN
1	A	160	TYR
1	A	170	ILE
1	A	176	LEU
1	A	177	TYR
1	A	178	THR
1	A	182	THR
1	A	184	VAL
1	A	193	VAL
1	A	195	GLN
1	A	203	ASP
1	A	204	TRP
1	A	206	VAL
1	A	207	VAL
1	A	212	VAL
1	A	214	VAL
1	A	215	GLU
1	A	216	LEU
1	A	217	ARG
1	A	218	ASP
1	A	221	GLN
1	A	226	THR
1	A	233	THR
1	A	234	LEU
1	A	236	VAL
1	A	249	LEU
1	A	251	GLU
1	A	259	GLN
1	A	261	GLU
1	A	262	CYS

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Mol	Chain	Res	Type
1	A	272	ARG
1	A	298	ASP
1	A	300	ASP
1	A	321	ILE
1	A	328	THR
1	A	335	GLU
1	A	338	LEU
1	A	340	TRP
1	A	344	HIS
1	A	347	VAL
1	A	355	VAL
1	A	359	LEU
1	A	373	GLU
1	A	375	TYR
1	A	377	GLU
1	A	398	ARG
1	A	400	LYS
1	A	446	VAL
1	A	450	ASP
1	A	456	ILE
1	A	461	ASP
1	A	469	TYR
1	A	473	VAL
1	A	487	LYS
1	A	488	GLU
1	A	494	GLU
1	A	530	LEU
1	A	531	ASP
1	A	536	VAL
1	A	539	ARG
1	A	563	VAL
1	A	570	ILE
1	A	598	GLN
1	A	603	GLN
1	B	0	HIS
1	B	1	MSE
1	B	8	PRO
1	B	10	ARG
1	B	14	LYS
1	B	16	ASP
1	B	18	LEU
1	B	26	GLU

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Mol	Chain	Res	Type
1	B	28	CYS
1	B	31	ASP
1	B	37	SER
1	B	39	LEU
1	B	40	GLN
1	B	43	ARG
1	B	45	ILE
1	B	61	ARG
1	B	67	VAL
1	B	69	TYR
1	B	87	ARG
1	B	89	ASP
1	B	101	ASN
1	B	102	GLN
1	B	114	PHE
1	B	115	GLU
1	B	119	THR
1	B	122	VAL
1	B	123	ILE
1	B	127	SER
1	B	129	ARG
1	B	134	VAL
1	B	143	ILE
1	B	144	PRO
1	B	147	MSE
1	B	148	VAL
1	B	149	ILE
1	B	155	LYS
1	B	163	ASP
1	B	175	MSE
1	B	176	LEU
1	B	178	THR
1	B	179	THR
1	B	182	THR
1	B	190	VAL
1	B	192	HIS
1	B	193	VAL
1	B	196	ASP
1	B	198	ASN
1	B	199	HIS
1	B	209	ASN
1	B	211	ASP

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Mol	Chain	Res	Type
1	B	216	LEU
1	B	223	VAL
1	B	234	LEU
1	B	235	GLN
1	B	240	HIS
1	B	241	LEU
1	B	243	GLN
1	B	246	GLU
1	B	248	TYR
1	B	249	LEU
1	B	252	LEU
1	B	259	GLN
1	B	260	THR
1	B	262	CYS
1	B	267	LEU
1	B	268	ARG
1	B	269	VAL
1	B	272	ARG
1	B	276	VAL
1	B	282	LEU
1	B	283	ILE
1	B	288	PHE
1	B	295	ARG
1	B	319	ASP
1	B	327	ARG
1	B	328	THR
1	B	330	HIS
1	B	348	VAL
1	B	350	ASP
1	B	361	LEU
1	B	372	LYS
1	B	373	GLU
1	B	375	TYR
1	B	392	ILE
1	B	395	LEU
1	B	416	THR
1	B	422	ARG
1	B	425	PHE
1	B	434	LYS
1	B	441	ILE
1	B	445	ASN
1	B	446	VAL

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Mol	Chain	Res	Type
1	B	448	PHE
1	B	449	CYS
1	B	452	HIS
1	B	455	THR
1	B	458	ASP
1	B	459	LEU
1	B	461	ASP
1	B	463	LEU
1	B	465	LEU
1	B	467	ARG
1	B	472	TYR
1	B	509	THR
1	B	513	LEU
1	B	517	TYR
1	B	520	MSE
1	B	530	LEU
1	B	537	PHE
1	B	558	GLN
1	B	562	ARG
1	B	573	ARG
1	B	598	GLN
1	B	599	GLN
1	B	603	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	40	GLN
1	A	52	ASN
1	A	70	GLN
1	A	82	GLN
1	A	107	HIS
1	A	108	GLN
1	A	136	ASN
1	A	141	GLN
1	A	199	HIS
1	A	228	GLN
1	A	259	GLN
1	A	313	HIS
1	A	330	HIS
1	A	402	HIS
1	A	412	ASN

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Mol	Chain	Res	Type
1	A	474	GLN
1	A	493	GLN
1	A	497	HIS
1	A	547	GLN
1	B	32	GLN
1	B	52	ASN
1	B	54	GLN
1	B	93	HIS
1	B	101	ASN
1	B	102	GLN
1	B	107	HIS
1	B	192	HIS
1	B	199	HIS
1	B	222	GLN
1	B	228	GLN
1	B	240	HIS
1	B	259	GLN
1	B	315	HIS
1	B	385	GLN
1	B	402	HIS
1	B	412	ASN
1	B	466	ASN
1	B	497	HIS
1	B	498	GLN
1	B	514	HIS
1	B	526	GLN
1	B	550	ASN
1	B	592	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	584/605 (96%)	0.10	29 (4%) 28 25	18, 45, 78, 103	0
1	B	584/605 (96%)	0.47	44 (7%) 14 11	39, 70, 89, 99	0
All	All	1168/1210 (96%)	0.28	73 (6%) 20 16	18, 61, 86, 103	0

All (73) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	227	GLY	6.4
1	B	204	TRP	6.2
1	B	206	VAL	5.9
1	A	98	TRP	5.0
1	B	469	TYR	4.8
1	A	601	GLY	4.7
1	B	207	VAL	4.5
1	A	454	ASP	4.3
1	B	209	ASN	4.0
1	B	465	LEU	3.8
1	A	603	GLN	3.8
1	B	211	ASP	3.6
1	A	207	VAL	3.5
1	A	216	LEU	3.4
1	B	228	GLN	3.4
1	B	240	HIS	3.3
1	B	470	GLY	3.3
1	A	456	ILE	3.3
1	A	97	VAL	3.2
1	B	456	ILE	3.1
1	B	290	PHE	3.1
1	B	173	SER	3.1
1	A	214	VAL	3.0
1	B	266	PRO	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	235	GLN	3.0
1	A	182	THR	2.9
1	A	117	ASP	2.9
1	A	199	HIS	2.8
1	A	254	VAL	2.8
1	A	209	ASN	2.8
1	B	257	LYS	2.8
1	B	289	TYR	2.8
1	A	470	GLY	2.7
1	B	443	CYS	2.7
1	A	252	LEU	2.6
1	B	444	VAL	2.6
1	B	457	SER	2.6
1	A	602	LYS	2.6
1	B	225	ALA	2.6
1	B	375	TYR	2.5
1	A	205	GLN	2.5
1	B	237	VAL	2.4
1	B	154	GLY	2.4
1	B	545	GLY	2.4
1	B	253	CYS	2.4
1	B	489	LEU	2.3
1	A	236	VAL	2.3
1	A	212	VAL	2.3
1	B	31	ASP	2.3
1	A	230	THR	2.3
1	B	410	ILE	2.3
1	A	131	THR	2.2
1	B	496	LEU	2.2
1	A	100	ASN	2.2
1	B	600	GLY	2.2
1	B	445	ASN	2.2
1	B	238	ASN	2.2
1	B	587	ARG	2.2
1	B	529	TRP	2.1
1	B	462	VAL	2.1
1	B	243	GLN	2.1
1	B	424	TYR	2.1
1	A	256	ALA	2.1
1	B	229	GLY	2.1
1	A	226	THR	2.1
1	A	469	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	425	PHE	2.1
1	A	104	VAL	2.1
1	B	467	ARG	2.0
1	B	500	ILE	2.0
1	B	536	VAL	2.0
1	A	237	VAL	2.0
1	B	230	THR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.