



Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 01:45 am BST

PDB ID : 2Y9E
Title : Structural basis for the allosteric interference of myosin function by mutants G680A and G680V of Dictyostelium myosin-2
Authors : Preller, M.; Bauer, S.; Adamek, N.; Fujita-Becker, S.; Fedorov, R.; Geeves, M.A.; Manstein, D.J.
Deposited on : 2011-02-14
Resolution : 3.40 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
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

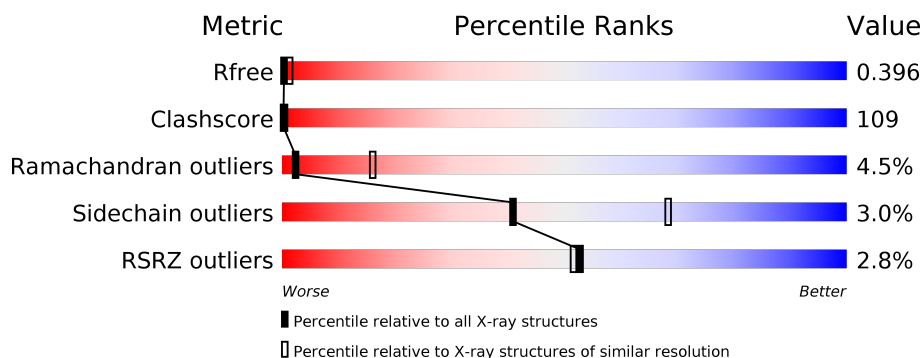
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 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	1026 (3.48-3.32)
Clashscore	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)
RSRZ outliers	127900	2173 (3.50-3.30)

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	X	758	<div> <div>3%</div> <div>19%</div> <div>67%</div> <div>13%</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6348 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 MYOSIN-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	X	758	Total	C	N	O	S	0	0	0
			6092	3870	1053	1153	16			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X	680	VAL	GLY	engineered mutation	UNP P08799

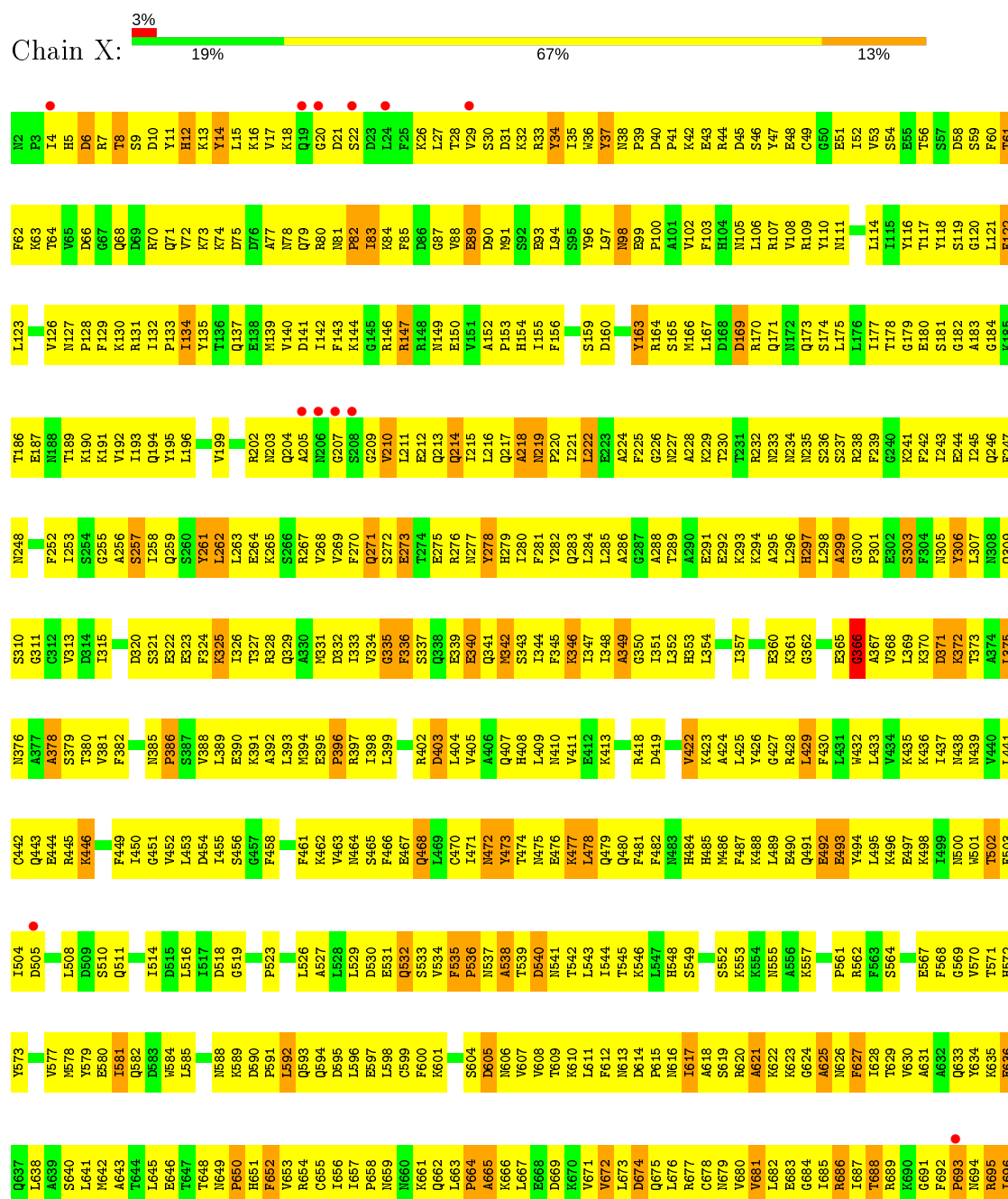
- Molecule 2 is water.

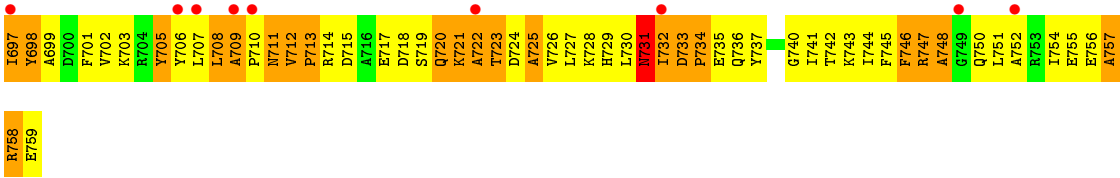
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	X	256	Total	O	0	0
			256	256		

3 Residue-property plots

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

• Molecule 1: MYOSIN-2





4 Data and refinement statistics

Property	Value	Source
Space group	P 2 ₁ 2 ₁ 2 ₁	Depositor
Cell constants a, b, c, α , β , γ	55.00Å 105.80Å 180.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.96 – 3.40 19.96 – 3.40	Depositor EDS
% Data completeness (in resolution range)	99.7 (19.96-3.40) 99.7 (19.96-3.40)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.64 (at 3.36Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.282 , 0.372 0.292 , 0.396	Depositor DCC
R_{free} test set	760 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	40.2	Xtriage
Anisotropy	0.296	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.23 , 68.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.21$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.77	EDS
Total number of atoms	6348	wwPDB-VP
Average B, all atoms (Å ²)	14.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.43% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	X	0.50	0/6212	1.09	76/8382 (0.9%)

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	X	0	2

There are no bond length outliers.

All (76) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	X	532	GLN	N-CA-CB	-11.79	89.38	110.60
1	X	581	ILE	CB-CA-C	-11.27	89.07	111.60
1	X	403	ASP	N-CA-CB	-10.86	91.05	110.60
1	X	502	THR	N-CA-C	-10.20	83.47	111.00
1	X	581	ILE	N-CA-C	8.98	135.24	111.00
1	X	98	ASN	N-CA-C	-8.18	88.91	111.00
1	X	235	ASN	N-CA-CB	-8.17	95.89	110.60
1	X	271	GLN	CB-CA-C	-8.10	94.21	110.40
1	X	184	GLY	N-CA-C	-8.04	93.01	113.10
1	X	286	ALA	CB-CA-C	7.59	121.48	110.10
1	X	720	GLN	N-CA-C	7.50	131.26	111.00
1	X	218	ALA	N-CA-CB	-7.30	99.88	110.10
1	X	472	ASN	CB-CA-C	-7.20	95.99	110.40
1	X	718	ASP	N-CA-CB	7.12	123.42	110.60
1	X	366	GLY	N-CA-C	-7.12	95.30	113.10
1	X	299	ALA	N-CA-CB	7.09	120.03	110.10
1	X	752	ALA	N-CA-CB	-7.06	100.21	110.10
1	X	747	ARG	N-CA-C	-7.06	91.95	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	621	ALA	CB-CA-C	6.94	120.50	110.10
1	X	688	THR	N-CA-C	6.88	129.56	111.00
1	X	263	LEU	CB-CA-C	6.76	123.05	110.20
1	X	371	ASP	CB-CA-C	-6.74	96.92	110.40
1	X	757	ALA	CB-CA-C	-6.69	100.06	110.10
1	X	627	PHE	N-CA-CB	-6.65	98.62	110.60
1	X	733	ASP	N-CA-CB	-6.63	98.67	110.60
1	X	222	LEU	CB-CA-C	-6.58	97.70	110.20
1	X	372	LYS	N-CA-CB	-6.47	98.95	110.60
1	X	758	ARG	N-CA-C	6.47	128.48	111.00
1	X	83	ILE	N-CA-C	-6.39	93.75	111.00
1	X	340	GLU	CB-CA-C	-6.30	97.81	110.40
1	X	446	LYS	N-CA-C	6.27	127.94	111.00
1	X	262	LEU	N-CA-CB	6.25	122.90	110.40
1	X	375	LEU	CB-CA-C	-6.24	98.34	110.20
1	X	349	ALA	N-CA-CB	-6.17	101.46	110.10
1	X	444	GLU	N-CA-C	6.14	127.59	111.00
1	X	477	LYS	CB-CA-C	6.11	122.62	110.40
1	X	733	ASP	N-CA-C	6.11	127.49	111.00
1	X	429	LEU	N-CA-CB	-5.98	98.44	110.40
1	X	478	LEU	CB-CA-C	-5.97	98.85	110.20
1	X	708	LEU	CB-CA-C	5.97	121.55	110.20
1	X	444	GLU	CB-CA-C	-5.97	98.46	110.40
1	X	712	VAL	N-CA-C	-5.96	94.91	111.00
1	X	466	PHE	CB-CA-C	-5.89	98.62	110.40
1	X	592	LEU	N-CA-CB	-5.88	98.64	110.40
1	X	734	PRO	CB-CA-C	-5.83	97.42	112.00
1	X	697	ILE	N-CA-C	-5.83	95.26	111.00
1	X	723	THR	N-CA-C	5.83	126.73	111.00
1	X	473	TYR	CB-CA-C	-5.80	98.80	110.40
1	X	204	GLN	N-CA-C	5.75	126.52	111.00
1	X	538	ALA	N-CA-C	-5.75	95.48	111.00
1	X	725	ALA	N-CA-CB	5.71	118.09	110.10
1	X	349	ALA	CB-CA-C	-5.68	101.58	110.10
1	X	325	LYS	CB-CA-C	5.65	121.69	110.40
1	X	163	TYR	CB-CA-C	-5.54	99.32	110.40
1	X	311	GLY	N-CA-C	5.51	126.89	113.10
1	X	705	TYR	N-CA-CB	5.44	120.39	110.60
1	X	478	LEU	N-CA-C	5.38	125.54	111.00
1	X	278	TYR	CB-CA-C	5.38	121.17	110.40
1	X	257	SER	CB-CA-C	5.38	120.33	110.10
1	X	746	PHE	CB-CA-C	5.38	121.15	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	61	THR	N-CA-CB	5.34	120.45	110.30
1	X	740	GLY	N-CA-C	-5.34	99.76	113.10
1	X	748	ALA	N-CA-C	-5.32	96.63	111.00
1	X	664	PRO	N-CA-C	-5.31	98.28	112.10
1	X	342	MET	CB-CA-C	-5.28	99.83	110.40
1	X	681	VAL	CB-CA-C	-5.28	101.37	111.40
1	X	720	GLN	CB-CA-C	-5.27	99.85	110.40
1	X	205	ALA	N-CA-CB	-5.27	102.72	110.10
1	X	617	ILE	CB-CA-C	-5.26	101.09	111.60
1	X	82	PRO	N-CA-C	-5.17	98.65	112.10
1	X	257	SER	N-CA-C	-5.16	97.07	111.00
1	X	386	PRO	CB-CA-C	-5.12	99.20	112.00
1	X	705	TYR	CB-CA-C	-5.04	100.31	110.40
1	X	422	VAL	CB-CA-C	5.04	120.98	111.40
1	X	17	VAL	N-CA-C	-5.02	97.45	111.00
1	X	758	ARG	N-CA-CB	-5.02	101.57	110.60

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	X	169	ASP	Peptide
1	X	696	ILE	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	X	6092	0	6051	1324	4
2	X	256	0	0	84	0
All	All	6348	0	6051	1324	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 109.

All (1324) 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:X:242:PHE:CE2	1:X:244:GLU:HG3	1.39	1.54
1:X:163:TYR:CE1	1:X:167:LEU:HD11	1.44	1.49
1:X:242:PHE:CE2	1:X:244:GLU:CG	1.97	1.46
1:X:247:PHE:CD1	1:X:253:ILE:HA	1.48	1.46
1:X:242:PHE:CE2	1:X:244:GLU:CB	2.00	1.44
1:X:689:ARG:CB	1:X:695:ARG:HH21	1.31	1.42
1:X:78:ASN:HB3	1:X:98:ASN:ND2	1.14	1.41
1:X:685:ILE:HG21	1:X:689:ARG:NH2	1.23	1.40
1:X:503:PHE:CE1	1:X:504:ILE:CD1	2.06	1.37
1:X:685:ILE:HG21	1:X:689:ARG:CZ	1.55	1.37
1:X:78:ASN:CB	1:X:98:ASN:ND2	1.86	1.36
1:X:230:THR:CG2	1:X:238:ARG:HH22	1.36	1.36
1:X:626:ASN:OD1	1:X:627:PHE:CD2	1.79	1.34
1:X:242:PHE:CZ	1:X:451:GLY:HA3	1.62	1.33
1:X:503:PHE:CE1	1:X:504:ILE:HD12	1.63	1.33
1:X:682:LEU:HD12	1:X:683:GLU:N	1.43	1.33
1:X:689:ARG:CB	1:X:695:ARG:NH2	1.88	1.32
1:X:614:ASP:OD1	1:X:615:PRO:CD	1.79	1.31
1:X:242:PHE:CZ	1:X:244:GLU:HG3	1.66	1.30
1:X:539:THR:O	1:X:541:ASN:N	1.62	1.29
1:X:695:ARG:HG2	2:X:2226:HOH:O	1.21	1.29
1:X:464:ASN:CB	1:X:468:GLN:HG2	1.62	1.29
1:X:709:ALA:HB1	1:X:710:PRO:CD	1.61	1.28
1:X:609:THR:O	1:X:613:ASN:HB2	1.23	1.28
1:X:296:LEU:C	1:X:297:HIS:ND1	1.84	1.28
1:X:503:PHE:CD1	1:X:504:ILE:HD12	1.67	1.28
1:X:242:PHE:CE2	1:X:244:GLU:HB2	1.64	1.28
1:X:698:TYR:CE2	1:X:699:ALA:HB3	1.69	1.28
1:X:135:TYR:CD2	1:X:191:LYS:HE3	1.71	1.26
1:X:477:LYS:O	1:X:480:GLN:NE2	1.69	1.25
1:X:98:ASN:OD1	1:X:100:PRO:HD2	1.30	1.24
1:X:137:GLN:O	1:X:140:VAL:HG22	1.30	1.24
1:X:725:ALA:HB1	1:X:729:HIS:NE2	1.53	1.23
1:X:692:PHE:CD1	1:X:745:PHE:HB2	1.73	1.22
1:X:29:VAL:CG1	1:X:758:ARG:HB3	1.66	1.22
1:X:477:LYS:O	1:X:480:GLN:CD	1.78	1.22
1:X:464:ASN:HB2	1:X:468:GLN:CG	1.70	1.22
1:X:325:LYS:O	1:X:329:GLN:HB2	1.32	1.21
1:X:641:LEU:O	1:X:645:LEU:HD13	1.41	1.20
1:X:210:VAL:CG2	1:X:214:GLN:OE1	1.88	1.20
1:X:477:LYS:O	1:X:480:GLN:OE1	1.55	1.20
1:X:242:PHE:HE2	1:X:244:GLU:CG	1.40	1.20

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:685:ILE:CG2	1:X:689:ARG:CZ	2.20	1.19
1:X:725:ALA:HB1	1:X:729:HIS:CD2	1.78	1.19
1:X:137:GLN:O	1:X:140:VAL:CG2	1.90	1.19
1:X:692:PHE:HD1	1:X:745:PHE:CB	1.57	1.17
1:X:64:THR:HG21	1:X:68:GLN:O	1.45	1.16
1:X:375:LEU:HD13	1:X:375:LEU:O	1.45	1.16
1:X:709:ALA:HB1	1:X:710:PRO:HD2	1.17	1.15
1:X:510:SER:O	1:X:514:ILE:HD12	1.46	1.15
1:X:29:VAL:CG1	1:X:758:ARG:CB	2.24	1.14
1:X:362:GLY:HA3	1:X:366:GLY:O	1.46	1.14
1:X:64:THR:CG2	1:X:68:GLN:O	1.95	1.14
1:X:689:ARG:HE	1:X:695:ARG:CZ	1.59	1.14
1:X:751:LEU:HD12	1:X:751:LEU:O	1.46	1.14
1:X:626:ASN:OD1	1:X:627:PHE:N	1.79	1.13
1:X:689:ARG:HB3	1:X:695:ARG:NH2	1.50	1.13
1:X:247:PHE:CD1	1:X:253:ILE:CA	2.30	1.12
1:X:64:THR:HG23	1:X:66:ASP:O	1.50	1.12
1:X:48:GLU:HG3	1:X:49:CYS:H	1.11	1.11
1:X:238:ARG:CZ	1:X:267:ARG:NH2	2.13	1.11
1:X:681:VAL:HG23	1:X:682:LEU:H	1.05	1.10
1:X:581:ILE:O	1:X:584:TRP:CD1	2.05	1.10
1:X:230:THR:HG23	1:X:238:ARG:NH2	1.66	1.09
1:X:592:LEU:O	1:X:592:LEU:HD12	1.49	1.09
1:X:29:VAL:HG11	1:X:758:ARG:CB	1.82	1.09
1:X:210:VAL:HG13	1:X:211:LEU:H	1.13	1.09
1:X:85:PHE:HD1	1:X:88:VAL:HG21	1.15	1.09
1:X:135:TYR:CE2	1:X:191:LYS:HE3	1.88	1.09
1:X:365:GLU:HG3	1:X:366:GLY:H	1.11	1.09
1:X:98:ASN:OD1	1:X:100:PRO:CD	2.00	1.08
1:X:137:GLN:NE2	1:X:140:VAL:HG21	1.66	1.08
1:X:230:THR:CG2	1:X:238:ARG:NH2	2.16	1.08
1:X:689:ARG:HB2	1:X:695:ARG:NH2	1.69	1.08
1:X:163:TYR:HE1	1:X:167:LEU:CD1	1.66	1.08
1:X:246:GLN:HE21	1:X:443:GLN:HB2	0.98	1.07
1:X:691:GLY:HA2	1:X:747:ARG:NH1	1.68	1.07
1:X:163:TYR:CE1	1:X:167:LEU:CD1	2.37	1.07
1:X:298:LEU:HD12	1:X:299:ALA:N	1.69	1.07
1:X:230:THR:HG23	1:X:238:ARG:HH22	1.06	1.07
1:X:291:GLU:HB2	2:X:2099:HOH:O	1.52	1.06
1:X:424:ALA:O	1:X:428:ARG:CG	2.02	1.06
1:X:685:ILE:HG22	1:X:689:ARG:NH1	1.69	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:210:VAL:HG21	1:X:214:GLN:OE1	1.56	1.06
1:X:614:ASP:OD1	1:X:615:PRO:HD2	0.90	1.05
1:X:503:PHE:CZ	1:X:504:ILE:HD11	1.89	1.05
1:X:238:ARG:NH1	1:X:267:ARG:HH21	1.51	1.05
1:X:685:ILE:CG2	1:X:689:ARG:NH1	2.18	1.05
1:X:8:THR:HG22	1:X:8:THR:O	1.52	1.05
1:X:701:PHE:CZ	1:X:713:PRO:O	2.09	1.05
1:X:464:ASN:HB2	1:X:468:GLN:HG2	1.06	1.04
1:X:526:LEU:HD22	1:X:631:ALA:HB1	1.40	1.04
1:X:709:ALA:CB	1:X:710:PRO:CD	2.32	1.04
1:X:230:THR:HG21	1:X:238:ARG:HH22	1.20	1.03
1:X:675:GLN:HA	1:X:678:CYS:HB2	1.40	1.03
1:X:741:ILE:HG23	1:X:742:THR:CG2	1.87	1.03
1:X:741:ILE:CG2	1:X:742:THR:HG23	1.87	1.03
1:X:705:TYR:CD1	1:X:705:TYR:O	2.11	1.03
1:X:698:TYR:CE2	1:X:699:ALA:CB	2.41	1.03
1:X:692:PHE:CE1	1:X:745:PHE:HB2	1.92	1.03
1:X:60:PHE:HB3	1:X:72:VAL:O	1.59	1.02
1:X:709:ALA:O	2:X:2234:HOH:O	1.75	1.02
1:X:458:PHE:HE1	1:X:475:ASN:HB3	1.21	1.02
1:X:365:GLU:CG	1:X:366:GLY:H	1.72	1.02
1:X:503:PHE:CE1	1:X:504:ILE:HD11	1.92	1.02
1:X:296:LEU:O	1:X:297:HIS:ND1	1.91	1.02
1:X:203:ASN:HB2	1:X:207:GLY:O	1.58	1.02
1:X:698:TYR:CG	1:X:699:ALA:N	2.26	1.02
1:X:210:VAL:HG22	1:X:214:GLN:OE1	1.57	1.01
1:X:56:THR:HB	1:X:59:SER:O	1.60	1.01
1:X:681:VAL:HG23	1:X:682:LEU:N	1.70	1.01
1:X:238:ARG:NH1	1:X:267:ARG:NH2	2.06	1.01
1:X:685:ILE:CG2	1:X:689:ARG:NH2	2.19	1.01
1:X:78:ASN:CB	1:X:98:ASN:HD22	1.59	1.01
1:X:689:ARG:HB3	1:X:695:ARG:HH21	0.85	1.01
1:X:247:PHE:HD1	1:X:253:ILE:HA	1.18	1.01
1:X:726:VAL:HG23	1:X:730:LEU:HD21	1.41	1.00
1:X:243:ILE:HG23	1:X:258:ILE:HG13	1.41	1.00
1:X:692:PHE:CD1	1:X:745:PHE:CB	2.37	1.00
1:X:741:ILE:HG23	1:X:742:THR:HG23	1.00	0.99
1:X:424:ALA:O	1:X:428:ARG:HG3	1.62	0.99
1:X:726:VAL:O	1:X:730:LEU:HG	1.62	0.99
1:X:242:PHE:CD2	1:X:244:GLU:HB2	1.98	0.98
1:X:693:PRO:HG2	1:X:748:ALA:H	1.22	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:87:GLY:HA2	1:X:109:ARG:HD3	1.43	0.98
1:X:11:TYR:O	1:X:15:LEU:HB2	1.62	0.98
1:X:682:LEU:O	2:X:2217:HOH:O	1.80	0.98
1:X:424:ALA:O	1:X:428:ARG:CD	2.12	0.98
1:X:85:PHE:CD1	1:X:88:VAL:HG21	1.99	0.98
1:X:474:THR:O	1:X:478:LEU:HD13	1.64	0.97
1:X:490:GLU:O	1:X:494:TYR:HD2	1.47	0.97
1:X:13:LYS:HA	1:X:18:LYS:HD2	1.43	0.97
1:X:682:LEU:CD1	1:X:683:GLU:N	2.27	0.96
1:X:480:GLN:HB2	1:X:508:LEU:CD2	1.94	0.96
1:X:685:ILE:HG21	1:X:689:ARG:HH22	1.19	0.96
1:X:736:GLN:O	1:X:747:ARG:CG	2.14	0.96
1:X:247:PHE:HD1	1:X:253:ILE:CA	1.75	0.96
1:X:98:ASN:OD1	1:X:99:GLU:N	1.99	0.95
1:X:75:ASP:OD1	2:X:2041:HOH:O	1.83	0.95
1:X:242:PHE:CZ	1:X:451:GLY:CA	2.49	0.95
1:X:698:TYR:CZ	1:X:699:ALA:HB2	2.00	0.95
1:X:724:ASP:OD2	2:X:2243:HOH:O	1.84	0.95
1:X:736:GLN:O	1:X:747:ARG:HG3	1.64	0.95
1:X:609:THR:O	1:X:613:ASN:CB	2.15	0.95
1:X:121:LEU:HD13	1:X:652:PHE:CE2	2.02	0.95
1:X:350:GLY:O	1:X:354:LEU:HG	1.67	0.95
1:X:641:LEU:O	1:X:645:LEU:CD1	2.14	0.95
1:X:424:ALA:O	1:X:428:ARG:HD2	1.66	0.94
1:X:242:PHE:HZ	1:X:451:GLY:HA3	1.19	0.94
1:X:504:ILE:HD12	1:X:505:ASP:H	1.32	0.94
1:X:626:ASN:OD1	1:X:627:PHE:HD2	1.26	0.94
1:X:689:ARG:NE	1:X:695:ARG:CZ	2.29	0.94
1:X:709:ALA:CB	1:X:710:PRO:HD2	1.94	0.94
1:X:183:ALA:HB1	1:X:655:CYS:HB3	1.47	0.93
1:X:682:LEU:HD12	1:X:683:GLU:CA	1.98	0.93
1:X:485:HIS:HE1	1:X:650:PRO:HD2	1.33	0.93
1:X:748:ALA:O	1:X:751:LEU:HG	1.66	0.93
1:X:337:SER:HB3	1:X:340:GLU:HG2	1.50	0.93
1:X:581:ILE:O	1:X:584:TRP:HD1	1.51	0.93
1:X:689:ARG:NE	1:X:695:ARG:NH2	2.15	0.93
1:X:78:ASN:CA	1:X:98:ASN:HD22	1.81	0.92
1:X:689:ARG:CD	1:X:695:ARG:NH2	2.33	0.92
1:X:698:TYR:CZ	1:X:699:ALA:CB	2.53	0.92
1:X:37:TYR:HE1	1:X:39:PRO:HA	1.33	0.92
1:X:246:GLN:NE2	1:X:443:GLN:HB2	1.84	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:87:GLY:HA2	1:X:109:ARG:CD	1.99	0.92
1:X:229:LYS:HB2	1:X:234:ASN:O	1.71	0.91
1:X:294:LYS:HD2	1:X:297:HIS:HA	1.50	0.91
1:X:7:ARG:HE	1:X:18:LYS:HB3	1.35	0.91
1:X:242:PHE:CZ	1:X:244:GLU:CG	2.37	0.91
1:X:166:MET:O	1:X:170:ARG:HA	1.71	0.91
1:X:98:ASN:CG	1:X:100:PRO:HD2	1.90	0.91
1:X:238:ARG:CZ	1:X:267:ARG:HH21	1.78	0.90
1:X:362:GLY:CA	1:X:366:GLY:O	2.19	0.90
1:X:48:GLU:HG3	1:X:49:CYS:N	1.85	0.90
1:X:135:TYR:CD2	1:X:191:LYS:CE	2.53	0.90
1:X:29:VAL:HG13	1:X:758:ARG:CB	2.00	0.90
1:X:539:THR:O	1:X:539:THR:HG23	1.70	0.90
1:X:56:THR:HG22	1:X:59:SER:H	1.37	0.89
1:X:393:LEU:HD12	1:X:596:LEU:HD21	1.55	0.89
1:X:548:HIS:O	1:X:552:SER:OG	1.89	0.89
1:X:474:THR:O	1:X:478:LEU:CD1	2.20	0.89
1:X:681:VAL:CG2	1:X:682:LEU:H	1.86	0.89
1:X:210:VAL:HG13	1:X:211:LEU:N	1.88	0.89
1:X:458:PHE:CE1	1:X:475:ASN:HB3	2.07	0.88
1:X:588:ASN:O	1:X:630:VAL:HG22	1.73	0.88
1:X:398:ILE:HD13	1:X:407:GLN:HG3	1.56	0.88
1:X:532:GLN:OE1	1:X:543:LEU:HD13	1.74	0.88
1:X:725:ALA:CB	1:X:729:HIS:CD2	2.56	0.88
1:X:689:ARG:HB2	1:X:695:ARG:HH22	1.36	0.88
1:X:698:TYR:CD1	2:X:2227:HOH:O	2.26	0.88
1:X:241:LYS:CE	1:X:243:ILE:HD11	2.05	0.87
1:X:709:ALA:HB1	1:X:710:PRO:HD3	1.55	0.87
1:X:117:THR:O	1:X:123:LEU:HD12	1.74	0.87
1:X:379:SER:OG	1:X:389:LEU:HD22	1.75	0.87
1:X:710:PRO:O	1:X:711:ASN:HB2	1.73	0.87
1:X:29:VAL:HG13	1:X:758:ARG:HB3	1.57	0.87
1:X:379:SER:OG	1:X:389:LEU:CD2	2.22	0.87
1:X:247:PHE:CE1	1:X:253:ILE:HA	2.09	0.87
1:X:255:GLY:HA3	1:X:443:GLN:HG3	1.54	0.87
1:X:685:ILE:HD13	1:X:689:ARG:NH2	1.90	0.87
1:X:689:ARG:HE	1:X:695:ARG:NH2	1.71	0.86
1:X:485:HIS:CE1	1:X:650:PRO:HD2	2.10	0.86
1:X:539:THR:HG23	1:X:541:ASN:HB3	1.55	0.86
1:X:693:PRO:HG2	1:X:748:ALA:N	1.91	0.86
1:X:11:TYR:CE2	1:X:16:LYS:HB2	2.10	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:666:LYS:O	2:X:2213:HOH:O	1.92	0.86
1:X:84:LYS:CE	1:X:85:PHE:CE2	2.59	0.86
1:X:121:LEU:HD11	1:X:482:PHE:CE2	2.10	0.85
1:X:7:ARG:NH2	2:X:2002:HOH:O	2.09	0.85
1:X:7:ARG:O	1:X:8:THR:HB	1.74	0.85
1:X:474:THR:HG23	1:X:638:LEU:HD13	1.58	0.85
1:X:33:ARG:HD2	1:X:52:ILE:CG2	2.06	0.85
1:X:365:GLU:HG3	1:X:366:GLY:N	1.91	0.85
1:X:298:LEU:CD1	1:X:299:ALA:O	2.24	0.85
1:X:691:GLY:HA2	1:X:747:ARG:HH12	1.32	0.85
1:X:16:LYS:HD2	1:X:152:ALA:HB2	1.57	0.85
1:X:29:VAL:CG1	1:X:758:ARG:HB2	2.03	0.85
1:X:510:SER:O	1:X:514:ILE:CD1	2.22	0.85
1:X:137:GLN:C	1:X:140:VAL:HG22	1.96	0.85
1:X:428:ARG:HH12	1:X:618:ALA:HA	1.40	0.85
1:X:8:THR:CG2	1:X:8:THR:O	2.24	0.85
1:X:121:LEU:HD21	1:X:486:MET:SD	2.17	0.84
1:X:313:VAL:O	1:X:315:ILE:HG13	1.77	0.84
1:X:534:VAL:HG23	1:X:535:PHE:CE2	2.11	0.84
1:X:35:ILE:HB	1:X:52:ILE:HD11	1.56	0.84
1:X:293:LYS:HE2	1:X:298:LEU:HD11	1.58	0.84
1:X:285:LEU:HD13	1:X:301:PRO:HB3	1.57	0.84
1:X:134:ILE:O	1:X:134:ILE:HG13	1.78	0.83
1:X:29:VAL:HG11	1:X:758:ARG:HB2	1.60	0.83
1:X:244:GLU:HG2	1:X:451:GLY:CA	2.09	0.83
1:X:485:HIS:CE1	1:X:650:PRO:CD	2.62	0.83
1:X:84:LYS:HE3	1:X:85:PHE:CE2	2.14	0.83
1:X:689:ARG:CG	1:X:695:ARG:HH21	1.90	0.83
1:X:465:SER:N	1:X:468:GLN:OE1	2.09	0.83
1:X:11:TYR:OH	1:X:152:ALA:HB3	1.77	0.83
1:X:726:VAL:HG23	1:X:730:LEU:CD2	2.09	0.83
1:X:219:ASN:H	1:X:220:PRO:HD2	1.42	0.83
1:X:725:ALA:C	1:X:729:HIS:HD2	1.82	0.83
1:X:203:ASN:ND2	1:X:207:GLY:HA3	1.95	0.82
1:X:651:HIS:HE1	2:X:2207:HOH:O	1.62	0.82
1:X:705:TYR:CG	1:X:705:TYR:O	2.31	0.82
1:X:689:ARG:HD2	1:X:695:ARG:NE	1.94	0.82
1:X:470:CYS:HB3	1:X:634:TYR:CZ	2.14	0.82
1:X:147:ARG:N	1:X:150:GLU:OE2	2.12	0.82
1:X:243:ILE:HG23	1:X:258:ILE:CG1	2.10	0.82
1:X:693:PRO:CG	1:X:748:ALA:H	1.92	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:239:PHE:CE2	1:X:241:LYS:HD3	2.16	0.81
1:X:325:LYS:O	1:X:329:GLN:CB	2.24	0.81
1:X:604:SER:O	1:X:605:ASP:CG	2.19	0.81
1:X:464:ASN:HB3	1:X:468:GLN:HG2	1.59	0.81
1:X:490:GLU:O	1:X:494:TYR:CD2	2.32	0.81
1:X:689:ARG:HD2	1:X:695:ARG:HE	1.43	0.81
1:X:246:GLN:HE21	1:X:443:GLN:CB	1.89	0.81
1:X:475:ASN:O	1:X:478:LEU:HB2	1.80	0.81
1:X:607:VAL:HA	1:X:610:LYS:HB3	1.63	0.81
1:X:46:SER:OG	1:X:669:ASP:OD2	1.99	0.81
1:X:572:HIS:CD2	1:X:577:VAL:HG21	2.16	0.81
1:X:492:GLU:O	1:X:495:LEU:HG	1.80	0.80
1:X:464:ASN:HB2	1:X:468:GLN:CB	2.11	0.80
1:X:102:VAL:O	1:X:106:LEU:HB2	1.82	0.80
1:X:369:LEU:HD11	1:X:372:LYS:HE3	1.62	0.80
1:X:682:LEU:HD12	1:X:683:GLU:H	1.43	0.80
1:X:211:LEU:HB3	2:X:2087:HOH:O	1.82	0.80
1:X:331:MET:O	1:X:336:PHE:HB2	1.82	0.80
1:X:13:LYS:HD3	1:X:18:LYS:NZ	1.97	0.80
1:X:609:THR:HG23	1:X:613:ASN:ND2	1.97	0.80
1:X:121:LEU:HD13	1:X:652:PHE:HE2	1.47	0.80
1:X:677:ARG:HA	2:X:2218:HOH:O	1.80	0.80
1:X:541:ASN:O	1:X:545:THR:HG23	1.81	0.79
1:X:38:ASN:HB2	1:X:47:TYR:CE1	2.16	0.79
1:X:754:ILE:HG23	1:X:755:GLU:N	1.97	0.79
1:X:279:HIS:O	1:X:283:GLN:HG2	1.83	0.79
1:X:285:LEU:HD23	1:X:298:LEU:HD22	1.65	0.79
1:X:126:VAL:HG23	1:X:656:ILE:O	1.83	0.79
1:X:582:GLN:HB2	2:X:2186:HOH:O	1.82	0.79
1:X:242:PHE:HE2	1:X:244:GLU:CB	1.67	0.79
1:X:7:ARG:HH21	1:X:18:LYS:HE2	1.47	0.79
1:X:84:LYS:HE2	1:X:85:PHE:CE2	2.18	0.79
1:X:375:LEU:CD1	1:X:375:LEU:O	2.29	0.79
1:X:64:THR:HG22	1:X:68:GLN:O	1.83	0.79
1:X:518:ASP:HB2	1:X:635:LYS:NZ	1.97	0.79
1:X:679:ASN:HB2	1:X:681:VAL:HG13	1.62	0.79
1:X:539:THR:C	1:X:541:ASN:H	1.86	0.79
1:X:230:THR:HB	1:X:275:GLU:OE2	1.83	0.78
1:X:736:GLN:O	1:X:747:ARG:CD	2.31	0.78
1:X:488:LYS:O	1:X:491:GLN:HB3	1.84	0.78
1:X:226:GLY:O	1:X:238:ARG:HB3	1.84	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:733:ASP:HB2	1:X:734:PRO:HD2	1.65	0.78
1:X:689:ARG:CD	1:X:695:ARG:HH21	1.95	0.78
1:X:33:ARG:HD2	1:X:52:ILE:HG21	1.64	0.78
1:X:132:ILE:O	1:X:134:ILE:HG23	1.83	0.78
1:X:20:GLY:HA3	2:X:2011:HOH:O	1.84	0.78
1:X:247:PHE:HD1	1:X:253:ILE:N	1.81	0.78
1:X:701:PHE:HZ	1:X:713:PRO:O	1.66	0.78
1:X:121:LEU:HD11	1:X:482:PHE:HE2	1.46	0.77
1:X:365:GLU:CG	1:X:366:GLY:N	2.45	0.77
1:X:202:ARG:HG2	1:X:252:PHE:HD2	1.49	0.77
1:X:219:ASN:H	1:X:220:PRO:CD	1.97	0.77
1:X:477:LYS:HD3	1:X:638:LEU:HD21	1.64	0.77
1:X:680:VAL:HG22	1:X:684:GLY:HA2	1.65	0.77
1:X:121:LEU:HD13	1:X:652:PHE:CD2	2.19	0.77
1:X:152:ALA:HB1	1:X:153:PRO:HD2	1.66	0.77
1:X:539:THR:C	1:X:541:ASN:N	2.34	0.77
1:X:36:TRP:HE3	1:X:48:GLU:O	1.65	0.77
1:X:241:LYS:HE2	1:X:243:ILE:HD11	1.65	0.77
1:X:282:TYR:HB3	2:X:2098:HOH:O	1.84	0.77
1:X:562:ARG:NH1	2:X:2178:HOH:O	2.17	0.77
1:X:717:GLU:HG2	1:X:717:GLU:O	1.85	0.77
1:X:751:LEU:O	1:X:751:LEU:CD1	2.31	0.77
1:X:343:SER:HA	1:X:346:LYS:HB2	1.65	0.77
1:X:503:PHE:CD1	1:X:504:ILE:CD1	2.51	0.77
1:X:81:ASN:HB3	1:X:82:PRO:HD2	1.65	0.77
1:X:391:LYS:O	1:X:395:GLU:O	2.02	0.77
1:X:484:HIS:O	1:X:487:PHE:HB3	1.83	0.77
1:X:203:ASN:HB2	1:X:207:GLY:C	2.04	0.76
1:X:187:GLU:HA	1:X:190:LYS:HB2	1.67	0.76
1:X:272:SER:OG	1:X:273:GLU:N	2.19	0.76
1:X:146:ARG:HA	1:X:150:GLU:OE2	1.86	0.76
1:X:12:HIS:HB3	1:X:18:LYS:HG2	1.66	0.76
1:X:247:PHE:HE1	1:X:253:ILE:HB	1.50	0.76
1:X:664:PRO:O	1:X:665:ALA:CB	2.33	0.76
1:X:701:PHE:HD2	2:X:2229:HOH:O	1.68	0.76
1:X:7:ARG:O	1:X:8:THR:CB	2.34	0.76
1:X:5:HIS:O	1:X:6:ASP:HB2	1.84	0.75
1:X:698:TYR:CE1	1:X:699:ALA:HB2	2.20	0.75
1:X:210:VAL:CG1	1:X:211:LEU:H	1.97	0.75
1:X:386:PRO:O	1:X:390:GLU:HG2	1.86	0.75
1:X:491:GLN:O	2:X:2155:HOH:O	2.04	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:626:ASN:OD1	1:X:627:PHE:CG	2.38	0.75
1:X:56:THR:CG2	1:X:59:SER:H	2.00	0.75
1:X:651:HIS:CE1	2:X:2207:HOH:O	2.37	0.75
1:X:85:PHE:HD1	1:X:88:VAL:CG2	1.99	0.75
1:X:12:HIS:O	1:X:18:LYS:HG3	1.85	0.75
1:X:432:TRP:CZ2	1:X:610:LYS:HD3	2.22	0.75
1:X:78:ASN:CG	1:X:98:ASN:ND2	2.39	0.75
1:X:5:HIS:O	1:X:6:ASP:CB	2.34	0.75
1:X:675:GLN:HA	1:X:678:CYS:CB	2.17	0.75
1:X:294:LYS:HB3	1:X:294:LYS:HZ2	1.51	0.74
1:X:490:GLU:HA	1:X:493:GLU:HB2	1.69	0.74
1:X:540:ASP:OD1	1:X:585:LEU:HD12	1.87	0.74
1:X:546:LYS:HB3	2:X:2172:HOH:O	1.86	0.74
1:X:597:GLU:C	1:X:601:LYS:HG3	2.08	0.74
1:X:247:PHE:CE1	1:X:253:ILE:CA	2.70	0.74
1:X:33:ARG:HG3	1:X:52:ILE:HB	1.69	0.74
1:X:344:ILE:O	1:X:348:ILE:HG12	1.87	0.74
1:X:480:GLN:HB2	1:X:508:LEU:HD21	1.70	0.74
1:X:87:GLY:CA	1:X:109:ARG:HD3	2.18	0.74
1:X:698:TYR:CD2	1:X:699:ALA:HB3	2.22	0.74
1:X:494:TYR:HB3	1:X:500:ASN:CG	2.09	0.74
1:X:464:ASN:CB	1:X:468:GLN:CG	2.46	0.73
1:X:375:LEU:C	1:X:375:LEU:HD13	2.09	0.73
1:X:685:ILE:O	1:X:688:THR:N	2.20	0.73
1:X:369:LEU:O	1:X:369:LEU:HD12	1.86	0.73
1:X:15:LEU:HD21	1:X:139:MET:SD	2.29	0.73
1:X:244:GLU:HG2	1:X:451:GLY:HA2	1.70	0.73
1:X:242:PHE:CD2	1:X:244:GLU:CB	2.62	0.73
1:X:539:THR:O	1:X:541:ASN:CA	2.37	0.73
1:X:685:ILE:HG21	1:X:689:ARG:NH1	1.94	0.73
1:X:129:PHE:HE2	1:X:658:PRO:HG2	1.52	0.73
1:X:228:ALA:HA	1:X:279:HIS:CE1	2.23	0.73
1:X:428:ARG:NH1	1:X:618:ALA:HA	2.04	0.73
1:X:582:GLN:NE2	1:X:582:GLN:HA	2.04	0.73
1:X:728:LYS:HA	1:X:734:PRO:HD3	1.69	0.73
1:X:78:ASN:HB3	1:X:98:ASN:HD21	0.92	0.73
1:X:163:TYR:CD1	1:X:167:LEU:HD11	2.18	0.72
1:X:132:ILE:HD12	1:X:132:ILE:N	2.04	0.72
1:X:626:ASN:CG	1:X:627:PHE:HD2	1.91	0.72
1:X:702:VAL:HA	1:X:714:ARG:O	1.89	0.72
1:X:215:ILE:HG12	1:X:441:LEU:HD22	1.72	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:743:LYS:HD3	2:X:2248:HOH:O	1.89	0.72
1:X:298:LEU:HD12	1:X:299:ALA:O	1.87	0.72
1:X:90:ASP:HA	1:X:118:TYR:HB2	1.71	0.72
1:X:342:MET:O	1:X:342:MET:SD	2.48	0.72
1:X:479:GLN:NE2	1:X:573:TYR:CD2	2.58	0.72
1:X:597:GLU:O	1:X:601:LYS:HG3	1.90	0.72
1:X:332:ASP:HB3	1:X:336:PHE:O	1.89	0.72
1:X:56:THR:HB	1:X:59:SER:C	2.09	0.72
1:X:99:GLU:O	1:X:102:VAL:HG12	1.90	0.72
1:X:213:GLN:HA	1:X:216:LEU:HD13	1.70	0.72
1:X:224:ALA:O	1:X:280:ILE:HG23	1.90	0.71
1:X:306:TYR:HE2	1:X:422:VAL:HG11	1.53	0.71
1:X:84:LYS:HE3	1:X:85:PHE:CZ	2.25	0.71
1:X:122:PHE:CE1	1:X:652:PHE:HB2	2.25	0.71
1:X:156:PHE:HA	1:X:159:SER:OG	1.90	0.71
1:X:294:LYS:HE2	1:X:297:HIS:HB3	1.71	0.71
1:X:572:HIS:HD2	1:X:577:VAL:HG21	1.55	0.71
1:X:642:MET:SD	1:X:645:LEU:HD22	2.30	0.71
1:X:331:MET:C	1:X:336:PHE:HB2	2.11	0.71
1:X:347:ILE:HA	1:X:382:PHE:HE1	1.54	0.71
1:X:389:LEU:HD13	1:X:600:PHE:CZ	2.25	0.71
1:X:298:LEU:HD13	1:X:299:ALA:O	1.90	0.71
1:X:242:PHE:CE1	1:X:451:GLY:HA3	2.23	0.71
1:X:458:PHE:HE1	1:X:475:ASN:CB	2.02	0.71
1:X:728:LYS:HG2	1:X:734:PRO:HG3	1.72	0.71
1:X:534:VAL:HG23	1:X:535:PHE:CD2	2.25	0.71
1:X:245:ILE:HD11	1:X:450:ILE:HB	1.72	0.71
1:X:7:ARG:NE	1:X:18:LYS:HB3	2.05	0.71
1:X:245:ILE:O	1:X:245:ILE:HD12	1.91	0.70
1:X:692:PHE:HD1	1:X:745:PHE:CG	2.08	0.70
1:X:698:TYR:CD2	1:X:699:ALA:N	2.52	0.70
1:X:247:PHE:CE1	1:X:253:ILE:HB	2.27	0.70
1:X:641:LEU:C	1:X:645:LEU:HD13	2.11	0.70
1:X:193:ILE:HD11	2:X:2072:HOH:O	1.91	0.70
1:X:29:VAL:HG11	1:X:758:ARG:HD2	1.73	0.70
1:X:490:GLU:HB3	1:X:494:TYR:HE2	1.56	0.70
1:X:474:THR:HG23	1:X:638:LEU:CD1	2.22	0.70
1:X:736:GLN:O	1:X:747:ARG:HD2	1.91	0.70
1:X:129:PHE:HB2	1:X:664:PRO:HB3	1.72	0.70
1:X:721:LYS:HE2	2:X:2241:HOH:O	1.91	0.70
1:X:238:ARG:HG2	1:X:278:TYR:OH	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:48:GLU:CG	1:X:49:CYS:H	1.96	0.70
1:X:590:ASP:N	1:X:591:PRO:HD3	2.05	0.70
1:X:532:GLN:OE1	1:X:543:LEU:CD1	2.39	0.70
1:X:296:LEU:C	1:X:297:HIS:CG	2.65	0.70
1:X:685:ILE:HD13	1:X:689:ARG:HH21	1.56	0.70
1:X:105:ASN:O	1:X:109:ARG:HG2	1.92	0.70
1:X:36:TRP:CE3	1:X:48:GLU:O	2.44	0.70
1:X:326:ILE:HG23	2:X:2114:HOH:O	1.90	0.70
1:X:283:GLN:HB2	1:X:324:PHE:HD1	1.56	0.69
1:X:38:ASN:HB2	1:X:47:TYR:CD1	2.26	0.69
1:X:490:GLU:HB3	1:X:494:TYR:CE2	2.27	0.69
1:X:508:LEU:HA	2:X:2161:HOH:O	1.91	0.69
1:X:389:LEU:CD1	1:X:600:PHE:CZ	2.75	0.69
1:X:130:LYS:HG2	1:X:131:ARG:H	1.57	0.69
1:X:691:GLY:CA	1:X:747:ARG:NH1	2.53	0.69
1:X:109:ARG:O	1:X:114:LEU:HB2	1.91	0.69
1:X:375:LEU:CD1	1:X:375:LEU:C	2.61	0.69
1:X:13:LYS:HD3	1:X:18:LYS:HZ3	1.57	0.69
1:X:28:THR:HG22	1:X:29:VAL:N	2.07	0.69
1:X:535:PHE:HB2	1:X:536:PRO:HD2	1.75	0.69
1:X:130:LYS:HB3	1:X:132:ILE:HD11	1.75	0.69
1:X:155:ILE:HG23	1:X:156:PHE:HD1	1.58	0.69
1:X:134:ILE:HG13	1:X:135:TYR:CD1	2.27	0.68
1:X:7:ARG:HH21	1:X:18:LYS:CE	2.06	0.68
1:X:389:LEU:CD1	1:X:600:PHE:HZ	2.06	0.68
1:X:33:ARG:CD	1:X:52:ILE:HB	2.24	0.68
1:X:692:PHE:HD1	1:X:745:PHE:HB3	1.57	0.68
1:X:708:LEU:O	1:X:709:ALA:O	2.10	0.68
1:X:380:THR:HG22	1:X:380:THR:O	1.93	0.68
1:X:438:ASN:O	1:X:442:CYS:HB2	1.93	0.68
1:X:516:LEU:HD22	1:X:555:ASN:OD1	1.93	0.68
1:X:137:GLN:NE2	1:X:140:VAL:CG2	2.51	0.68
1:X:238:ARG:CZ	1:X:267:ARG:CZ	2.70	0.68
1:X:461:PHE:HB2	2:X:2145:HOH:O	1.93	0.68
1:X:393:LEU:HD12	1:X:596:LEU:CD2	2.23	0.68
1:X:728:LYS:HG3	1:X:737:TYR:OH	1.94	0.68
1:X:202:ARG:HG2	1:X:252:PHE:CD2	2.28	0.68
1:X:98:ASN:OD1	1:X:98:ASN:C	2.31	0.68
1:X:174:SER:OG	1:X:650:PRO:HA	1.93	0.68
1:X:238:ARG:O	1:X:238:ARG:HG3	1.92	0.68
1:X:493:GLU:OE1	1:X:493:GLU:HA	1.92	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:389:LEU:HD13	1:X:600:PHE:CE1	2.29	0.68
1:X:165:SER:O	1:X:169:ASP:N	2.25	0.68
1:X:255:GLY:HA3	1:X:443:GLN:CG	2.24	0.68
1:X:480:GLN:HG3	2:X:2150:HOH:O	1.92	0.68
1:X:518:ASP:HB2	1:X:635:LYS:HZ2	1.55	0.68
1:X:455:ILE:HG22	1:X:456:SER:N	2.09	0.68
1:X:675:GLN:O	1:X:678:CYS:N	2.26	0.68
1:X:52:ILE:HG12	1:X:60:PHE:CZ	2.29	0.68
1:X:7:ARG:NH2	1:X:18:LYS:CE	2.58	0.67
1:X:238:ARG:NH2	1:X:267:ARG:NH2	2.41	0.67
1:X:37:TYR:CE1	1:X:39:PRO:HA	2.23	0.67
1:X:332:ASP:HA	1:X:336:PHE:H	1.58	0.67
1:X:357:ILE:N	1:X:418:ARG:HH12	1.93	0.67
1:X:322:GLU:HB2	2:X:2111:HOH:O	1.94	0.67
1:X:381:VAL:O	2:X:2126:HOH:O	2.13	0.67
1:X:494:TYR:HB3	1:X:500:ASN:ND2	2.09	0.67
1:X:526:LEU:CD2	1:X:631:ALA:HB1	2.22	0.67
1:X:225:PHE:CG	1:X:280:ILE:HG21	2.29	0.67
1:X:283:GLN:HB2	1:X:324:PHE:CD1	2.29	0.67
1:X:33:ARG:HD2	1:X:52:ILE:CB	2.23	0.67
1:X:604:SER:O	1:X:605:ASP:CB	2.41	0.67
1:X:146:ARG:CA	1:X:150:GLU:OE2	2.41	0.67
1:X:392:ALA:HB3	1:X:596:LEU:HD23	1.76	0.67
1:X:496:LYS:O	1:X:742:THR:OG1	2.13	0.67
1:X:22:SER:HB3	1:X:26:LYS:NZ	2.09	0.67
1:X:379:SER:OG	1:X:389:LEU:HD23	1.94	0.67
1:X:682:LEU:CD1	1:X:683:GLU:H	2.00	0.67
1:X:689:ARG:CD	1:X:695:ARG:CZ	2.69	0.67
1:X:110:TYR:HE2	1:X:126:VAL:HG13	1.60	0.67
1:X:135:TYR:CE2	1:X:191:LYS:CE	2.75	0.67
1:X:692:PHE:CD1	1:X:745:PHE:CG	2.83	0.67
1:X:119:SER:HB2	1:X:122:PHE:CB	2.24	0.66
1:X:385:ASN:O	1:X:388:VAL:HB	1.96	0.66
1:X:609:THR:CG2	1:X:613:ASN:HD22	2.07	0.66
1:X:186:THR:O	1:X:190:LYS:HG3	1.95	0.66
1:X:432:TRP:O	1:X:435:LYS:HB3	1.95	0.66
1:X:43:GLU:HG3	1:X:45:ASP:H	1.60	0.66
1:X:97:LEU:HD12	1:X:97:LEU:O	1.94	0.66
1:X:503:PHE:CD1	1:X:505:ASP:N	2.63	0.66
1:X:52:ILE:CG1	1:X:60:PHE:CZ	2.78	0.66
1:X:296:LEU:CA	1:X:297:HIS:ND1	2.58	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:385:ASN:HB3	1:X:388:VAL:HG21	1.77	0.66
1:X:503:PHE:HD1	1:X:505:ASP:H	1.42	0.66
1:X:592:LEU:O	1:X:592:LEU:CD1	2.36	0.66
1:X:736:GLN:HG2	1:X:747:ARG:HB2	1.78	0.66
1:X:210:VAL:CG2	1:X:214:GLN:CD	2.64	0.66
1:X:389:LEU:O	1:X:393:LEU:HD13	1.95	0.66
1:X:121:LEU:CD1	1:X:482:PHE:HE2	2.08	0.66
1:X:33:ARG:CG	1:X:52:ILE:HB	2.25	0.66
1:X:33:ARG:HD2	1:X:52:ILE:HB	1.78	0.66
1:X:664:PRO:O	1:X:665:ALA:HB3	1.96	0.66
1:X:84:LYS:HE2	1:X:85:PHE:HE2	1.59	0.66
1:X:247:PHE:CE1	1:X:253:ILE:CB	2.78	0.66
1:X:229:LYS:HD3	1:X:276:ARG:HD3	1.76	0.66
1:X:353:HIS:CB	1:X:378:ALA:HB2	2.26	0.66
1:X:399:LEU:HD12	1:X:403:ASP:O	1.96	0.66
1:X:698:TYR:HE2	1:X:720:GLN:HE22	1.43	0.66
1:X:183:ALA:HB1	1:X:655:CYS:CB	2.23	0.65
1:X:539:THR:CG2	1:X:539:THR:O	2.42	0.65
1:X:56:THR:CG2	1:X:58:ASP:OD1	2.43	0.65
1:X:532:GLN:HE22	1:X:543:LEU:HB2	1.61	0.65
1:X:685:ILE:CG2	1:X:689:ARG:HH12	2.06	0.65
1:X:691:GLY:HA2	1:X:747:ARG:HH11	1.60	0.65
1:X:473:TYR:HE2	1:X:638:LEU:HD23	1.62	0.65
1:X:691:GLY:CA	1:X:747:ARG:HH12	2.08	0.65
1:X:701:PHE:CD2	2:X:2229:HOH:O	2.47	0.65
1:X:726:VAL:O	1:X:730:LEU:N	2.27	0.65
1:X:143:PHE:O	1:X:146:ARG:HG2	1.97	0.65
1:X:241:LYS:HE2	1:X:243:ILE:CD1	2.26	0.65
1:X:710:PRO:HB2	2:X:2235:HOH:O	1.97	0.65
1:X:239:PHE:HE2	1:X:241:LYS:HD3	1.59	0.65
1:X:464:ASN:HA	1:X:468:GLN:CD	2.17	0.65
1:X:182:GLY:HA3	1:X:657:ILE:HD12	1.80	0.64
1:X:609:THR:HG23	1:X:613:ASN:HD22	1.61	0.64
1:X:572:HIS:HD2	1:X:577:VAL:CG2	2.11	0.64
1:X:533:SER:O	1:X:589:LYS:HE2	1.96	0.64
1:X:485:HIS:CE1	1:X:650:PRO:CG	2.80	0.64
1:X:155:ILE:HG23	1:X:156:PHE:CD1	2.31	0.64
1:X:504:ILE:HD12	1:X:505:ASP:N	2.10	0.64
1:X:29:VAL:HG13	1:X:758:ARG:HB2	1.74	0.64
1:X:98:ASN:HD21	1:X:100:PRO:HG2	1.62	0.64
1:X:623:LYS:HG3	1:X:624:GLY:H	1.62	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:93:GLU:OE1	1:X:694:ASN:CG	2.36	0.64
1:X:298:LEU:HD12	1:X:299:ALA:CA	2.28	0.64
1:X:37:TYR:O	1:X:48:GLU:N	2.31	0.64
1:X:623:LYS:O	1:X:626:ASN:O	2.16	0.64
1:X:725:ALA:CA	1:X:729:HIS:HD2	2.10	0.64
1:X:160:ASP:O	1:X:163:TYR:HB3	1.99	0.63
1:X:33:ARG:HG2	2:X:2016:HOH:O	1.98	0.63
1:X:477:LYS:C	1:X:480:GLN:OE1	2.34	0.63
1:X:246:GLN:HG2	1:X:255:GLY:HA3	1.79	0.63
1:X:519:GLY:O	1:X:523:PRO:HA	1.99	0.63
1:X:730:LEU:HD12	1:X:730:LEU:C	2.18	0.63
1:X:146:ARG:HD3	2:X:2061:HOH:O	1.97	0.63
1:X:70:ARG:HB2	2:X:2037:HOH:O	1.98	0.63
1:X:689:ARG:HD2	1:X:695:ARG:CZ	2.29	0.63
1:X:701:PHE:CD2	1:X:701:PHE:O	2.52	0.63
1:X:30:SER:O	1:X:756:GLU:O	2.16	0.63
1:X:432:TRP:CZ2	1:X:436:LYS:HE2	2.34	0.63
1:X:711:ASN:C	1:X:713:PRO:HD3	2.19	0.63
1:X:552:SER:O	1:X:553:LYS:HB2	1.99	0.62
1:X:90:ASP:OD1	1:X:120:GLY:N	2.28	0.62
1:X:354:LEU:O	1:X:418:ARG:HD2	1.98	0.62
1:X:539:THR:HG22	1:X:542:THR:CG2	2.28	0.62
1:X:477:LYS:HD3	1:X:638:LEU:CD2	2.29	0.62
1:X:11:TYR:HA	1:X:15:LEU:HD13	1.81	0.62
1:X:222:LEU:O	1:X:226:GLY:N	2.33	0.62
1:X:593:GLN:HA	1:X:593:GLN:OE1	1.99	0.62
1:X:701:PHE:CD1	2:X:2231:HOH:O	2.51	0.62
1:X:538:ALA:HA	2:X:2171:HOH:O	1.98	0.62
1:X:297:HIS:ND1	1:X:297:HIS:N	2.47	0.62
1:X:624:GLY:O	1:X:625:ALA:HB3	1.99	0.62
1:X:685:ILE:HG13	1:X:686:ARG:N	2.14	0.62
1:X:492:GLU:HA	1:X:495:LEU:CD2	2.30	0.62
1:X:503:PHE:HD1	1:X:505:ASP:N	1.97	0.62
1:X:93:GLU:OE1	1:X:694:ASN:OD1	2.16	0.62
1:X:230:THR:HG21	1:X:238:ARG:NH2	1.96	0.62
1:X:544:ILE:HD11	1:X:548:HIS:CE1	2.35	0.62
1:X:698:TYR:CD2	1:X:699:ALA:CB	2.81	0.62
1:X:117:THR:HG22	1:X:118:TYR:H	1.65	0.61
1:X:294:LYS:HB3	1:X:294:LYS:NZ	2.14	0.61
1:X:620:ARG:HH22	1:X:630:VAL:HG13	1.65	0.61
1:X:671:VAL:HG23	1:X:672:VAL:H	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:171:GLN:NE2	2:X:2069:HOH:O	2.33	0.61
1:X:436:LYS:O	1:X:439:ASN:OD1	2.18	0.61
1:X:93:GLU:OE1	1:X:694:ASN:ND2	2.33	0.61
1:X:272:SER:O	1:X:310:SER:HB2	2.00	0.61
1:X:532:GLN:C	1:X:534:VAL:H	2.03	0.61
1:X:680:VAL:O	1:X:684:GLY:HA3	2.00	0.61
1:X:689:ARG:CG	1:X:695:ARG:NH2	2.54	0.61
1:X:342:MET:HG3	1:X:346:LYS:HG3	1.83	0.61
1:X:103:PHE:O	1:X:107:ARG:HG3	1.99	0.61
1:X:242:PHE:CE2	1:X:244:GLU:HB3	2.22	0.61
1:X:54:SER:HB2	1:X:61:THR:O	2.00	0.61
1:X:473:TYR:CE2	1:X:638:LEU:HD23	2.36	0.61
1:X:35:ILE:HG13	1:X:36:TRP:O	2.01	0.61
1:X:491:GLN:HA	1:X:491:GLN:OE1	2.00	0.61
1:X:11:TYR:OH	1:X:152:ALA:CB	2.46	0.61
1:X:12:HIS:O	1:X:18:LYS:CG	2.49	0.61
1:X:219:ASN:HA	1:X:222:LEU:HG	1.83	0.61
1:X:736:GLN:HG3	1:X:750:GLN:HB2	1.82	0.61
1:X:78:ASN:HA	1:X:98:ASN:HD22	1.63	0.61
1:X:293:LYS:CE	1:X:298:LEU:HD11	2.31	0.61
1:X:504:ILE:CD1	1:X:505:ASP:H	2.12	0.61
1:X:134:ILE:O	1:X:135:TYR:HD1	1.83	0.61
1:X:300:GLY:O	1:X:303:SER:HB3	2.00	0.61
1:X:332:ASP:HA	1:X:336:PHE:N	2.16	0.61
1:X:367:ALA:HB2	1:X:411:VAL:N	2.16	0.61
1:X:339:GLU:O	1:X:342:MET:HB3	2.00	0.61
1:X:480:GLN:HB2	1:X:508:LEU:HD22	1.81	0.61
1:X:14:TYR:CE1	1:X:133:PRO:HG2	2.35	0.60
1:X:730:LEU:HD12	1:X:731:ASN:HB2	1.82	0.60
1:X:91:MET:O	1:X:94:LEU:HG	2.01	0.60
1:X:607:VAL:O	1:X:611:LEU:N	2.34	0.60
1:X:306:TYR:CE2	1:X:422:VAL:HG11	2.35	0.60
1:X:244:GLU:OE2	1:X:449:PHE:HB2	2.01	0.60
1:X:322:GLU:O	1:X:326:ILE:HD13	2.02	0.60
1:X:432:TRP:CZ2	1:X:610:LYS:CD	2.85	0.60
1:X:139:MET:O	1:X:143:PHE:CD2	2.54	0.60
1:X:165:SER:HA	2:X:2067:HOH:O	2.01	0.60
1:X:238:ARG:NH2	1:X:267:ARG:CZ	2.65	0.60
1:X:278:TYR:O	1:X:281:PHE:HB2	2.02	0.60
1:X:581:ILE:HG22	1:X:581:ILE:O	1.97	0.60
1:X:107:ARG:O	1:X:111:ASN:N	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:346:LYS:HD3	2:X:2126:HOH:O	2.02	0.60
1:X:219:ASN:N	1:X:220:PRO:HD2	2.17	0.60
1:X:324:PHE:HE2	1:X:328:ARG:NH1	2.00	0.60
1:X:597:GLU:HB3	1:X:601:LYS:HD2	1.83	0.60
1:X:661:LYS:O	1:X:662:GLN:HB2	2.02	0.60
1:X:696:ILE:HB	1:X:697:ILE:O	2.02	0.60
1:X:246:GLN:HG2	1:X:255:GLY:CA	2.32	0.60
1:X:105:ASN:O	1:X:109:ARG:CG	2.50	0.59
1:X:698:TYR:HE2	1:X:720:GLN:NE2	1.98	0.59
1:X:366:GLY:HA2	1:X:408:HIS:CE1	2.37	0.59
1:X:392:ALA:CB	1:X:596:LEU:HD23	2.31	0.59
1:X:7:ARG:NE	1:X:18:LYS:HE3	2.17	0.59
1:X:8:THR:O	1:X:9:SER:OG	2.20	0.59
1:X:385:ASN:HB3	1:X:388:VAL:CG2	2.31	0.59
1:X:492:GLU:HA	1:X:495:LEU:HD23	1.84	0.59
1:X:597:GLU:O	1:X:601:LYS:N	2.32	0.59
1:X:636:GLU:HG2	1:X:636:GLU:O	1.99	0.59
1:X:97:LEU:HD11	1:X:686:ARG:HG3	1.85	0.59
1:X:21:ASP:HA	2:X:2012:HOH:O	2.02	0.59
1:X:455:ILE:CG2	1:X:456:SER:N	2.65	0.59
1:X:495:LEU:HA	2:X:2158:HOH:O	2.02	0.59
1:X:680:VAL:O	1:X:684:GLY:CA	2.50	0.59
1:X:708:LEU:HD22	1:X:712:VAL:HG13	1.85	0.59
1:X:289:THR:C	1:X:291:GLU:N	2.55	0.59
1:X:458:PHE:HZ	1:X:479:GLN:OE1	1.85	0.59
1:X:79:GLN:OE1	1:X:96:TYR:HD2	1.85	0.59
1:X:353:HIS:HB3	1:X:378:ALA:HB2	1.85	0.59
1:X:429:LEU:HD23	1:X:430:PHE:N	2.18	0.59
1:X:617:ILE:HG22	1:X:617:ILE:O	2.02	0.59
1:X:481:PHE:HE1	1:X:646:GLU:HA	1.67	0.59
1:X:476:GLU:OE2	1:X:573:TYR:HB2	2.02	0.59
1:X:52:ILE:CG1	1:X:60:PHE:HZ	2.16	0.59
1:X:130:LYS:HG2	1:X:131:ARG:N	2.17	0.59
1:X:147:ARG:O	1:X:150:GLU:HG2	2.03	0.59
1:X:539:THR:HG22	1:X:542:THR:HG23	1.84	0.59
1:X:52:ILE:HG12	1:X:60:PHE:HZ	1.68	0.58
1:X:682:LEU:CG	1:X:683:GLU:H	2.16	0.58
1:X:192:VAL:HG23	1:X:193:ILE:N	2.18	0.58
1:X:397:ARG:HA	1:X:405:VAL:O	2.03	0.58
1:X:210:VAL:HG23	1:X:214:GLN:HG3	1.85	0.58
1:X:37:TYR:HE1	1:X:39:PRO:CA	2.11	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:492:GLU:O	1:X:494:TYR:N	2.36	0.58
1:X:701:PHE:O	1:X:701:PHE:CG	2.54	0.58
1:X:353:HIS:HB2	1:X:378:ALA:HB2	1.85	0.58
1:X:409:LEU:HD22	1:X:413:LYS:HB2	1.85	0.58
1:X:127:ASN:O	1:X:658:PRO:HG3	2.03	0.58
1:X:347:ILE:C	1:X:349:ALA:N	2.56	0.58
1:X:44:ARG:HA	1:X:44:ARG:HH11	1.69	0.58
1:X:210:VAL:CG2	1:X:214:GLN:HG3	2.34	0.58
1:X:680:VAL:HG22	1:X:684:GLY:CA	2.32	0.58
1:X:163:TYR:C	1:X:163:TYR:CD1	2.77	0.58
1:X:233:ASN:OD1	1:X:234:ASN:N	2.34	0.58
1:X:347:ILE:C	1:X:349:ALA:H	2.07	0.58
1:X:477:LYS:C	1:X:480:GLN:HE22	2.06	0.58
1:X:725:ALA:CA	1:X:729:HIS:CD2	2.86	0.58
1:X:754:ILE:HG23	1:X:755:GLU:H	1.68	0.58
1:X:759:GLU:HG2	1:X:759:GLU:OXT	2.03	0.58
1:X:13:LYS:HD3	1:X:18:LYS:HZ2	1.69	0.58
1:X:398:ILE:HD13	1:X:407:GLN:CG	2.33	0.58
1:X:71:GLN:N	1:X:71:GLN:OE1	2.37	0.58
1:X:723:THR:O	1:X:723:THR:OG1	2.15	0.58
1:X:164:ARG:HD3	1:X:167:LEU:HD12	1.84	0.57
1:X:64:THR:CG2	1:X:66:ASP:O	2.40	0.57
1:X:682:LEU:CG	1:X:683:GLU:N	2.66	0.57
1:X:692:PHE:CB	2:X:2226:HOH:O	2.52	0.57
1:X:247:PHE:CD1	1:X:253:ILE:N	2.65	0.57
1:X:29:VAL:HG11	1:X:758:ARG:CD	2.34	0.57
1:X:501:TRP:HB3	2:X:2160:HOH:O	2.03	0.57
1:X:425:LEU:CD2	1:X:612:PHE:HZ	2.17	0.57
1:X:373:THR:HA	1:X:376:ASN:HD22	1.69	0.57
1:X:81:ASN:CB	1:X:82:PRO:HD2	2.31	0.57
1:X:453:LEU:HD12	1:X:454:ASP:N	2.19	0.57
1:X:672:VAL:O	1:X:675:GLN:HG2	2.04	0.57
1:X:685:ILE:CD1	1:X:689:ARG:NH2	2.67	0.57
1:X:309:GLN:HB2	2:X:2107:HOH:O	2.05	0.57
1:X:491:GLN:CA	1:X:491:GLN:OE1	2.52	0.57
1:X:689:ARG:HD2	1:X:695:ARG:NH2	2.20	0.57
1:X:41:PRO:HD3	1:X:70:ARG:HH12	1.70	0.57
1:X:217:GLN:C	1:X:220:PRO:HD2	2.24	0.57
1:X:4:ILE:CG2	1:X:4:ILE:O	2.52	0.57
1:X:484:HIS:NE2	1:X:488:LYS:NZ	2.51	0.57
1:X:99:GLU:HG2	1:X:673:LEU:HD11	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:147:ARG:H	1:X:150:GLU:CD	2.07	0.57
1:X:289:THR:C	1:X:291:GLU:H	2.08	0.57
1:X:527:ALA:O	1:X:531:GLU:CG	2.53	0.57
1:X:282:TYR:CD1	1:X:282:TYR:N	2.72	0.57
1:X:544:ILE:HD11	1:X:548:HIS:NE2	2.20	0.57
1:X:154:HIS:ND1	1:X:156:PHE:HB2	2.20	0.56
1:X:160:ASP:O	1:X:163:TYR:N	2.35	0.56
1:X:733:ASP:HB2	1:X:734:PRO:CD	2.35	0.56
1:X:193:ILE:CG1	1:X:194:GLN:N	2.67	0.56
1:X:245:ILE:HD12	1:X:450:ILE:H	1.70	0.56
1:X:342:MET:O	1:X:345:PHE:HB2	2.05	0.56
1:X:60:PHE:CE2	1:X:62:PHE:CD2	2.92	0.56
1:X:680:VAL:HG22	1:X:680:VAL:O	2.06	0.56
1:X:28:THR:HG22	1:X:29:VAL:H	1.69	0.56
1:X:754:ILE:CG2	1:X:755:GLU:N	2.68	0.56
1:X:362:GLY:N	1:X:366:GLY:O	2.39	0.56
1:X:375:LEU:HD11	1:X:389:LEU:HD23	1.87	0.56
1:X:702:VAL:HG13	1:X:715:ASP:HB2	1.87	0.56
1:X:143:PHE:HD1	2:X:2060:HOH:O	1.88	0.56
1:X:539:THR:O	1:X:541:ASN:CB	2.53	0.56
1:X:626:ASN:CG	1:X:627:PHE:CD2	2.70	0.56
1:X:707:LEU:HD11	2:X:2046:HOH:O	2.05	0.56
1:X:461:PHE:HD1	1:X:462:LYS:N	2.03	0.56
1:X:15:LEU:CD2	1:X:139:MET:SD	2.94	0.56
1:X:577:VAL:HG11	1:X:579:TYR:CZ	2.41	0.56
1:X:61:THR:HG22	1:X:62:PHE:N	2.21	0.56
1:X:736:GLN:CG	1:X:747:ARG:HB2	2.35	0.56
1:X:285:LEU:HD23	1:X:298:LEU:CD2	2.35	0.56
1:X:736:GLN:HG2	1:X:747:ARG:H	1.71	0.56
1:X:4:ILE:HG22	1:X:4:ILE:O	2.04	0.56
1:X:81:ASN:OD1	1:X:96:TYR:HB2	2.06	0.56
1:X:285:LEU:HD23	1:X:298:LEU:HB2	1.88	0.55
1:X:164:ARG:HA	1:X:167:LEU:HD12	1.88	0.55
1:X:225:PHE:CD2	1:X:280:ILE:HG21	2.41	0.55
1:X:642:MET:HA	1:X:645:LEU:HD22	1.88	0.55
1:X:99:GLU:HG2	1:X:673:LEU:CD1	2.35	0.55
1:X:267:ARG:HG2	1:X:267:ARG:O	2.06	0.55
1:X:588:ASN:OD1	2:X:2188:HOH:O	2.18	0.55
1:X:7:ARG:HE	1:X:18:LYS:CB	2.15	0.55
1:X:37:TYR:O	1:X:47:TYR:HB3	2.05	0.55
1:X:745:PHE:HD1	2:X:2224:HOH:O	1.90	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:347:ILE:HG21	1:X:429:LEU:HD12	1.87	0.55
1:X:455:ILE:CG2	1:X:456:SER:H	2.20	0.55
1:X:535:PHE:HB2	1:X:536:PRO:CD	2.37	0.55
1:X:432:TRP:O	1:X:435:LYS:N	2.39	0.55
1:X:37:TYR:C	1:X:47:TYR:HD1	2.09	0.55
1:X:529:LEU:O	1:X:533:SER:OG	2.22	0.55
1:X:693:PRO:HD2	1:X:746:PHE:O	2.07	0.55
1:X:98:ASN:HD21	1:X:100:PRO:CG	2.20	0.55
1:X:219:ASN:N	1:X:220:PRO:CD	2.62	0.55
1:X:399:LEU:HD13	1:X:404:LEU:HB3	1.89	0.55
1:X:402:ARG:HG2	1:X:402:ARG:O	2.06	0.54
1:X:679:ASN:CB	1:X:681:VAL:HG13	2.33	0.54
1:X:230:THR:HG22	1:X:275:GLU:OE1	2.07	0.54
1:X:244:GLU:CG	1:X:451:GLY:CA	2.83	0.54
1:X:527:ALA:O	1:X:531:GLU:HG2	2.07	0.54
1:X:609:THR:CG2	1:X:613:ASN:ND2	2.68	0.54
1:X:638:LEU:O	1:X:641:LEU:HB3	2.08	0.54
1:X:685:ILE:C	1:X:687:ILE:N	2.57	0.54
1:X:242:PHE:HZ	1:X:244:GLU:HG3	1.55	0.54
1:X:390:GLU:HG3	1:X:391:LYS:N	2.21	0.54
1:X:265:LYS:O	1:X:423:LYS:HG2	2.07	0.54
1:X:691:GLY:O	1:X:747:ARG:NH1	2.40	0.54
1:X:712:VAL:N	1:X:713:PRO:HD3	2.21	0.54
1:X:486:MET:CE	1:X:689:ARG:HH11	2.21	0.54
1:X:351:ILE:O	1:X:354:LEU:HB2	2.07	0.54
1:X:461:PHE:CD1	1:X:462:LYS:N	2.75	0.54
1:X:518:ASP:HB2	1:X:635:LYS:HZ1	1.72	0.54
1:X:616:ASN:O	1:X:617:ILE:HD13	2.07	0.54
1:X:7:ARG:CZ	1:X:18:LYS:HE3	2.38	0.54
1:X:398:ILE:CG2	1:X:399:LEU:N	2.70	0.54
1:X:569:GLY:HA3	1:X:578:MET:SD	2.48	0.54
1:X:641:LEU:HG	1:X:645:LEU:HD11	1.88	0.54
1:X:726:VAL:O	1:X:730:LEU:CG	2.48	0.54
1:X:497:GLU:OE2	1:X:744:ILE:HA	2.08	0.54
1:X:163:TYR:CD1	1:X:167:LEU:CD1	2.84	0.54
1:X:529:LEU:HD23	1:X:631:ALA:HB2	1.90	0.54
1:X:110:TYR:CE2	1:X:126:VAL:HG13	2.42	0.54
1:X:210:VAL:HG22	1:X:214:GLN:CD	2.28	0.54
1:X:373:THR:HA	1:X:376:ASN:ND2	2.22	0.54
1:X:357:ILE:H	1:X:418:ARG:HH12	1.56	0.54
1:X:35:ILE:CB	1:X:52:ILE:HD11	2.34	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:61:THR:HG23	1:X:71:GLN:HG3	1.90	0.54
1:X:35:ILE:HD11	1:X:77:ALA:HB1	1.90	0.53
1:X:699:ALA:HB3	1:X:720:GLN:OE1	2.08	0.53
1:X:692:PHE:HE1	1:X:745:PHE:HB2	1.68	0.53
1:X:345:PHE:O	1:X:347:ILE:N	2.41	0.53
1:X:245:ILE:CD1	1:X:450:ILE:HB	2.38	0.53
1:X:56:THR:CB	1:X:59:SER:O	2.45	0.53
1:X:689:ARG:NH1	2:X:2221:HOH:O	2.23	0.53
1:X:692:PHE:HB3	2:X:2226:HOH:O	2.06	0.53
1:X:189:THR:O	1:X:192:VAL:HG22	2.08	0.53
1:X:144:LYS:HE2	1:X:199:VAL:HG12	1.90	0.53
1:X:470:CYS:HB3	1:X:634:TYR:CE2	2.43	0.53
1:X:98:ASN:OD1	1:X:100:PRO:N	2.41	0.53
1:X:238:ARG:HG2	1:X:278:TYR:CE1	2.44	0.53
1:X:326:ILE:HD12	1:X:326:ILE:N	2.23	0.53
1:X:667:LEU:HD23	1:X:667:LEU:C	2.28	0.53
1:X:119:SER:N	1:X:122:PHE:O	2.41	0.53
1:X:212:GLU:O	1:X:216:LEU:CD1	2.57	0.53
1:X:119:SER:HB2	1:X:122:PHE:HB2	1.88	0.53
1:X:424:ALA:O	1:X:428:ARG:CB	2.57	0.53
1:X:582:GLN:HE21	1:X:582:GLN:HA	1.70	0.53
1:X:276:ARG:NH2	1:X:282:TYR:CG	2.77	0.53
1:X:711:ASN:O	1:X:713:PRO:HD3	2.09	0.53
1:X:743:LYS:C	1:X:744:ILE:HG23	2.29	0.53
1:X:398:ILE:HG22	1:X:399:LEU:N	2.24	0.53
1:X:121:LEU:HD11	1:X:482:PHE:CZ	2.44	0.53
1:X:215:ILE:O	1:X:218:ALA:HB3	2.09	0.53
1:X:285:LEU:HD23	1:X:298:LEU:HD13	1.90	0.53
1:X:432:TRP:CH2	1:X:436:LYS:HE2	2.43	0.53
1:X:623:LYS:HG3	1:X:624:GLY:N	2.24	0.53
1:X:626:ASN:OD1	1:X:627:PHE:CB	2.56	0.53
1:X:175:LEU:HD23	1:X:651:HIS:HB2	1.91	0.53
1:X:685:ILE:O	1:X:687:ILE:N	2.42	0.53
1:X:689:ARG:CD	1:X:695:ARG:NE	2.69	0.53
1:X:743:LYS:O	1:X:744:ILE:CG2	2.57	0.53
1:X:289:THR:O	1:X:291:GLU:N	2.42	0.52
1:X:203:ASN:CB	1:X:207:GLY:C	2.77	0.52
1:X:461:PHE:CE1	1:X:462:LYS:HG2	2.44	0.52
1:X:486:MET:CE	1:X:689:ARG:NH1	2.72	0.52
1:X:228:ALA:O	1:X:236:SER:N	2.35	0.52
1:X:31:ASP:OD1	1:X:757:ALA:HA	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:244:GLU:CG	1:X:451:GLY:HA2	2.38	0.52
1:X:667:LEU:HD23	1:X:667:LEU:O	2.09	0.52
1:X:743:LYS:O	1:X:744:ILE:HG23	2.09	0.52
1:X:241:LYS:HE3	1:X:243:ILE:HD11	1.89	0.52
1:X:345:PHE:C	1:X:347:ILE:N	2.63	0.52
1:X:29:VAL:HG12	1:X:758:ARG:HB3	1.77	0.52
1:X:514:ILE:CG2	1:X:518:ASP:OD2	2.58	0.52
1:X:134:ILE:CD1	1:X:154:HIS:HE2	2.23	0.52
1:X:508:LEU:HD13	2:X:2150:HOH:O	2.09	0.52
1:X:542:THR:OG1	1:X:543:LEU:N	2.40	0.52
1:X:129:PHE:CE2	1:X:658:PRO:HG2	2.41	0.52
1:X:89:GLU:H	1:X:89:GLU:CD	2.09	0.52
1:X:63:LYS:HG2	1:X:64:THR:H	1.75	0.52
1:X:82:PRO:O	1:X:84:LYS:N	2.36	0.52
1:X:134:ILE:CG1	1:X:135:TYR:CE1	2.93	0.52
1:X:213:GLN:C	1:X:215:ILE:N	2.62	0.52
1:X:345:PHE:CD1	1:X:345:PHE:N	2.71	0.52
1:X:498:LYS:HA	2:X:2159:HOH:O	2.09	0.52
1:X:570:VAL:CG1	1:X:571:THR:N	2.72	0.52
1:X:119:SER:HB2	1:X:122:PHE:HB3	1.90	0.51
1:X:195:TYR:O	1:X:196:LEU:C	2.47	0.51
1:X:221:ILE:HG22	1:X:222:LEU:N	2.25	0.51
1:X:474:THR:O	1:X:478:LEU:HD12	2.06	0.51
1:X:577:VAL:HG11	1:X:579:TYR:OH	2.10	0.51
1:X:60:PHE:CE2	1:X:62:PHE:HD2	2.29	0.51
1:X:153:PRO:O	1:X:154:HIS:HB2	2.10	0.51
1:X:294:LYS:C	1:X:296:LEU:N	2.63	0.51
1:X:471:ILE:O	1:X:475:ASN:OD1	2.29	0.51
1:X:599:CYS:C	1:X:600:PHE:HD1	2.14	0.51
1:X:530:ASP:OD1	1:X:629:THR:OG1	2.28	0.51
1:X:193:ILE:HG12	1:X:194:GLN:H	1.75	0.51
1:X:428:ARG:HB3	1:X:611:LEU:HD22	1.91	0.51
1:X:298:LEU:HD12	1:X:299:ALA:H	1.67	0.51
1:X:38:ASN:ND2	1:X:43:GLU:O	2.43	0.51
1:X:470:CYS:O	1:X:634:TYR:OH	2.29	0.51
1:X:526:LEU:O	1:X:530:ASP:OD2	2.29	0.51
1:X:193:ILE:CG1	1:X:194:GLN:H	2.24	0.51
1:X:486:MET:HE3	1:X:689:ARG:NH1	2.26	0.51
1:X:708:LEU:HB3	1:X:712:VAL:HG22	1.93	0.51
1:X:727:LEU:HD13	1:X:736:GLN:OE1	2.11	0.51
1:X:742:THR:O	1:X:743:LYS:HD2	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:230:THR:O	1:X:233:ASN:O	2.29	0.51
1:X:699:ALA:O	1:X:719:SER:O	2.28	0.51
1:X:98:ASN:OD1	1:X:99:GLU:CA	2.58	0.51
1:X:267:ARG:CG	1:X:267:ARG:O	2.59	0.51
1:X:468:GLN:O	1:X:472:ASN:ND2	2.44	0.51
1:X:557:LYS:HD2	1:X:571:THR:HB	1.93	0.51
1:X:107:ARG:O	1:X:110:TYR:N	2.39	0.50
1:X:280:ILE:O	1:X:284:LEU:HB2	2.11	0.50
1:X:37:TYR:CE1	1:X:39:PRO:CA	2.91	0.50
1:X:724:ASP:O	2:X:2244:HOH:O	2.20	0.50
1:X:134:ILE:HD12	1:X:154:HIS:HE2	1.76	0.50
1:X:229:LYS:HG3	1:X:234:ASN:HA	1.91	0.50
1:X:485:HIS:ND1	1:X:650:PRO:CG	2.74	0.50
1:X:516:LEU:HD13	1:X:555:ASN:ND2	2.26	0.50
1:X:606:ASN:O	1:X:610:LYS:HB2	2.11	0.50
1:X:741:ILE:HG23	1:X:742:THR:N	2.27	0.50
1:X:203:ASN:ND2	1:X:207:GLY:CA	2.73	0.50
1:X:213:GLN:O	1:X:215:ILE:N	2.44	0.50
1:X:277:ASN:N	1:X:282:TYR:OH	2.43	0.50
1:X:285:LEU:CD2	1:X:298:LEU:HB2	2.41	0.50
1:X:28:THR:CG2	1:X:29:VAL:N	2.73	0.50
1:X:91:MET:SD	1:X:106:LEU:CD1	2.99	0.50
1:X:296:LEU:O	1:X:297:HIS:CG	2.64	0.50
1:X:29:VAL:HG11	1:X:758:ARG:CG	2.40	0.50
1:X:177:ILE:HD12	1:X:189:THR:HG22	1.93	0.50
1:X:298:LEU:HD12	1:X:299:ALA:C	2.31	0.50
1:X:372:LYS:O	1:X:376:ASN:ND2	2.45	0.50
1:X:43:GLU:OE2	1:X:45:ASP:HB2	2.11	0.50
1:X:22:SER:HB3	1:X:26:LYS:HZ3	1.76	0.50
1:X:392:ALA:HA	1:X:595:ASP:OD2	2.11	0.50
1:X:93:GLU:HA	1:X:694:ASN:ND2	2.27	0.50
1:X:228:ALA:HB2	1:X:278:TYR:CD1	2.46	0.50
1:X:453:LEU:HD12	1:X:454:ASP:H	1.75	0.50
1:X:675:GLN:O	1:X:678:CYS:HB3	2.12	0.50
1:X:131:ARG:C	1:X:132:ILE:HD12	2.32	0.49
1:X:293:LYS:HG3	1:X:298:LEU:HG	1.93	0.49
1:X:429:LEU:CD2	1:X:430:PHE:N	2.75	0.49
1:X:617:ILE:CG2	1:X:617:ILE:O	2.60	0.49
1:X:682:LEU:CD1	1:X:683:GLU:HB3	2.41	0.49
1:X:264:GLU:OE1	1:X:267:ARG:NH2	2.45	0.49
1:X:333:ILE:C	1:X:335:GLY:H	2.14	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:386:PRO:C	1:X:388:VAL:H	2.15	0.49
1:X:396:PRO:HA	1:X:595:ASP:OD2	2.12	0.49
1:X:470:CYS:O	1:X:473:TYR:HB3	2.12	0.49
1:X:641:LEU:HG	1:X:645:LEU:CD1	2.41	0.49
1:X:126:VAL:HG13	1:X:126:VAL:O	2.13	0.49
1:X:485:HIS:HE1	1:X:650:PRO:CD	2.05	0.49
1:X:82:PRO:C	1:X:84:LYS:H	2.15	0.49
1:X:336:PHE:HB3	1:X:341:GLN:NE2	2.27	0.49
1:X:706:TYR:O	1:X:706:TYR:CD1	2.65	0.49
1:X:394:MET:C	1:X:396:PRO:HD3	2.32	0.49
1:X:429:LEU:HD21	1:X:433:LEU:HD12	1.95	0.49
1:X:5:HIS:O	1:X:6:ASP:CG	2.50	0.49
1:X:116:TYR:CE2	1:X:154:HIS:CD2	3.00	0.49
1:X:128:PRO:O	1:X:129:PHE:HB2	2.13	0.49
1:X:40:ASP:HB3	1:X:42:LYS:CG	2.43	0.49
1:X:35:ILE:HD12	1:X:78:ASN:O	2.12	0.49
1:X:91:MET:HB3	2:X:2049:HOH:O	2.12	0.49
1:X:15:LEU:O	1:X:114:LEU:HD22	2.13	0.49
1:X:135:TYR:HD2	1:X:191:LYS:NZ	2.10	0.49
1:X:227:ASN:OD1	1:X:237:SER:HA	2.13	0.49
1:X:336:PHE:HB3	1:X:341:GLN:HE21	1.77	0.49
1:X:484:HIS:CD2	1:X:488:LYS:NZ	2.79	0.49
1:X:633:GLN:C	1:X:635:LYS:N	2.66	0.49
1:X:726:VAL:CG2	1:X:730:LEU:HD21	2.29	0.49
1:X:584:TRP:O	1:X:588:ASN:HB2	2.13	0.49
1:X:186:THR:CG2	1:X:187:GLU:N	2.75	0.49
1:X:296:LEU:HA	1:X:297:HIS:CE1	2.48	0.49
1:X:329:GLN:O	1:X:333:ILE:CG1	2.60	0.49
1:X:187:GLU:CA	1:X:190:LYS:HB2	2.42	0.49
1:X:342:MET:C	1:X:342:MET:SD	2.88	0.49
1:X:61:THR:HG22	1:X:62:PHE:H	1.78	0.49
1:X:219:ASN:HB2	1:X:220:PRO:HD3	1.93	0.48
1:X:736:GLN:CG	1:X:750:GLN:HB2	2.43	0.48
1:X:135:TYR:CD2	1:X:191:LYS:NZ	2.80	0.48
1:X:27:LEU:O	1:X:28:THR:OG1	2.19	0.48
1:X:728:LYS:HG3	1:X:737:TYR:HH	1.75	0.48
1:X:481:PHE:O	1:X:485:HIS:HB2	2.13	0.48
1:X:425:LEU:HD21	1:X:612:PHE:HZ	1.77	0.48
1:X:110:TYR:CE2	1:X:126:VAL:CG1	2.96	0.48
1:X:210:VAL:CG2	1:X:214:GLN:CG	2.91	0.48
1:X:353:HIS:HB2	1:X:378:ALA:CB	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:680:VAL:HA	1:X:683:GLU:CD	2.33	0.48
1:X:339:GLU:HB3	2:X:2117:HOH:O	2.13	0.48
1:X:486:MET:HE3	1:X:689:ARG:HH11	1.79	0.48
1:X:501:TRP:O	1:X:502:THR:C	2.49	0.48
1:X:544:ILE:CG1	1:X:548:HIS:CE1	2.97	0.48
1:X:428:ARG:HB3	1:X:611:LEU:CD2	2.43	0.48
1:X:369:LEU:C	1:X:369:LEU:HD12	2.33	0.48
1:X:91:MET:SD	1:X:106:LEU:HD13	2.54	0.48
1:X:134:ILE:HG13	1:X:135:TYR:CE1	2.49	0.48
1:X:229:LYS:HD3	1:X:276:ARG:CD	2.42	0.48
1:X:270:PHE:C	1:X:271:GLN:NE2	2.67	0.48
1:X:294:LYS:CB	1:X:294:LYS:NZ	2.76	0.48
1:X:329:GLN:O	1:X:333:ILE:HG13	2.14	0.48
1:X:449:PHE:CZ	1:X:648:THR:HG21	2.49	0.48
1:X:568:PHE:O	1:X:578:MET:SD	2.71	0.48
1:X:701:PHE:HD1	1:X:705:TYR:CZ	2.32	0.48
1:X:87:GLY:CA	1:X:109:ARG:CD	2.84	0.48
1:X:298:LEU:CD1	1:X:299:ALA:N	2.59	0.48
1:X:332:ASP:CB	1:X:336:PHE:O	2.61	0.48
1:X:353:HIS:HD2	1:X:378:ALA:HA	1.78	0.48
1:X:35:ILE:CD1	1:X:77:ALA:HB1	2.44	0.48
1:X:367:ALA:N	1:X:408:HIS:HE1	2.12	0.48
1:X:428:ARG:O	1:X:429:LEU:C	2.49	0.48
1:X:590:ASP:N	1:X:591:PRO:CD	2.77	0.48
1:X:620:ARG:NH2	1:X:630:VAL:CG1	2.77	0.48
1:X:682:LEU:HD12	1:X:682:LEU:C	2.23	0.48
1:X:243:ILE:HG12	1:X:258:ILE:CG2	2.44	0.47
1:X:623:LYS:HB3	1:X:628:ILE:HG23	1.95	0.47
1:X:667:LEU:CD2	1:X:667:LEU:O	2.62	0.47
1:X:675:GLN:O	1:X:676:LEU:C	2.51	0.47
1:X:347:ILE:HA	1:X:382:PHE:CE1	2.43	0.47
1:X:492:GLU:C	1:X:494:TYR:N	2.66	0.47
1:X:73:LYS:O	1:X:75:ASP:N	2.47	0.47
1:X:117:THR:HG22	1:X:118:TYR:N	2.29	0.47
1:X:135:TYR:N	1:X:139:MET:HG3	2.29	0.47
1:X:210:VAL:O	1:X:213:GLN:N	2.31	0.47
1:X:539:THR:O	1:X:540:ASP:C	2.43	0.47
1:X:546:LYS:O	1:X:549:SER:HB2	2.15	0.47
1:X:327:THR:OG1	1:X:328:ARG:N	2.46	0.47
1:X:398:ILE:CG2	1:X:399:LEU:H	2.27	0.47
1:X:495:LEU:HB3	2:X:2155:HOH:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:22:SER:CB	1:X:26:LYS:HZ3	2.28	0.47
1:X:271:GLN:HG2	1:X:276:ARG:O	2.15	0.47
1:X:343:SER:HA	1:X:346:LYS:CB	2.42	0.47
1:X:390:GLU:O	1:X:393:LEU:HB2	2.14	0.47
1:X:674:ASP:OD2	2:X:2215:HOH:O	2.20	0.47
1:X:682:LEU:HG	1:X:683:GLU:H	1.80	0.47
1:X:245:ILE:HD11	1:X:450:ILE:CB	2.44	0.47
1:X:267:ARG:HB3	1:X:278:TYR:CE2	2.50	0.47
1:X:365:GLU:OE1	1:X:366:GLY:N	2.47	0.47
1:X:629:THR:CB	2:X:2188:HOH:O	2.62	0.47
1:X:726:VAL:HG23	1:X:730:LEU:CG	2.43	0.47
1:X:28:THR:CG2	1:X:29:VAL:H	2.26	0.47
1:X:465:SER:OG	1:X:467:GLU:OE1	2.32	0.47
1:X:641:LEU:CD2	1:X:645:LEU:HD11	2.44	0.47
1:X:701:PHE:CE2	1:X:722:ALA:HB3	2.50	0.47
1:X:154:HIS:CE1	1:X:156:PHE:CD1	3.02	0.47
1:X:285:LEU:HD23	1:X:298:LEU:CG	2.45	0.47
1:X:532:GLN:C	1:X:534:VAL:N	2.66	0.47
1:X:614:ASP:OD1	1:X:615:PRO:N	2.44	0.47
1:X:642:MET:O	1:X:645:LEU:HB2	2.15	0.47
1:X:689:ARG:HD2	1:X:695:ARG:HH21	1.78	0.47
1:X:71:GLN:HB2	2:X:2038:HOH:O	2.15	0.47
1:X:544:ILE:HG13	1:X:548:HIS:CE1	2.50	0.47
1:X:567:GLU:HB3	1:X:580:GLU:HA	1.97	0.47
1:X:620:ARG:NH2	1:X:630:VAL:HG13	2.30	0.47
1:X:140:VAL:HG23	1:X:141:ASP:N	2.29	0.47
1:X:243:ILE:CG2	1:X:258:ILE:HG13	2.29	0.47
1:X:28:THR:O	1:X:29:VAL:HG23	2.15	0.47
1:X:306:TYR:O	1:X:307:LEU:HD23	2.14	0.47
1:X:322:GLU:C	1:X:324:PHE:N	2.67	0.47
1:X:367:ALA:HB1	1:X:411:VAL:CG2	2.45	0.47
1:X:473:TYR:O	1:X:477:LYS:HB2	2.15	0.47
1:X:514:ILE:HG23	1:X:518:ASP:OD2	2.15	0.47
1:X:323:GLU:O	1:X:326:ILE:HB	2.15	0.46
1:X:366:GLY:CA	1:X:408:HIS:CE1	2.97	0.46
1:X:419:ASP:O	1:X:423:LYS:HE2	2.14	0.46
1:X:121:LEU:CD2	1:X:486:MET:SD	2.98	0.46
1:X:623:LYS:HB3	1:X:628:ILE:CG2	2.45	0.46
1:X:730:LEU:HD12	1:X:730:LEU:O	2.15	0.46
1:X:122:PHE:CE1	1:X:654:ARG:HG2	2.50	0.46
1:X:300:GLY:CA	1:X:303:SER:HB3	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:385:ASN:OD1	1:X:388:VAL:HG23	2.15	0.46
1:X:390:GLU:CG	1:X:391:LYS:N	2.78	0.46
1:X:508:LEU:CD1	2:X:2150:HOH:O	2.63	0.46
1:X:572:HIS:CD2	1:X:577:VAL:CG2	2.89	0.46
1:X:675:GLN:C	1:X:678:CYS:H	2.18	0.46
1:X:82:PRO:C	1:X:84:LYS:N	2.66	0.46
1:X:288:ALA:HB1	1:X:292:GLU:HG2	1.97	0.46
1:X:351:ILE:HG22	1:X:352:LEU:N	2.29	0.46
1:X:608:VAL:HG13	1:X:612:PHE:HE2	1.81	0.46
1:X:629:THR:HB	2:X:2188:HOH:O	2.14	0.46
1:X:134:ILE:HG13	1:X:135:TYR:HD1	1.80	0.46
1:X:14:TYR:CZ	2:X:2008:HOH:O	2.56	0.46
1:X:177:ILE:O	1:X:178:THR:HG23	2.15	0.46
1:X:224:ALA:C	1:X:280:ILE:HG23	2.35	0.46
1:X:294:LYS:CD	1:X:297:HIS:HA	2.35	0.46
1:X:371:ASP:OD1	1:X:372:LYS:N	2.42	0.46
1:X:391:LYS:HD3	1:X:391:LYS:HA	1.70	0.46
1:X:52:ILE:HA	1:X:62:PHE:HB3	1.96	0.46
1:X:432:TRP:HA	1:X:435:LYS:HB3	1.97	0.46
1:X:485:HIS:CD2	2:X:2153:HOH:O	2.68	0.46
1:X:707:LEU:O	1:X:708:LEU:C	2.53	0.46
1:X:244:GLU:OE2	1:X:449:PHE:CD1	2.69	0.46
1:X:532:GLN:HE22	1:X:543:LEU:CB	2.26	0.46
1:X:588:ASN:ND2	1:X:630:VAL:HG23	2.31	0.46
1:X:703:LYS:HG3	1:X:714:ARG:NH2	2.30	0.46
1:X:721:LYS:HD3	2:X:2243:HOH:O	2.15	0.46
1:X:38:ASN:N	1:X:47:TYR:HD1	2.14	0.46
1:X:474:THR:C	1:X:478:LEU:HD13	2.34	0.46
1:X:173:GLN:NE2	1:X:649:ASN:HB3	2.31	0.46
1:X:186:THR:HG23	1:X:187:GLU:N	2.31	0.46
1:X:294:LYS:HA	1:X:297:HIS:H	1.80	0.46
1:X:327:THR:O	1:X:331:MET:HG3	2.15	0.46
1:X:418:ARG:O	1:X:422:VAL:HG23	2.16	0.46
1:X:593:GLN:OE1	1:X:593:GLN:CA	2.64	0.46
1:X:624:GLY:O	1:X:625:ALA:CB	2.63	0.46
1:X:685:ILE:O	1:X:686:ARG:C	2.54	0.46
1:X:230:THR:CB	1:X:275:GLU:OE2	2.60	0.46
1:X:324:PHE:HE2	1:X:328:ARG:CZ	2.29	0.46
1:X:284:LEU:HD22	1:X:348:ILE:CG2	2.46	0.46
1:X:461:PHE:CD1	1:X:463:VAL:HG13	2.51	0.46
1:X:52:ILE:HG13	1:X:60:PHE:CZ	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:63:LYS:HG2	1:X:64:THR:N	2.30	0.46
1:X:12:HIS:HA	1:X:16:LYS:HB3	1.98	0.46
1:X:296:LEU:HD12	1:X:296:LEU:C	2.36	0.46
1:X:476:GLU:OE2	1:X:573:TYR:N	2.49	0.46
1:X:682:LEU:HD11	1:X:683:GLU:HB3	1.97	0.46
1:X:116:TYR:CD2	1:X:154:HIS:CD2	3.03	0.45
1:X:149:ASN:ND2	1:X:697:ILE:HD11	2.31	0.45
1:X:166:MET:O	1:X:170:ARG:HD3	2.16	0.45
1:X:213:GLN:O	1:X:216:LEU:N	2.49	0.45
1:X:343:SER:O	1:X:347:ILE:N	2.48	0.45
1:X:508:LEU:HD23	2:X:2161:HOH:O	2.14	0.45
1:X:596:LEU:O	1:X:599:CYS:N	2.44	0.45
1:X:98:ASN:CG	1:X:99:GLU:N	2.62	0.45
1:X:243:ILE:HG12	1:X:258:ILE:HG23	1.98	0.45
1:X:44:ARG:NH1	1:X:47:TYR:OH	2.49	0.45
1:X:682:LEU:HD12	1:X:683:GLU:CB	2.46	0.45
1:X:698:TYR:CE1	2:X:2227:HOH:O	2.60	0.45
1:X:187:GLU:O	1:X:190:LYS:HB2	2.17	0.45
1:X:21:ASP:HB3	2:X:2003:HOH:O	2.15	0.45
1:X:380:THR:O	1:X:380:THR:CG2	2.63	0.45
1:X:215:ILE:CG1	1:X:441:LEU:HD22	2.43	0.45
1:X:446:LYS:NZ	2:X:2143:HOH:O	2.48	0.45
1:X:473:TYR:OH	1:X:477:LYS:NZ	2.43	0.45
1:X:496:LYS:HB2	2:X:2248:HOH:O	2.17	0.45
1:X:52:ILE:CG2	1:X:53:VAL:N	2.79	0.45
1:X:692:PHE:HB2	2:X:2226:HOH:O	2.14	0.45
1:X:226:GLY:HA3	1:X:239:PHE:CE1	2.52	0.45
1:X:570:VAL:HG12	1:X:571:THR:N	2.31	0.45
1:X:588:ASN:HD22	1:X:630:VAL:CG2	2.30	0.45
1:X:126:VAL:CG2	1:X:656:ILE:O	2.62	0.45
1:X:177:ILE:HD12	1:X:189:THR:CG2	2.46	0.45
1:X:324:PHE:CE2	1:X:328:ARG:CZ	2.99	0.45
1:X:346:LYS:HB3	2:X:2126:HOH:O	2.15	0.45
1:X:357:ILE:H	1:X:418:ARG:NH1	2.14	0.45
1:X:410:ASN:N	1:X:410:ASN:OD1	2.50	0.45
1:X:588:ASN:HD22	1:X:630:VAL:HG23	1.82	0.45
1:X:449:PHE:HZ	1:X:648:THR:HG21	1.81	0.45
1:X:594:GLN:NE2	2:X:2190:HOH:O	2.49	0.45
1:X:54:SER:OG	1:X:61:THR:HB	2.16	0.45
1:X:108:VAL:C	1:X:110:TYR:H	2.20	0.45
1:X:12:HIS:O	1:X:16:LYS:O	2.35	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:179:GLY:O	1:X:180:GLU:C	2.55	0.45
1:X:429:LEU:HD21	1:X:433:LEU:CD1	2.46	0.45
1:X:285:LEU:HD23	1:X:298:LEU:CB	2.46	0.45
1:X:458:PHE:CE1	1:X:475:ASN:CB	2.88	0.45
1:X:477:LYS:CD	1:X:638:LEU:HD21	2.43	0.45
1:X:706:TYR:O	1:X:706:TYR:HD1	2.00	0.45
1:X:12:HIS:ND1	1:X:18:LYS:HA	2.31	0.45
1:X:423:LYS:HE3	1:X:423:LYS:HB2	1.78	0.45
1:X:12:HIS:CB	1:X:18:LYS:HG2	2.43	0.45
1:X:409:LEU:HD23	1:X:409:LEU:HA	1.79	0.45
1:X:34:TYR:HD1	1:X:51:GLU:HG2	1.82	0.45
1:X:529:LEU:HD21	1:X:588:ASN:ND2	2.32	0.45
1:X:730:LEU:O	1:X:731:ASN:HB2	2.17	0.45
1:X:83:ILE:HG22	1:X:83:ILE:O	2.17	0.45
1:X:257:SER:HA	1:X:438:ASN:ND2	2.32	0.44
1:X:276:ARG:NH2	1:X:282:TYR:CD1	2.85	0.44
1:X:238:ARG:HG2	1:X:278:TYR:CZ	2.52	0.44
1:X:347:ILE:O	1:X:349:ALA:N	2.50	0.44
1:X:354:LEU:HD12	1:X:422:VAL:HG22	1.99	0.44
1:X:597:GLU:HB3	1:X:601:LYS:CG	2.47	0.44
1:X:620:ARG:HH22	1:X:630:VAL:CG1	2.28	0.44
1:X:219:ASN:HA	1:X:222:LEU:CG	2.45	0.44
1:X:283:GLN:HB3	1:X:320:ASP:OD1	2.16	0.44
1:X:285:LEU:CD2	1:X:298:LEU:HD22	2.43	0.44
1:X:345:PHE:C	1:X:347:ILE:H	2.21	0.44
1:X:367:ALA:HB1	1:X:411:VAL:HG22	1.99	0.44
1:X:461:PHE:CD1	1:X:462:LYS:HG2	2.53	0.44
1:X:121:LEU:CD1	1:X:482:PHE:CE2	2.87	0.44
1:X:192:VAL:HG23	1:X:193:ILE:H	1.81	0.44
1:X:552:SER:O	1:X:553:LYS:CB	2.61	0.44
1:X:712:VAL:O	1:X:712:VAL:CG2	2.64	0.44
1:X:8:THR:HA	1:X:13:LYS:NZ	2.32	0.44
1:X:116:TYR:CD2	1:X:154:HIS:HA	2.53	0.44
1:X:155:ILE:CG2	1:X:156:PHE:HD1	2.27	0.44
1:X:335:GLY:HA2	2:X:2115:HOH:O	2.17	0.44
1:X:731:ASN:OD1	1:X:754:ILE:HB	2.17	0.44
1:X:292:GLU:HA	1:X:295:ALA:CB	2.48	0.44
1:X:360:GLU:HB2	1:X:370:LYS:HE2	2.00	0.44
1:X:368:VAL:HA	1:X:394:MET:SD	2.58	0.44
1:X:561:PRO:HG2	1:X:564:SER:O	2.17	0.44
1:X:139:MET:HG2	2:X:2058:HOH:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:567:GLU:CB	1:X:580:GLU:HA	2.47	0.44
1:X:123:LEU:HD23	1:X:653:VAL:HG13	1.99	0.44
1:X:163:TYR:CE1	1:X:167:LEU:CG	2.99	0.44
1:X:44:ARG:NH1	2:X:2025:HOH:O	2.50	0.44
1:X:49:CYS:SG	1:X:80:ARG:CD	3.06	0.44
1:X:555:ASN:O	2:X:2175:HOH:O	2.21	0.44
1:X:745:PHE:CD1	2:X:2224:HOH:O	2.57	0.44
1:X:685:ILE:HG22	1:X:689:ARG:CZ	2.14	0.44
1:X:134:ILE:CG1	1:X:135:TYR:CD1	3.00	0.43
1:X:272:SER:O	1:X:275:GLU:HB2	2.18	0.43
1:X:135:TYR:HD2	2:X:2073:HOH:O	2.01	0.43
1:X:265:LYS:O	1:X:268:VAL:HG12	2.18	0.43
1:X:366:GLY:HA2	1:X:408:HIS:ND1	2.33	0.43
1:X:659:ASN:ND2	1:X:663:LEU:O	2.48	0.43
1:X:725:ALA:CB	1:X:729:HIS:HD2	2.17	0.43
1:X:16:LYS:CD	1:X:152:ALA:HB2	2.39	0.43
1:X:492:GLU:C	1:X:494:TYR:H	2.20	0.43
1:X:33:ARG:CD	1:X:52:ILE:CB	2.91	0.43
1:X:577:VAL:CG1	1:X:579:TYR:CZ	3.00	0.43
1:X:129:PHE:CB	1:X:664:PRO:HB3	2.43	0.43
1:X:694:ASN:OD1	1:X:694:ASN:O	2.36	0.43
1:X:256:ALA:HB3	1:X:441:LEU:HB3	2.01	0.43
1:X:375:LEU:HA	1:X:378:ALA:HB3	2.00	0.43
1:X:245:ILE:O	1:X:449:PHE:HA	2.18	0.43
1:X:529:LEU:HG	1:X:588:ASN:OD1	2.18	0.43
1:X:577:VAL:HB	1:X:579:TYR:CE1	2.53	0.43
1:X:641:LEU:CD2	1:X:645:LEU:CD1	2.96	0.43
1:X:11:TYR:CE2	1:X:16:LYS:CB	2.93	0.43
1:X:134:ILE:C	1:X:139:MET:HG3	2.39	0.43
1:X:193:ILE:HD11	2:X:2080:HOH:O	2.18	0.43
1:X:294:LYS:HZ1	1:X:297:HIS:CD2	2.37	0.43
1:X:300:GLY:HA3	1:X:303:SER:HB3	2.01	0.43
1:X:37:TYR:C	1:X:37:TYR:CD1	2.92	0.43
1:X:132:ILE:CD1	1:X:132:ILE:N	2.75	0.43
1:X:262:LEU:HD11	1:X:634:TYR:CE2	2.54	0.43
1:X:532:GLN:HE22	1:X:543:LEU:CA	2.32	0.43
1:X:732:ILE:HG13	1:X:733:ASP:N	2.33	0.43
1:X:326:ILE:CD1	1:X:326:ILE:N	2.81	0.43
1:X:426:TYR:O	1:X:427:GLY:C	2.57	0.43
1:X:56:THR:HG22	1:X:58:ASP:OD1	2.15	0.43
1:X:389:LEU:HD11	1:X:600:PHE:HZ	1.79	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:4:ILE:HD13	1:X:142:ILE:HA	2.00	0.43
1:X:193:ILE:HG13	1:X:194:GLN:N	2.32	0.43
1:X:259:GLN:HB2	2:X:2090:HOH:O	2.18	0.43
1:X:305:ASN:C	1:X:307:LEU:H	2.21	0.43
1:X:481:PHE:O	1:X:485:HIS:CB	2.67	0.43
1:X:49:CYS:SG	1:X:80:ARG:HD3	2.59	0.43
1:X:508:LEU:C	1:X:510:SER:H	2.22	0.43
1:X:393:LEU:CD1	1:X:596:LEU:CD2	2.95	0.43
1:X:682:LEU:C	2:X:2217:HOH:O	2.38	0.43
1:X:230:THR:HG21	1:X:267:ARG:NH2	2.33	0.43
1:X:633:GLN:C	1:X:635:LYS:H	2.21	0.43
1:X:675:GLN:O	1:X:678:CYS:CB	2.67	0.43
1:X:679:ASN:HB2	1:X:681:VAL:CG1	2.39	0.43
1:X:155:ILE:O	1:X:159:SER:HB3	2.19	0.42
1:X:672:VAL:HA	1:X:675:GLN:HE21	1.83	0.42
1:X:689:ARG:HE	1:X:695:ARG:NH1	2.09	0.42
1:X:28:THR:O	1:X:29:VAL:CG2	2.67	0.42
1:X:340:GLU:HG3	1:X:341:GLN:N	2.33	0.42
1:X:353:HIS:CD2	1:X:378:ALA:HA	2.54	0.42
1:X:485:HIS:CE1	1:X:650:PRO:HG2	2.53	0.42
1:X:620:ARG:O	1:X:621:ALA:C	2.58	0.42
1:X:357:ILE:O	1:X:418:ARG:NH1	2.52	0.42
1:X:389:LEU:CD1	1:X:600:PHE:CE1	2.98	0.42
1:X:455:ILE:HG22	1:X:456:SER:H	1.79	0.42
1:X:474:THR:HG22	1:X:478:LEU:HD11	2.00	0.42
1:X:532:GLN:NE2	1:X:543:LEU:HB2	2.29	0.42
1:X:597:GLU:O	1:X:600:PHE:N	2.51	0.42
1:X:640:SER:O	1:X:643:ALA:HB3	2.19	0.42
1:X:661:LYS:HB3	1:X:663:LEU:HG	2.01	0.42
1:X:36:TRP:HB2	1:X:78:ASN:O	2.19	0.42
1:X:679:ASN:C	1:X:681:VAL:H	2.21	0.42
1:X:222:LEU:O	1:X:226:GLY:CA	2.68	0.42
1:X:40:ASP:C	1:X:42:LYS:H	2.23	0.42
1:X:437:ILE:HG13	1:X:438:ASN:N	2.35	0.42
1:X:710:PRO:O	1:X:711:ASN:CB	2.54	0.42
1:X:708:LEU:HB3	1:X:712:VAL:CG2	2.49	0.42
1:X:9:SER:O	1:X:13:LYS:HG2	2.20	0.42
1:X:300:GLY:C	1:X:303:SER:HB3	2.39	0.42
1:X:423:LYS:O	1:X:427:GLY:N	2.51	0.42
1:X:97:LEU:HD12	1:X:97:LEU:C	2.40	0.42
1:X:107:ARG:O	1:X:110:TYR:HB3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:137:GLN:HE21	1:X:140:VAL:CG2	2.31	0.42
1:X:360:GLU:O	1:X:361:LYS:C	2.58	0.42
1:X:245:ILE:CD1	1:X:450:ILE:O	2.67	0.42
1:X:728:LYS:HA	1:X:734:PRO:CD	2.43	0.42
1:X:381:VAL:HG23	1:X:382:PHE:N	2.34	0.42
1:X:389:LEU:HD13	1:X:600:PHE:HE1	1.84	0.42
1:X:375:LEU:CD1	1:X:389:LEU:HD23	2.50	0.42
1:X:730:LEU:CD1	1:X:730:LEU:C	2.88	0.42
1:X:322:GLU:C	1:X:324:PHE:H	2.23	0.42
1:X:598:LEU:HA	1:X:598:LEU:HD23	1.76	0.42
1:X:701:PHE:HE2	1:X:722:ALA:HB3	1.85	0.42
1:X:726:VAL:HG22	1:X:730:LEU:HD11	2.01	0.42
1:X:698:TYR:HE1	1:X:744:ILE:O	2.01	0.42
1:X:180:GLU:O	1:X:181:SER:C	2.57	0.42
1:X:269:VAL:HA	1:X:306:TYR:CE1	2.55	0.42
1:X:544:ILE:CD1	1:X:548:HIS:CE1	3.02	0.42
1:X:735:GLU:O	1:X:736:GLN:C	2.57	0.42
1:X:36:TRP:N	1:X:78:ASN:O	2.50	0.42
1:X:220:PRO:O	1:X:224:ALA:HB2	2.20	0.41
1:X:362:GLY:H	1:X:367:ALA:HA	1.84	0.41
1:X:487:PHE:C	1:X:489:LEU:N	2.73	0.41
1:X:22:SER:HB3	1:X:26:LYS:CE	2.49	0.41
1:X:429:LEU:HD23	1:X:429:LEU:C	2.41	0.41
1:X:597:GLU:HB3	1:X:601:LYS:CD	2.49	0.41
1:X:619:SER:OG	1:X:620:ARG:N	2.54	0.41
1:X:664:PRO:O	1:X:665:ALA:HB2	2.16	0.41
1:X:73:LYS:C	1:X:75:ASP:N	2.74	0.41
1:X:361:LYS:HD3	1:X:361:LYS:HA	1.85	0.41
1:X:210:VAL:HG13	1:X:211:LEU:HG	2.02	0.41
1:X:261:TYR:N	1:X:261:TYR:CD1	2.87	0.41
1:X:292:GLU:HA	1:X:295:ALA:HB2	2.02	0.41
1:X:334:VAL:O	1:X:334:VAL:HG13	2.20	0.41
1:X:464:ASN:HA	1:X:468:GLN:NE2	2.35	0.41
1:X:501:TRP:O	1:X:503:PHE:N	2.52	0.41
1:X:604:SER:O	1:X:605:ASP:HB2	2.16	0.41
1:X:673:LEU:HA	1:X:676:LEU:HG	2.01	0.41
1:X:78:ASN:CA	1:X:98:ASN:ND2	2.56	0.41
1:X:452:VAL:O	1:X:452:VAL:HG23	2.19	0.41
1:X:526:LEU:HD22	1:X:631:ALA:CB	2.29	0.41
1:X:219:ASN:O	1:X:222:LEU:N	2.53	0.41
1:X:273:GLU:OE2	2:X:2095:HOH:O	2.22	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:411:VAL:O	1:X:413:LYS:N	2.53	0.41
1:X:439:ASN:OD1	1:X:439:ASN:C	2.59	0.41
1:X:243:ILE:O	1:X:452:VAL:HG22	2.20	0.41
1:X:498:LYS:O	1:X:500:ASN:OD1	2.38	0.41
1:X:504:ILE:CD1	1:X:505:ASP:N	2.78	0.41
1:X:508:LEU:HB3	1:X:511:GLN:H	1.86	0.41
1:X:622:LYS:O	1:X:622:LYS:HG2	2.21	0.41
1:X:754:ILE:CG2	1:X:755:GLU:H	2.33	0.41
1:X:110:TYR:CD2	1:X:126:VAL:HG11	2.56	0.41
1:X:210:VAL:HG22	1:X:214:GLN:CG	2.51	0.41
1:X:626:ASN:ND2	1:X:627:PHE:HD2	2.18	0.41
1:X:121:LEU:CD1	1:X:652:PHE:CD2	2.99	0.41
1:X:685:ILE:HG13	1:X:686:ARG:H	1.84	0.41
1:X:110:TYR:OH	1:X:128:PRO:HA	2.20	0.41
1:X:108:VAL:C	1:X:110:TYR:N	2.74	0.41
1:X:209:GLY:O	1:X:210:VAL:C	2.60	0.41
1:X:35:ILE:HD12	1:X:79:GLN:HA	2.03	0.41
1:X:127:ASN:OD1	1:X:127:ASN:C	2.59	0.41
1:X:134:ILE:HD12	1:X:154:HIS:NE2	2.36	0.41
1:X:147:ARG:HG2	1:X:150:GLU:OE2	2.21	0.41
1:X:178:THR:HA	1:X:455:ILE:O	2.21	0.41
1:X:192:VAL:CG2	1:X:193:ILE:N	2.84	0.41
1:X:305:ASN:HB3	1:X:309:GLN:HE21	1.86	0.41
1:X:365:GLU:O	1:X:366:GLY:O	2.39	0.41
1:X:588:ASN:ND2	2:X:2188:HOH:O	2.54	0.41
1:X:633:GLN:O	1:X:635:LYS:N	2.53	0.41
1:X:174:SER:HG	1:X:650:PRO:HA	1.85	0.41
1:X:671:VAL:O	1:X:674:ASP:HB3	2.19	0.41
1:X:98:ASN:ND2	1:X:100:PRO:CG	2.83	0.41
1:X:103:PHE:CE2	1:X:669:ASP:HB3	2.56	0.41
1:X:163:TYR:O	1:X:167:LEU:HG	2.21	0.41
1:X:265:LYS:O	1:X:423:LYS:CG	2.69	0.41
1:X:588:ASN:ND2	1:X:630:VAL:CG2	2.83	0.41
1:X:103:PHE:CZ	1:X:669:ASP:HB3	2.56	0.41
1:X:320:ASP:O	1:X:321:SER:C	2.58	0.40
1:X:329:GLN:O	1:X:333:ILE:HG12	2.22	0.40
1:X:93:GLU:CA	1:X:694:ASN:ND2	2.84	0.40
1:X:91:MET:CB	2:X:2049:HOH:O	2.69	0.40
1:X:212:GLU:O	1:X:216:LEU:HD13	2.21	0.40
1:X:685:ILE:HA	1:X:688:THR:OG1	2.21	0.40
1:X:248:ASN:HD21	1:X:252:PHE:HB2	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:685:ILE:CG2	1:X:689:ARG:HH22	2.08	0.40
1:X:146:ARG:HA	1:X:146:ARG:HD2	1.96	0.40
1:X:155:ILE:O	1:X:159:SER:CB	2.69	0.40
1:X:163:TYR:HE1	1:X:167:LEU:HD11	0.70	0.40
1:X:221:ILE:O	1:X:225:PHE:HD1	2.05	0.40
1:X:294:LYS:HA	1:X:294:LYS:HD2	1.91	0.40
1:X:280:ILE:CD1	1:X:348:ILE:HD12	2.51	0.40
1:X:610:LYS:HE3	1:X:610:LYS:HB2	1.86	0.40
1:X:736:GLN:O	1:X:747:ARG:CB	2.68	0.40
1:X:337:SER:HB3	1:X:340:GLU:CG	2.36	0.40
1:X:37:TYR:CD1	1:X:38:ASN:N	2.89	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:X:22:SER:OG	1:X:541:ASN:ND2[3_655]	2.04	0.16
1:X:403:ASP:OD1	1:X:405:VAL:CA[2_556]	2.04	0.16
1:X:445:ARG:NH1	1:X:582:GLN:OE1[1_455]	2.10	0.10
1:X:29:VAL:CG2	1:X:537:ASN:OD1[3_655]	2.18	0.02

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	X	756/758 (100%)	579 (77%)	143 (19%)	34 (4%)	2 16

All (34) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	X	6	ASP
1	X	8	THR

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Mol	Chain	Res	Type
1	X	32	LYS
1	X	210	VAL
1	X	540	ASP
1	X	605	ASP
1	X	665	ALA
1	X	693	PRO
1	X	698	TYR
1	X	709	ALA
1	X	711	ASN
1	X	722	ALA
1	X	732	ILE
1	X	214	GLN
1	X	346	LYS
1	X	74	LYS
1	X	378	ALA
1	X	695	ARG
1	X	303	SER
1	X	493	GLU
1	X	674	ASP
1	X	686	ARG
1	X	468	GLN
1	X	536	PRO
1	X	625	ALA
1	X	731	ASN
1	X	396	PRO
1	X	672	VAL
1	X	219	ASN
1	X	335	GLY
1	X	650	PRO
1	X	134	ILE
1	X	366	GLY
1	X	713	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	X	663/663 (100%)	643 (97%)	20 (3%)	41	68

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	X	10	ASP
1	X	12	HIS
1	X	14	TYR
1	X	34	TYR
1	X	37	TYR
1	X	89	GLU
1	X	122	PHE
1	X	147	ARG
1	X	232	ARG
1	X	261	TYR
1	X	273	GLU
1	X	297	HIS
1	X	306	TYR
1	X	336	PHE
1	X	492	GLU
1	X	535	PHE
1	X	636	GLU
1	X	652	PHE
1	X	721	LYS
1	X	731	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	X	111	ASN
1	X	137	GLN
1	X	149	ASN
1	X	172	ASN
1	X	203	ASN
1	X	234	ASN
1	X	271	GLN
1	X	305	ASN
1	X	308	ASN
1	X	309	GLN
1	X	341	GLN
1	X	353	HIS
1	X	376	ASN

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Mol	Chain	Res	Type
1	X	408	HIS
1	X	438	ASN
1	X	475	ASN
1	X	485	HIS
1	X	537	ASN
1	X	548	HIS
1	X	576	GLN
1	X	582	GLN
1	X	588	ASN
1	X	613	ASN
1	X	637	GLN
1	X	651	HIS
1	X	694	ASN
1	X	711	ASN
1	X	729	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no 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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	X	758/758 (100%)	-0.11	21 (2%) 53 51	0, 7, 48, 80	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	X	206	ASN	5.5
1	X	24	LEU	4.3
1	X	207	GLY	3.9
1	X	722	ALA	3.7
1	X	732	ILE	3.7
1	X	693	PRO	3.5
1	X	4	ILE	3.2
1	X	710	PRO	3.0
1	X	20	GLY	2.9
1	X	707	LEU	2.9
1	X	706	TYR	2.8
1	X	752	ALA	2.4
1	X	505	ASP	2.4
1	X	22	SER	2.3
1	X	749	GLY	2.2
1	X	709	ALA	2.2
1	X	19	GLN	2.1
1	X	29	VAL	2.0
1	X	205	ALA	2.0
1	X	697	ILE	2.0
1	X	208	SER	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.