



Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 05:47 pm BST

PDB ID : 3TON
Title : Crystal Structure of the C-terminal Subunit of Human Maltase-Glucoamylase
Authors : Shen, Y.; Qin, X.H.; Ren, L.M.
Deposited on : 2011-09-06
Resolution : 2.95 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

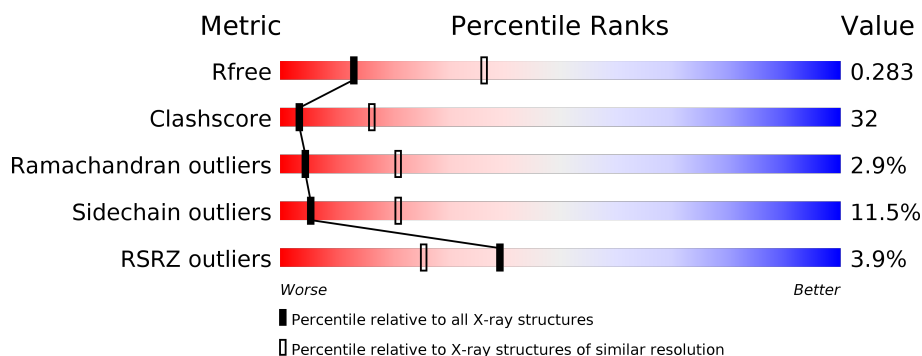
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.95 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	3104 (3.00-2.92)
Clashscore	141614	3462 (3.00-2.92)
Ramachandran outliers	138981	3340 (3.00-2.92)
Sidechain outliers	138945	3343 (3.00-2.92)
RSRZ outliers	127900	2986 (3.00-2.92)

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	908	<div> <div>2%</div> <div>48%</div> <div>42%</div> <div>8%</div> <div>.</div> </div>
1	B	908	<div> <div>6%</div> <div>48%</div> <div>42%</div> <div>8%</div> <div>.</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 14270 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 Maltase-glucoamylase, intestinal.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	890	Total	C	N	O	S	0	0	0
			7125	4569	1187	1338	31			
1	B	890	Total	C	N	O	S	0	0	0
			7125	4569	1187	1338	31			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	952	TRP	-	EXPRESSION TAG	UNP O43451
A	953	SER	-	EXPRESSION TAG	UNP O43451
A	954	HIS	-	EXPRESSION TAG	UNP O43451
A	955	PRO	-	EXPRESSION TAG	UNP O43451
A	956	GLN	-	EXPRESSION TAG	UNP O43451
A	957	PHE	-	EXPRESSION TAG	UNP O43451
A	958	GLU	-	EXPRESSION TAG	UNP O43451
A	959	LYS	-	EXPRESSION TAG	UNP O43451
A	1854	HIS	-	EXPRESSION TAG	UNP O43451
A	1855	HIS	-	EXPRESSION TAG	UNP O43451
A	1856	HIS	-	EXPRESSION TAG	UNP O43451
A	1857	HIS	-	EXPRESSION TAG	UNP O43451
A	1858	HIS	-	EXPRESSION TAG	UNP O43451
A	1859	HIS	-	EXPRESSION TAG	UNP O43451
B	952	TRP	-	EXPRESSION TAG	UNP O43451
B	953	SER	-	EXPRESSION TAG	UNP O43451
B	954	HIS	-	EXPRESSION TAG	UNP O43451
B	955	PRO	-	EXPRESSION TAG	UNP O43451
B	956	GLN	-	EXPRESSION TAG	UNP O43451
B	957	PHE	-	EXPRESSION TAG	UNP O43451
B	958	GLU	-	EXPRESSION TAG	UNP O43451
B	959	LYS	-	EXPRESSION TAG	UNP O43451
B	1854	HIS	-	EXPRESSION TAG	UNP O43451
B	1855	HIS	-	EXPRESSION TAG	UNP O43451
B	1856	HIS	-	EXPRESSION TAG	UNP O43451

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1857	HIS	-	EXPRESSION TAG	UNP O43451
B	1858	HIS	-	EXPRESSION TAG	UNP O43451
B	1859	HIS	-	EXPRESSION TAG	UNP O43451

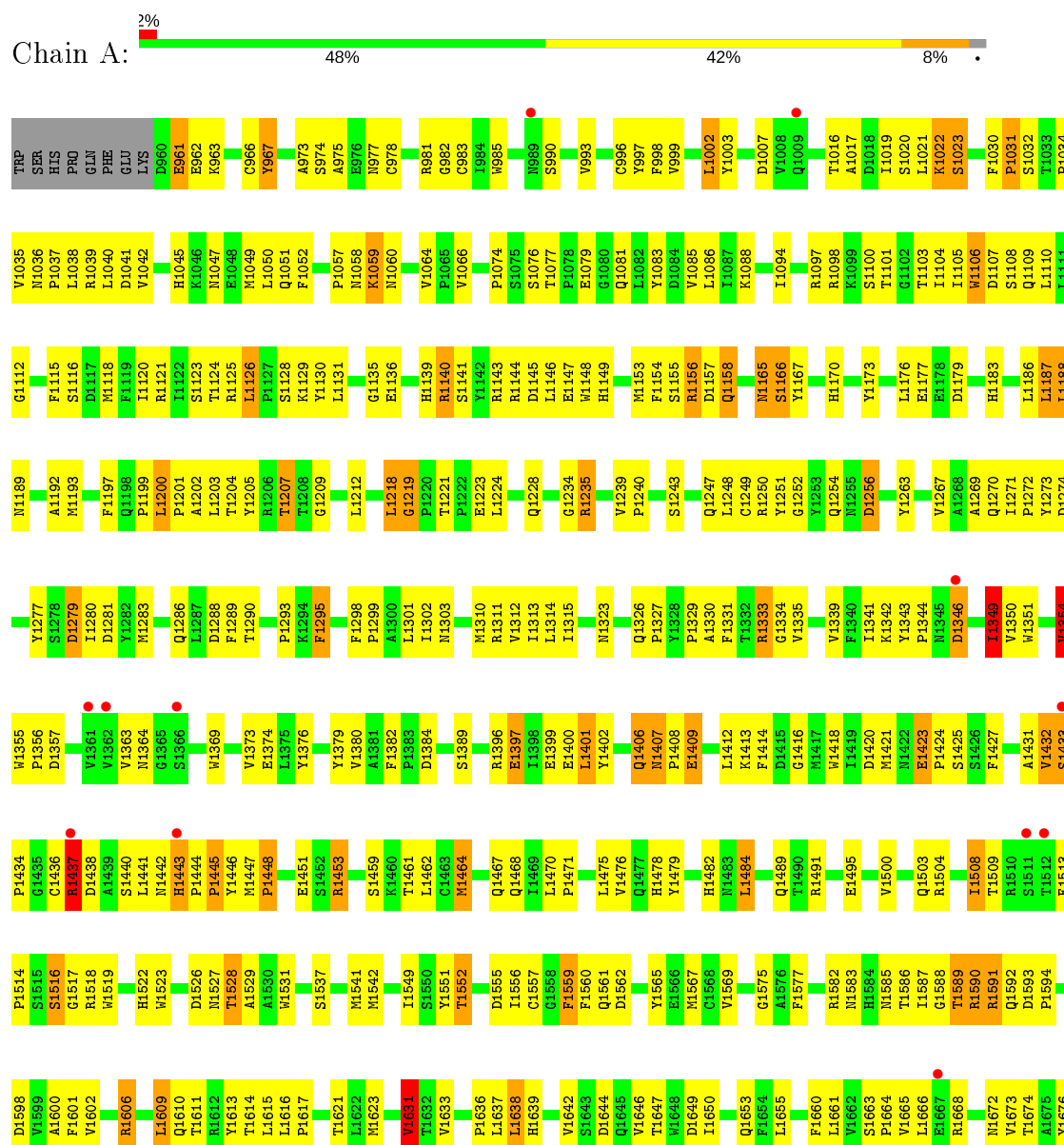
- Molecule 2 is water.

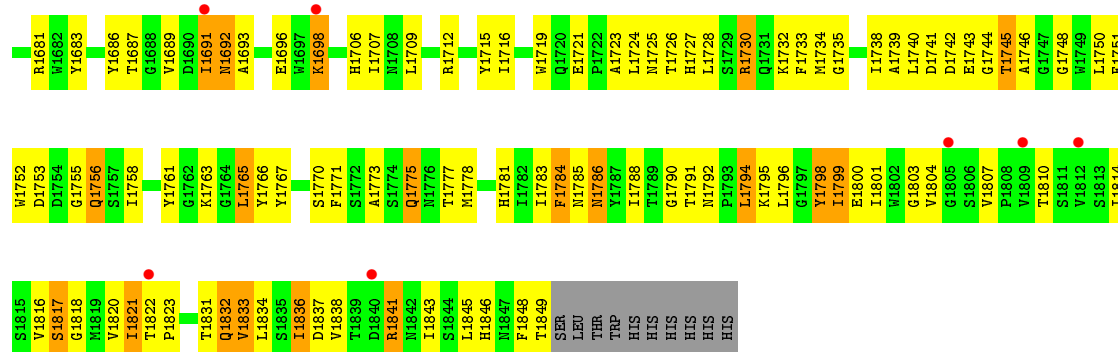
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	11	Total O 11 11	0	0
2	B	9	Total O 9 9	0	0

3 Residue-property plots

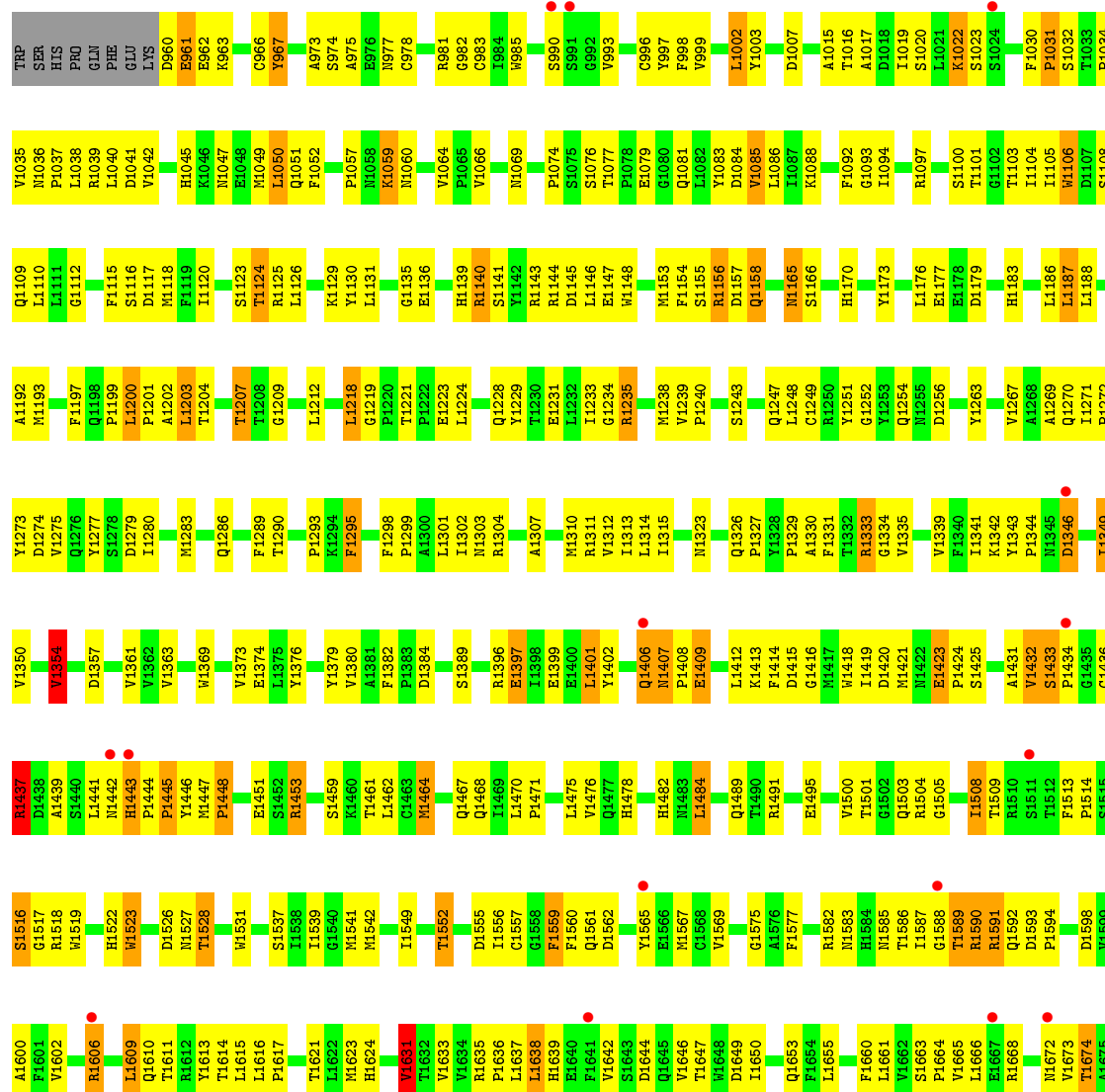
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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.

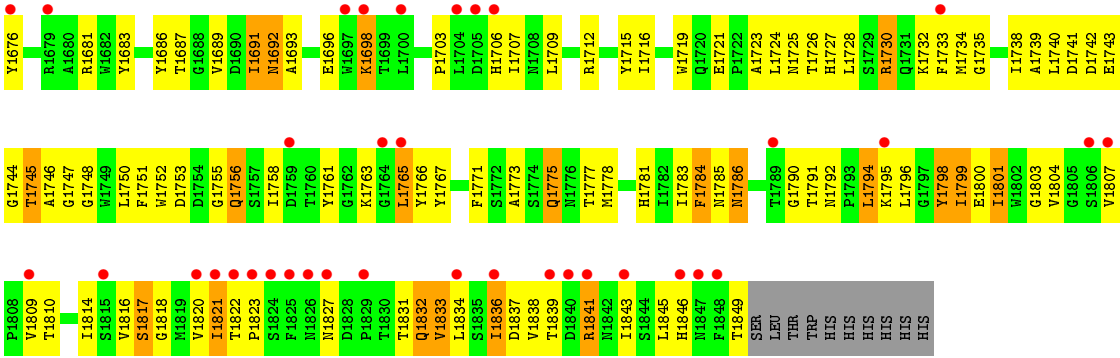
• Molecule 1: Maltase-glucoamylase, intestinal





• Molecule 1: Maltase-glucoamylase, intestinal





4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	106.23Å 106.23Å 517.56Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.17 – 2.95 37.17 – 2.95	Depositor EDS
% Data completeness (in resolution range)	73.5 (37.17-2.95) 78.5 (37.17-2.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.22 (at 2.95Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.4_486)	Depositor
R, R_{free}	0.232 , 0.288 0.227 , 0.283	Depositor DCC
R_{free} test set	2507 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	49.6	Xtriage
Anisotropy	0.693	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 35.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	14270	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.43% 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	A	0.48	5/7344 (0.1%)	0.64	1/10024 (0.0%)
1	B	0.48	4/7344 (0.1%)	0.64	1/10024 (0.0%)
All	All	0.48	9/14688 (0.1%)	0.64	2/20048 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
All	All	0	2

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1696	GLU	CD-OE2	6.73	1.33	1.25
1	B	1696	GLU	CD-OE1	6.41	1.32	1.25
1	A	1696	GLU	CD-OE1	5.66	1.31	1.25
1	A	1696	GLU	CG-CD	5.57	1.60	1.51
1	B	1696	GLU	CD-OE2	5.42	1.31	1.25
1	A	1698	LYS	CD-CE	5.40	1.64	1.51
1	B	1698	LYS	CD-CE	5.30	1.64	1.51
1	B	1696	GLU	CG-CD	5.11	1.59	1.51
1	A	1698	LYS	CE-NZ	5.03	1.61	1.49

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1219	GLY	N-CA-C	-5.50	99.35	113.10
1	B	1050	LEU	CB-CG-CD2	-5.29	102.01	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1431	ALA	Peptide
1	B	1431	ALA	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	A	7125	0	6755	454	0
1	B	7125	0	6755	448	0
2	A	11	0	0	0	0
2	B	9	0	0	0	0
All	All	14270	0	13510	898	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 32.

All (898) 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:A:1050:LEU:HD21	1:A:1083:TYR:CE1	1.99	0.97
1:A:1256:ASP:HB2	1:A:1295:PHE:HA	1.48	0.95
1:B:1256:ASP:HB2	1:B:1295:PHE:HA	1.48	0.94
1:B:1219:GLY:H	1:B:1228:GLN:HE22	1.07	0.94
1:B:1542:MET:HE3	1:B:1636:PRO:HB3	1.51	0.91
1:A:1219:GLY:H	1:A:1228:GLN:HE22	1.06	0.91
1:B:1235:ARG:HG2	1:B:1235:ARG:HH11	1.36	0.91
1:A:1734:MET:HE3	1:A:1794:LEU:HD21	1.54	0.90
1:B:1050:LEU:HD21	1:B:1083:TYR:CE1	2.06	0.90
1:B:1263:TYR:HE1	1:B:1310:MET:HG3	1.35	0.90
1:B:1765:LEU:HD23	1:B:1765:LEU:H	1.36	0.89
1:A:1765:LEU:HD23	1:A:1765:LEU:H	1.35	0.89
1:A:1468:GLN:HE21	1:A:1478:HIS:HD2	1.15	0.89
1:A:1235:ARG:HG2	1:A:1235:ARG:HH11	1.37	0.89
1:A:1468:GLN:NE2	1:A:1478:HIS:HD2	1.71	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1441:LEU:HD12	1:B:1464:MET:HB2	1.55	0.87
1:B:1047:ASN:HD21	1:B:1077:THR:H	1.20	0.87
1:B:1165:ASN:HD22	1:B:1165:ASN:H	1.21	0.86
1:A:1542:MET:HE3	1:A:1636:PRO:HB3	1.56	0.86
1:B:1035:VAL:HG23	1:B:1038:LEU:HD21	1.58	0.86
1:A:1047:ASN:HD21	1:A:1077:THR:H	1.20	0.86
1:B:1468:GLN:NE2	1:B:1478:HIS:HD2	1.74	0.85
1:A:1165:ASN:H	1:A:1165:ASN:HD22	1.24	0.85
1:B:1542:MET:CE	1:B:1636:PRO:HB3	2.06	0.84
1:B:1468:GLN:HE21	1:B:1478:HIS:HD2	1.21	0.84
1:B:961:GLU:HB3	1:B:1200:LEU:HB3	1.60	0.84
1:A:1123:SER:OG	1:A:1204:THR:HG23	1.77	0.83
1:B:1716:ILE:HD11	1:B:1771:PHE:CB	2.08	0.83
1:B:1734:MET:HE3	1:B:1794:LEU:HD21	1.58	0.83
1:A:1542:MET:CE	1:A:1636:PRO:HB3	2.07	0.83
1:A:1263:TYR:HE1	1:A:1310:MET:HG3	1.41	0.83
1:A:1687:THR:OG1	1:A:1689:VAL:HG12	1.79	0.83
1:A:1035:VAL:HG23	1:A:1038:LEU:HD21	1.58	0.82
1:A:1441:LEU:HD12	1:A:1464:MET:HB2	1.61	0.82
1:B:1441:LEU:CD1	1:B:1464:MET:H	1.93	0.82
1:A:961:GLU:HB3	1:A:1200:LEU:HB3	1.62	0.82
1:B:1687:THR:OG1	1:B:1689:VAL:HG12	1.79	0.82
1:A:1665:VAL:HG22	1:A:1673:VAL:HG11	1.62	0.81
1:A:1503:GLN:HE22	1:A:1756:GLN:CD	1.84	0.81
1:B:1156:ARG:HH11	1:B:1158:GLN:HG2	1.44	0.81
1:B:1784:PHE:HE2	1:B:1786:ASN:HB2	1.46	0.81
1:B:1503:GLN:HE22	1:B:1756:GLN:CD	1.85	0.80
1:A:1716:ILE:HD11	1:A:1771:PHE:CB	2.12	0.80
1:A:1156:ARG:HH11	1:A:1158:GLN:HG2	1.45	0.80
1:A:1653:GLN:HE22	1:A:1676:TYR:H	1.28	0.80
1:A:1798:TYR:N	1:A:1798:TYR:CD2	2.47	0.80
1:A:1636:PRO:HG2	1:A:1639:HIS:CD2	2.16	0.80
1:B:1156:ARG:HD3	1:B:1158:GLN:HG2	1.63	0.80
1:A:1441:LEU:CD1	1:A:1464:MET:H	1.95	0.79
1:A:1784:PHE:HE2	1:A:1786:ASN:HB2	1.46	0.79
1:A:1154:PHE:HZ	1:A:1464:MET:CE	1.97	0.78
1:B:1154:PHE:HZ	1:B:1464:MET:CE	1.96	0.78
1:B:1342:LYS:HB3	1:B:1349:ILE:HA	1.66	0.78
1:B:1653:GLN:HE22	1:B:1676:TYR:H	1.31	0.78
1:B:1665:VAL:HG22	1:B:1673:VAL:HG11	1.65	0.78
1:B:1617:PRO:O	1:B:1621:THR:HG23	1.83	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1326:GLN:HB3	1:B:1327:PRO:HD2	1.66	0.78
1:B:1399:GLU:HA	1:B:1500:VAL:HG21	1.66	0.77
1:B:1270:GLN:HA	1:B:1724:LEU:HD21	1.67	0.77
1:A:1329:PRO:O	1:A:1333:ARG:HG3	1.85	0.77
1:B:1423:GLU:N	1:B:1424:PRO:HA	1.99	0.76
1:A:1156:ARG:HD3	1:A:1158:GLN:HG2	1.67	0.76
1:B:1165:ASN:HD21	1:B:1451:GLU:H	1.32	0.76
1:B:1746:ALA:HB3	1:B:1773:ALA:HB3	1.68	0.76
1:A:1342:LYS:HB3	1:A:1349:ILE:HA	1.68	0.76
1:A:1165:ASN:HD21	1:A:1451:GLU:H	1.31	0.75
1:B:1716:ILE:HD11	1:B:1771:PHE:HB3	1.69	0.75
1:A:1270:GLN:HA	1:A:1724:LEU:HD21	1.67	0.75
1:B:1123:SER:OG	1:B:1204:THR:HG23	1.85	0.75
1:A:1343:TYR:HB3	1:A:1344:PRO:HD2	1.69	0.74
1:B:1798:TYR:CD2	1:B:1798:TYR:N	2.51	0.74
1:A:1399:GLU:HA	1:A:1500:VAL:HG21	1.69	0.74
1:B:1636:PRO:HG2	1:B:1639:HIS:CD2	2.22	0.74
1:B:1692:ASN:C	1:B:1698:LYS:HZ1	1.90	0.74
1:A:1614:THR:HG23	1:A:1719:TRP:HE3	1.53	0.73
1:B:1156:ARG:NH1	1:B:1158:GLN:HE21	1.86	0.73
1:B:1716:ILE:HD11	1:B:1771:PHE:HB2	1.70	0.73
1:A:1617:PRO:O	1:A:1621:THR:HG23	1.88	0.73
1:A:1156:ARG:NH1	1:A:1158:GLN:HE21	1.87	0.73
1:A:1746:ALA:HB3	1:A:1773:ALA:HB3	1.70	0.73
1:B:1606:ARG:O	1:B:1610:GLN:HG3	1.88	0.73
1:A:1235:ARG:HG2	1:A:1235:ARG:NH1	2.03	0.73
1:B:1614:THR:HG23	1:B:1719:TRP:HE3	1.51	0.72
1:B:967:TYR:CD1	1:B:973:ALA:HA	2.24	0.72
1:A:1606:ARG:O	1:A:1610:GLN:HG3	1.90	0.72
1:A:1050:LEU:HD21	1:A:1083:TYR:CZ	2.24	0.72
1:A:1326:GLN:HB3	1:A:1327:PRO:HD2	1.69	0.72
1:A:1716:ILE:HD11	1:A:1771:PHE:HB3	1.72	0.71
1:A:967:TYR:CD1	1:A:973:ALA:HA	2.24	0.71
1:A:1406:GLN:O	1:A:1408:PRO:HD3	1.90	0.71
1:A:1406:GLN:HE21	1:A:1406:GLN:HA	1.56	0.71
1:A:1379:TYR:CE1	1:A:1432:VAL:HG11	2.26	0.70
1:B:1263:TYR:CE1	1:B:1310:MET:HG3	2.23	0.70
1:A:1606:ARG:HH11	1:A:1606:ARG:CB	2.05	0.70
1:B:1716:ILE:HG22	1:B:1738:ILE:HA	1.74	0.70
1:B:1730:ARG:HH12	1:B:1755:GLY:HA3	1.55	0.70
1:B:1235:ARG:NH1	1:B:1235:ARG:HG2	2.04	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1406:GLN:O	1:B:1408:PRO:HD3	1.91	0.70
1:B:1219:GLY:N	1:B:1228:GLN:HE22	1.88	0.70
1:B:1517:GLY:HA3	1:B:1549:ILE:HG12	1.75	0.69
1:B:1433:SER:HB3	1:B:1434:PRO:CD	2.23	0.68
1:A:1433:SER:HB3	1:A:1434:PRO:CD	2.23	0.68
1:A:1513:PHE:H	1:A:1516:SER:HB2	1.58	0.68
1:B:1406:GLN:HE21	1:B:1406:GLN:HA	1.56	0.68
1:B:1165:ASN:ND2	1:B:1165:ASN:H	1.91	0.68
1:A:1526:ASP:HB3	1:A:1560:PHE:CE2	2.29	0.68
1:B:1526:ASP:HB3	1:B:1560:PHE:CE2	2.28	0.68
1:A:1606:ARG:HH11	1:A:1606:ARG:HB3	1.57	0.68
1:B:1606:ARG:HH11	1:B:1606:ARG:HB3	1.58	0.68
1:A:1459:SER:O	1:A:1461:THR:HG22	1.93	0.68
1:A:1263:TYR:CE1	1:A:1310:MET:HG3	2.28	0.67
1:A:1517:GLY:HA3	1:A:1549:ILE:HG12	1.75	0.67
1:A:1436:CYS:O	1:A:1437:ARG:HD3	1.93	0.67
1:A:1716:ILE:HD11	1:A:1771:PHE:HB2	1.73	0.67
1:A:1219:GLY:N	1:A:1228:GLN:HE22	1.87	0.67
1:A:1647:THR:HA	1:A:1650:ILE:HG22	1.76	0.67
1:A:1623:MET:HE2	1:A:1633:VAL:HG11	1.77	0.66
1:B:1252:GLY:HA3	1:B:1587:ILE:HD12	1.77	0.66
1:B:1765:LEU:H	1:B:1765:LEU:CD2	2.08	0.66
1:B:1329:PRO:O	1:B:1333:ARG:HG3	1.95	0.66
1:B:961:GLU:HG2	1:B:1200:LEU:H	1.61	0.66
1:A:1252:GLY:HA3	1:A:1587:ILE:HD12	1.77	0.66
1:B:1638:LEU:C	1:B:1638:LEU:HD12	2.16	0.66
1:B:1234:GLY:HA3	1:B:1518:ARG:HD3	1.77	0.66
1:B:1379:TYR:CE1	1:B:1432:VAL:HG11	2.30	0.66
1:B:1110:LEU:HD11	1:B:1125:ARG:HG2	1.78	0.66
1:A:1104:ILE:O	1:A:1104:ILE:HG13	1.96	0.65
1:A:1513:PHE:O	1:A:1516:SER:HB2	1.96	0.65
1:A:1423:GLU:N	1:A:1424:PRO:HA	2.10	0.65
1:A:1838:VAL:HG12	1:A:1838:VAL:O	1.95	0.65
1:B:1590:ARG:HD3	1:B:1591:ARG:O	1.96	0.65
1:B:1436:CYS:O	1:B:1437:ARG:HD3	1.95	0.65
1:A:1716:ILE:HG22	1:A:1738:ILE:HA	1.78	0.65
1:B:1050:LEU:HD21	1:B:1083:TYR:CZ	2.31	0.65
1:B:1614:THR:HG23	1:B:1719:TRP:CE3	2.31	0.65
1:A:1565:TYR:O	1:A:1569:VAL:HG23	1.96	0.65
1:B:1120:ILE:HB	1:B:1207:THR:HG22	1.78	0.65
1:A:1234:GLY:HA3	1:A:1518:ARG:HD3	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1513:PHE:H	1:B:1516:SER:HB2	1.63	0.64
1:B:1513:PHE:O	1:B:1516:SER:HB2	1.96	0.64
1:B:1838:VAL:O	1:B:1838:VAL:HG12	1.96	0.64
1:B:1606:ARG:HH11	1:B:1606:ARG:CB	2.10	0.64
1:A:1730:ARG:HH12	1:A:1755:GLY:HA3	1.62	0.64
1:B:1146:LEU:HA	1:B:1197:PHE:HB3	1.80	0.64
1:B:1083:TYR:HB3	1:B:1218:LEU:HD21	1.79	0.64
1:B:1343:TYR:HB3	1:B:1344:PRO:HD2	1.78	0.64
1:A:961:GLU:HG2	1:A:1200:LEU:H	1.63	0.64
1:B:1831:THR:O	1:B:1833:VAL:N	2.31	0.63
1:A:1590:ARG:HD3	1:A:1591:ARG:O	1.97	0.63
1:A:1816:VAL:HG22	1:A:1820:VAL:HG22	1.79	0.63
1:B:1750:LEU:HD23	1:B:1767:TYR:HE2	1.64	0.63
1:B:1758:ILE:N	1:B:1758:ILE:HD12	2.12	0.63
1:A:1120:ILE:HB	1:A:1207:THR:HG22	1.79	0.63
1:B:1623:MET:CE	1:B:1633:VAL:HG11	2.29	0.63
1:A:1249:CYS:HB2	1:A:1277:TYR:HB2	1.80	0.63
1:A:1803:GLY:H	1:A:1832:GLN:HB2	1.62	0.63
1:B:1040:LEU:HD12	1:B:1041:ASP:N	2.13	0.63
1:B:1803:GLY:H	1:B:1832:GLN:HB2	1.63	0.63
1:B:1647:THR:HA	1:B:1650:ILE:HG22	1.80	0.63
1:A:1807:VAL:O	1:A:1807:VAL:HG23	1.98	0.62
1:A:1681:ARG:HH11	1:A:1742:ASP:H	1.45	0.62
1:A:974:SER:OG	1:A:977:ASN:HB2	2.00	0.62
1:B:1354:VAL:HG23	1:B:1380:VAL:HG21	1.82	0.62
1:B:1565:TYR:O	1:B:1569:VAL:HG23	1.98	0.62
1:A:1614:THR:HG23	1:A:1719:TRP:CE3	2.34	0.62
1:B:1816:VAL:HG22	1:B:1820:VAL:HG22	1.80	0.62
1:A:1831:THR:O	1:A:1833:VAL:N	2.33	0.62
1:B:1503:GLN:HE22	1:B:1756:GLN:NE2	1.97	0.62
1:A:1468:GLN:HE21	1:A:1478:HIS:CD2	2.06	0.62
1:B:1723:ALA:HB1	1:B:1728:LEU:HB2	1.82	0.62
1:B:963:LYS:HE2	1:B:997:TYR:CE2	2.34	0.62
1:A:1271:ILE:HD11	1:A:1602:VAL:HG13	1.80	0.62
1:B:1459:SER:O	1:B:1461:THR:HG22	2.00	0.62
1:B:1740:LEU:HA	1:B:1745:THR:O	1.98	0.62
1:B:1800:GLU:O	1:B:1801:ILE:HG13	2.00	0.62
1:A:1165:ASN:ND2	1:A:1165:ASN:H	1.94	0.61
1:A:961:GLU:C	1:A:963:LYS:H	2.02	0.61
1:B:1444:PRO:O	1:B:1446:TYR:N	2.33	0.61
1:A:1740:LEU:HA	1:A:1745:THR:O	1.99	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1750:LEU:HD23	1:A:1767:TYR:HE2	1.64	0.61
1:A:1146:LEU:HA	1:A:1197:PHE:HB3	1.81	0.61
1:A:1289:PHE:CZ	1:A:1397:GLU:HB3	2.35	0.61
1:B:1047:ASN:ND2	1:B:1076:SER:HA	2.15	0.61
1:A:1040:LEU:HD12	1:A:1041:ASP:N	2.16	0.61
1:A:1606:ARG:HB3	1:A:1606:ARG:NH1	2.16	0.61
1:A:1283:MET:HA	1:A:1290:THR:O	2.01	0.61
1:B:1153:MET:HE3	1:B:1193:MET:SD	2.41	0.60
1:A:1513:PHE:CD2	1:A:1514:PRO:HD2	2.36	0.60
1:B:1200:LEU:HD12	1:B:1201:PRO:HD2	1.83	0.60
1:A:1047:ASN:ND2	1:A:1076:SER:HA	2.16	0.60
1:A:1765:LEU:CD2	1:A:1765:LEU:H	2.09	0.60
1:B:1156:ARG:HD3	1:B:1158:GLN:CG	2.29	0.60
1:B:1733:PHE:CD1	1:B:1795:LYS:HB3	2.36	0.60
1:A:1692:ASN:C	1:A:1698:LYS:HZ1	2.05	0.60
1:A:1758:ILE:N	1:A:1758:ILE:HD12	2.17	0.60
1:A:1816:VAL:HG12	1:A:1817:SER:N	2.17	0.60
1:A:1002:LEU:HD23	1:A:1002:LEU:N	2.17	0.59
1:A:1251:TYR:CD1	1:A:1587:ILE:HB	2.37	0.59
1:A:1468:GLN:NE2	1:A:1478:HIS:CD2	2.62	0.59
1:B:1513:PHE:CD2	1:B:1514:PRO:HD2	2.37	0.59
1:A:1638:LEU:HD12	1:A:1638:LEU:C	2.23	0.59
1:A:1733:PHE:CD1	1:A:1795:LYS:HB3	2.37	0.59
1:A:1834:LEU:O	1:A:1834:LEU:HG	2.02	0.59
1:B:961:GLU:CB	1:B:1200:LEU:HB3	2.32	0.59
1:B:1681:ARG:HH11	1:B:1742:ASP:H	1.49	0.59
1:B:1686:TYR:CE2	1:B:1706:HIS:CE1	2.91	0.59
1:B:961:GLU:C	1:B:963:LYS:H	2.04	0.59
1:A:1665:VAL:HG22	1:A:1673:VAL:CG1	2.32	0.59
1:A:1354:VAL:HG23	1:A:1380:VAL:HG21	1.83	0.59
1:A:1673:VAL:HG23	1:A:1673:VAL:O	2.02	0.59
1:B:1035:VAL:CG2	1:B:1038:LEU:HD21	2.32	0.59
1:A:1207:THR:HG23	1:A:1209:GLY:H	1.68	0.59
1:A:1503:GLN:HE22	1:A:1756:GLN:NE2	2.00	0.59
1:B:1002:LEU:N	1:B:1002:LEU:HD23	2.17	0.59
1:A:1047:ASN:HD21	1:A:1077:THR:N	1.96	0.58
1:B:1726:THR:O	1:B:1730:ARG:CG	2.51	0.58
1:A:1526:ASP:HB3	1:A:1560:PHE:HE2	1.68	0.58
1:B:1271:ILE:HD11	1:B:1602:VAL:HG13	1.85	0.58
1:A:1730:ARG:HB3	1:A:1752:TRP:HH2	1.66	0.58
1:B:1302:ILE:HD12	1:B:1312:VAL:HG21	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1407:ASN:HB3	1:B:1409:GLU:OE2	2.03	0.58
1:A:1003:TYR:HD2	1:A:1019:ILE:HG22	1.68	0.58
1:A:1140:ARG:HG3	1:A:1144:ARG:NH2	2.17	0.58
1:A:1200:LEU:HD12	1:A:1201:PRO:HD2	1.85	0.58
1:A:963:LYS:HE2	1:A:997:TYR:CE2	2.39	0.58
1:B:1691:ILE:HD11	1:B:1698:LYS:HD2	1.86	0.58
1:B:1726:THR:O	1:B:1730:ARG:HG3	2.03	0.58
1:B:1059:LYS:HD3	1:B:1060:ASN:H	1.68	0.58
1:A:1050:LEU:CD2	1:A:1083:TYR:CZ	2.87	0.58
1:A:1118:MET:HE1	1:A:1445:PRO:HD2	1.86	0.58
1:A:1531:TRP:CH2	1:A:1567:MET:HA	2.39	0.58
1:B:1283:MET:HA	1:B:1290:THR:O	2.04	0.58
1:B:1606:ARG:HB3	1:B:1606:ARG:NH1	2.19	0.58
1:A:1686:TYR:CE2	1:A:1706:HIS:CE1	2.91	0.58
1:A:1156:ARG:HD3	1:A:1158:GLN:CG	2.34	0.57
1:B:1623:MET:HE2	1:B:1633:VAL:HG11	1.84	0.57
1:A:1342:LYS:HA	1:A:1350:VAL:HG23	1.87	0.57
1:A:967:TYR:HD1	1:A:973:ALA:HA	1.69	0.57
1:B:1047:ASN:HD21	1:B:1077:THR:N	1.96	0.57
1:A:1444:PRO:O	1:A:1446:TYR:N	2.38	0.57
1:B:1526:ASP:HB3	1:B:1560:PHE:HE2	1.68	0.57
1:B:1784:PHE:CD2	1:B:1784:PHE:C	2.76	0.57
1:B:1104:ILE:HG13	1:B:1104:ILE:O	2.04	0.57
1:B:967:TYR:HD1	1:B:973:ALA:HA	1.70	0.57
1:B:1531:TRP:CH2	1:B:1567:MET:HA	2.39	0.57
1:B:1784:PHE:C	1:B:1784:PHE:HD2	2.07	0.57
1:B:1798:TYR:HD2	1:B:1798:TYR:N	2.02	0.57
1:A:1726:THR:O	1:A:1730:ARG:HG3	2.04	0.57
1:A:1816:VAL:CG1	1:A:1817:SER:N	2.67	0.57
1:B:1468:GLN:HE21	1:B:1478:HIS:CD2	2.12	0.57
1:A:990:SER:O	1:A:993:VAL:HG22	2.05	0.57
1:B:1059:LYS:HD3	1:B:1060:ASN:N	2.20	0.57
1:B:1298:PHE:HB3	1:B:1299:PRO:HD3	1.86	0.56
1:B:1342:LYS:HA	1:B:1350:VAL:HG23	1.87	0.56
1:B:1730:ARG:HB3	1:B:1752:TRP:HH2	1.69	0.56
1:A:961:GLU:CB	1:A:1200:LEU:HB3	2.35	0.56
1:B:961:GLU:HG2	1:B:1200:LEU:N	2.20	0.56
1:B:1251:TYR:CD1	1:B:1587:ILE:HB	2.41	0.56
1:B:1673:VAL:HG23	1:B:1673:VAL:O	2.03	0.56
1:A:1800:GLU:O	1:A:1801:ILE:HG13	2.05	0.56
1:B:1140:ARG:HG3	1:B:1144:ARG:NH2	2.19	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1059:LYS:HD3	1:A:1060:ASN:N	2.21	0.56
1:A:1007:ASP:O	1:A:1017:ALA:HA	2.06	0.56
1:A:1139:HIS:CD2	1:A:1144:ARG:HD2	2.41	0.56
1:B:1814:ILE:CB	1:B:1822:THR:HG22	2.35	0.56
1:A:1341:ILE:HG12	1:A:1384:ASP:HB2	1.86	0.56
1:A:1609:LEU:O	1:A:1613:TYR:HD2	1.89	0.56
1:A:961:GLU:HG2	1:A:1200:LEU:N	2.21	0.56
1:A:1537:SER:O	1:A:1541:MET:HG3	2.06	0.56
1:B:1045:HIS:CE1	1:B:1051:GLN:HE21	2.24	0.56
1:B:1423:GLU:N	1:B:1424:PRO:CA	2.67	0.56
1:B:1491:ARG:HG3	1:B:1519:TRP:CE2	2.41	0.56
1:A:1313:ILE:HG23	1:A:1416:GLY:O	2.06	0.55
1:A:1723:ALA:HB1	1:A:1728:LEU:HB2	1.86	0.55
1:A:1784:PHE:C	1:A:1784:PHE:HD2	2.08	0.55
1:B:1401:LEU:HD21	1:B:1412:LEU:HD12	1.87	0.55
1:A:1083:TYR:HB3	1:A:1218:LEU:HD21	1.87	0.55
1:B:1587:ILE:HG23	1:B:1588:GLY:H	1.71	0.55
1:B:1665:VAL:HG22	1:B:1673:VAL:CG1	2.36	0.55
1:B:1821:ILE:HD12	1:B:1841:ARG:NH1	2.22	0.55
1:A:1623:MET:CE	1:A:1633:VAL:HG11	2.35	0.55
1:A:1333:ARG:NH2	1:A:1396:ARG:HD3	2.21	0.55
1:A:1798:TYR:N	1:A:1798:TYR:HD2	1.98	0.55
1:A:1846:HIS:CD2	1:A:1846:HIS:H	2.24	0.55
1:A:1467:GLN:NE2	1:A:1475:LEU:HD13	2.22	0.55
1:A:1691:ILE:HD12	1:A:1698:LYS:HZ3	1.71	0.55
1:B:1433:SER:HB3	1:B:1434:PRO:HD3	1.89	0.55
1:B:1470:LEU:HD21	1:B:1476:VAL:HG21	1.88	0.55
1:A:1433:SER:HB3	1:A:1434:PRO:HD3	1.89	0.55
1:A:1821:ILE:HD12	1:A:1841:ARG:NH1	2.21	0.55
1:B:1807:VAL:O	1:B:1807:VAL:HG23	2.05	0.55
1:B:1118:MET:HE1	1:B:1445:PRO:HD2	1.88	0.55
1:A:1798:TYR:O	1:A:1799:ILE:HG12	2.07	0.55
1:A:1814:ILE:CB	1:A:1822:THR:HG22	2.37	0.55
1:B:1468:GLN:NE2	1:B:1478:HIS:CD2	2.66	0.55
1:B:1719:TRP:NE1	1:B:1735:GLY:HA3	2.22	0.55
1:B:1834:LEU:HG	1:B:1834:LEU:O	2.05	0.55
1:A:1302:ILE:HD12	1:A:1312:VAL:HG21	1.89	0.54
1:B:1326:GLN:HB3	1:B:1327:PRO:CD	2.37	0.54
1:B:1467:GLN:NE2	1:B:1475:LEU:HD13	2.22	0.54
1:A:1636:PRO:HG2	1:A:1639:HIS:CG	2.42	0.54
1:A:1784:PHE:CD2	1:A:1784:PHE:C	2.78	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1100:SER:OG	1:B:1101:THR:N	2.41	0.54
1:A:1059:LYS:HD3	1:A:1060:ASN:H	1.71	0.54
1:B:1513:PHE:CG	1:B:1514:PRO:HD2	2.42	0.54
1:B:1611:THR:O	1:B:1614:THR:HB	2.08	0.54
1:A:1003:TYR:CD2	1:A:1019:ILE:HG22	2.43	0.54
1:A:1726:THR:O	1:A:1730:ARG:CG	2.56	0.54
1:B:1846:HIS:CD2	1:B:1846:HIS:H	2.24	0.54
1:B:974:SER:OG	1:B:977:ASN:HB2	2.06	0.54
1:A:1664:PRO:HB2	1:A:1666:LEU:HD21	1.90	0.54
1:B:1035:VAL:CG2	1:B:1115:PHE:CD2	2.91	0.54
1:A:1401:LEU:HD21	1:A:1412:LEU:HD12	1.89	0.54
1:B:962:GLU:H	1:B:1200:LEU:HD23	1.72	0.54
1:A:1240:PRO:HA	1:A:1504:ARG:HH11	1.72	0.54
1:A:1263:TYR:O	1:A:1267:VAL:HG13	2.07	0.54
1:A:1587:ILE:HG23	1:A:1588:GLY:H	1.73	0.54
1:A:1646:VAL:HG11	1:A:1676:TYR:CE1	2.43	0.54
1:B:1333:ARG:NH2	1:B:1396:ARG:HD3	2.22	0.54
1:A:1165:ASN:ND2	1:A:1451:GLU:H	2.04	0.54
1:A:1637:LEU:HD11	1:A:1661:LEU:HD13	1.88	0.54
1:B:1341:ILE:HG12	1:B:1384:ASP:HB2	1.90	0.54
1:A:1110:LEU:HD11	1:A:1125:ARG:HG2	1.90	0.54
1:A:1154:PHE:HZ	1:A:1464:MET:HE3	1.72	0.54
1:B:1249:CYS:HB2	1:B:1277:TYR:HB2	1.90	0.54
1:B:1289:PHE:CZ	1:B:1397:GLU:HB3	2.43	0.54
1:B:1637:LEU:HD11	1:B:1661:LEU:HD13	1.90	0.53
1:B:1155:SER:HB2	1:B:1482:HIS:CD2	2.44	0.53
1:A:1587:ILE:HG23	1:A:1588:GLY:N	2.24	0.53
1:A:1741:ASP:CB	1:A:1744:GLY:H	2.21	0.53
1:A:1556:ILE:O	1:A:1557:CYS:HB2	2.09	0.53
1:A:1106:TRP:CZ3	1:A:1108:SER:HB3	2.43	0.53
1:A:1153:MET:HE3	1:A:1193:MET:SD	2.48	0.53
1:A:1131:LEU:CD2	1:A:1173:TYR:CD1	2.91	0.53
1:A:1542:MET:HE1	1:A:1636:PRO:HB3	1.88	0.53
1:B:1007:ASP:O	1:B:1017:ALA:HA	2.09	0.53
1:B:1145:ASP:O	1:B:1146:LEU:HB2	2.09	0.53
1:A:1691:ILE:HD11	1:A:1698:LYS:HD2	1.91	0.53
1:B:1088:LYS:HB3	1:B:1109:GLN:NE2	2.24	0.53
1:B:1461:THR:OG1	1:B:1462:LEU:N	2.40	0.53
1:A:1298:PHE:HB3	1:A:1299:PRO:HD3	1.90	0.53
1:A:1045:HIS:CE1	1:A:1051:GLN:HE21	2.27	0.53
1:A:1154:PHE:CZ	1:A:1464:MET:CE	2.86	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1585:ASN:ND2	1:A:1592:GLN:NE2	2.57	0.53
1:A:1721:GLU:OE1	1:A:1733:PHE:HB2	2.09	0.53
1:B:1609:LEU:O	1:B:1613:TYR:HD2	1.91	0.53
1:B:1154:PHE:HZ	1:B:1464:MET:HE1	1.74	0.52
1:B:1660:PHE:CZ	1:B:1709:LEU:HB3	2.44	0.52
1:A:1064:VAL:CG1	1:A:1066:VAL:HG13	2.39	0.52
1:A:1407:ASN:HB3	1:A:1409:GLU:OE2	2.09	0.52
1:B:1045:HIS:HE1	1:B:1051:GLN:HE21	1.57	0.52
1:B:1522:HIS:O	1:B:1552:THR:HA	2.08	0.52
1:A:1693:ALA:HB2	1:A:1698:LYS:HE3	1.91	0.52
1:A:1130:TYR:CD1	1:A:1143:ARG:HD2	2.44	0.52
1:A:1157:ASP:HB2	1:A:1425:SER:HB2	1.92	0.52
1:B:1587:ILE:HG23	1:B:1588:GLY:N	2.25	0.52
1:B:1644:ASP:OD1	1:B:1646:VAL:HG23	2.09	0.52
1:A:1326:GLN:HB3	1:A:1327:PRO:CD	2.40	0.52
1:A:1079:GLU:CD	1:A:1079:GLU:H	2.11	0.52
1:B:1130:TYR:CD1	1:B:1143:ARG:HD2	2.45	0.52
1:A:1035:VAL:CG2	1:A:1038:LEU:HD21	2.35	0.52
1:B:1664:PRO:HB2	1:B:1666:LEU:HD21	1.90	0.52
1:A:1045:HIS:HE1	1:A:1051:GLN:HE21	1.56	0.52
1:B:1693:ALA:N	1:B:1698:LYS:HZ1	2.08	0.52
1:A:1249:CYS:CB	1:A:1277:TYR:HB2	2.39	0.52
1:B:1039:ARG:HB3	1:B:1057:PRO:HG3	1.92	0.52
1:B:1734:MET:CE	1:B:1794:LEU:HD21	2.34	0.51
1:A:1816:VAL:CG1	1:A:1818:GLY:H	2.24	0.51
1:B:1275:VAL:HA	1:B:1311:ARG:O	2.10	0.51
1:A:1436:CYS:O	1:A:1437:ARG:CD	2.58	0.51
1:A:1436:CYS:O	1:A:1437:ARG:CG	2.58	0.51
1:A:981:ARG:O	1:A:983:CYS:N	2.43	0.51
1:B:1712:ARG:HD3	1:B:1715:TYR:CE2	2.46	0.51
1:A:1083:TYR:CD1	1:A:1083:TYR:C	2.83	0.51
1:A:962:GLU:H	1:A:1200:LEU:HD23	1.74	0.51
1:B:1314:LEU:HD12	1:B:1414:PHE:HB3	1.91	0.51
1:B:1615:LEU:HD11	1:B:1660:PHE:CZ	2.46	0.51
1:A:1100:SER:OG	1:A:1101:THR:N	2.44	0.51
1:A:1513:PHE:CG	1:A:1514:PRO:HD2	2.46	0.51
1:B:1814:ILE:CB	1:B:1822:THR:HA	2.40	0.51
1:B:1106:TRP:CZ3	1:B:1108:SER:HB3	2.46	0.51
1:B:1139:HIS:CD2	1:B:1144:ARG:HD2	2.46	0.51
1:B:1646:VAL:HG11	1:B:1676:TYR:CE1	2.45	0.51
1:A:1470:LEU:HD21	1:A:1476:VAL:HG21	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1442:ASN:O	1:B:1443:HIS:C	2.49	0.51
1:B:975:ALA:HA	1:B:985:TRP:CG	2.46	0.51
1:A:1186:LEU:HD12	1:A:1187:LEU:N	2.25	0.51
1:A:1734:MET:CE	1:A:1794:LEU:HD21	2.36	0.51
1:B:1293:PRO:C	1:B:1295:PHE:H	2.14	0.51
1:B:1716:ILE:HG12	1:B:1748:GLY:HA3	1.92	0.51
1:B:1816:VAL:CG1	1:B:1817:SER:N	2.74	0.51
1:A:1437:ARG:HG2	1:A:1437:ARG:O	2.11	0.51
1:A:1491:ARG:HG3	1:A:1519:TRP:CD2	2.46	0.51
1:B:1730:ARG:NH1	1:B:1755:GLY:HA3	2.24	0.51
1:B:1798:TYR:O	1:B:1799:ILE:HG12	2.11	0.51
1:B:990:SER:O	1:B:993:VAL:HG22	2.11	0.51
1:A:1107:ASP:HB3	1:A:1125:ARG:HG3	1.93	0.50
1:A:1611:THR:O	1:A:1614:THR:HB	2.11	0.50
1:B:1165:ASN:ND2	1:B:1451:GLU:H	2.05	0.50
1:B:1542:MET:HE1	1:B:1636:PRO:HB3	1.91	0.50
1:B:1816:VAL:HG12	1:B:1817:SER:N	2.25	0.50
1:A:1131:LEU:HD22	1:A:1173:TYR:CD1	2.46	0.50
1:A:1803:GLY:H	1:A:1832:GLN:CB	2.24	0.50
1:A:1145:ASP:O	1:A:1146:LEU:HB2	2.11	0.50
1:A:1442:ASN:O	1:A:1443:HIS:C	2.49	0.50
1:A:1660:PHE:CZ	1:A:1709:LEU:HB3	2.47	0.50
1:B:1154:PHE:CZ	1:B:1464:MET:CE	2.87	0.50
1:A:1681:ARG:HD3	1:A:1741:ASP:HA	1.94	0.50
1:A:967:TYR:HD1	1:A:973:ALA:CA	2.24	0.50
1:B:1560:PHE:O	1:B:1561:GLN:HB2	2.12	0.50
1:B:978:CYS:SG	1:B:978:CYS:O	2.68	0.50
1:B:1234:GLY:HA3	1:B:1518:ARG:CD	2.41	0.50
1:B:1399:GLU:HA	1:B:1500:VAL:CG2	2.39	0.50
1:B:1508:ILE:N	1:B:1508:ILE:CD1	2.74	0.50
1:B:1750:LEU:HD11	1:B:1752:TRP:HD1	1.76	0.50
1:A:1154:PHE:CE1	1:A:1192:ALA:HB2	2.47	0.50
1:A:1314:LEU:HD12	1:A:1414:PHE:HB3	1.93	0.50
1:B:1269:ALA:HB1	1:B:1602:VAL:CG1	2.42	0.50
1:B:1298:PHE:N	1:B:1299:PRO:CD	2.74	0.50
1:B:1436:CYS:O	1:B:1437:ARG:CG	2.60	0.50
1:A:1105:ILE:HG23	1:A:1183:HIS:CD2	2.47	0.50
1:A:1491:ARG:HD2	1:A:1495:GLU:OE1	2.12	0.50
1:B:1154:PHE:CE1	1:B:1192:ALA:HB2	2.46	0.50
1:B:1218:LEU:O	1:B:1219:GLY:C	2.49	0.50
1:B:1785:ASN:OD1	1:B:1786:ASN:N	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1621:THR:HG21	1:A:1750:LEU:HA	1.93	0.50
1:A:1814:ILE:CB	1:A:1822:THR:HA	2.41	0.50
1:B:1050:LEU:CD2	1:B:1083:TYR:CZ	2.95	0.50
1:A:1022:LYS:HD2	1:A:1022:LYS:O	2.11	0.49
1:A:1686:TYR:CD2	1:A:1706:HIS:HE1	2.29	0.49
1:B:1263:TYR:O	1:B:1267:VAL:HG13	2.11	0.49
1:A:1399:GLU:HA	1:A:1500:VAL:CG2	2.40	0.49
1:B:1003:TYR:HD2	1:B:1019:ILE:HG22	1.77	0.49
1:B:1077:THR:OG1	1:B:1079:GLU:HG2	2.12	0.49
1:B:1034:PRO:HA	1:B:1116:SER:HA	1.95	0.49
1:B:1030:PHE:O	1:B:1031:PRO:C	2.51	0.49
1:B:981:ARG:O	1:B:983:CYS:N	2.45	0.49
1:A:1719:TRP:NE1	1:A:1735:GLY:HA3	2.27	0.49
1:B:1423:GLU:H	1:B:1424:PRO:HA	1.72	0.49
1:B:1039:ARG:HG3	1:B:1040:LEU:N	2.28	0.49
1:A:1491:ARG:HG3	1:A:1519:TRP:CE2	2.48	0.49
1:A:1807:VAL:O	1:A:1807:VAL:CG2	2.61	0.49
1:B:1240:PRO:HA	1:B:1504:ARG:HH11	1.77	0.49
1:B:1741:ASP:CB	1:B:1744:GLY:H	2.24	0.49
1:B:1821:ILE:HG13	1:B:1823:PRO:HD3	1.95	0.49
1:A:1200:LEU:O	1:A:1201:PRO:C	2.50	0.49
1:B:1382:PHE:CD2	1:B:1462:LEU:HD21	2.48	0.49
1:B:1491:ARG:HG3	1:B:1519:TRP:CD2	2.47	0.49
1:B:1686:TYR:CD2	1:B:1706:HIS:HE1	2.30	0.49
1:B:1816:VAL:CG1	1:B:1818:GLY:H	2.26	0.49
1:A:1021:LEU:HB2	1:A:1036:ASN:ND2	2.27	0.49
1:B:1556:ILE:O	1:B:1557:CYS:HB2	2.13	0.49
1:A:1042:VAL:HG11	1:A:1085:VAL:HG21	1.94	0.49
1:A:1691:ILE:HG13	1:A:1698:LYS:NZ	2.28	0.49
1:B:1585:ASN:ND2	1:B:1592:GLN:NE2	2.61	0.49
1:B:1636:PRO:HG2	1:B:1639:HIS:CG	2.47	0.49
1:A:1796:LEU:HB3	1:A:1843:ILE:HG22	1.95	0.49
1:B:1621:THR:HG21	1:B:1750:LEU:HA	1.93	0.49
1:A:1034:PRO:HA	1:A:1116:SER:HA	1.95	0.48
1:A:1039:ARG:HB3	1:A:1057:PRO:HG3	1.95	0.48
1:A:1446:TYR:O	1:A:1448:PRO:HD3	2.12	0.48
1:A:1644:ASP:OD1	1:A:1646:VAL:HG23	2.13	0.48
1:A:1098:ARG:NH1	1:A:1177:GLU:OE2	2.42	0.48
1:A:1302:ILE:HD12	1:A:1312:VAL:HG11	1.93	0.48
1:A:1686:TYR:CE2	1:A:1706:HIS:HE1	2.32	0.48
1:B:1003:TYR:CD2	1:B:1019:ILE:HG22	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1615:LEU:HD11	1:A:1660:PHE:CZ	2.48	0.48
1:A:1660:PHE:HZ	1:A:1709:LEU:HD13	1.78	0.48
1:A:1765:LEU:HD23	1:A:1765:LEU:N	2.17	0.48
1:A:1785:ASN:OD1	1:A:1786:ASN:N	2.46	0.48
1:A:1836:ILE:HG22	1:A:1836:ILE:O	2.13	0.48
1:B:1681:ARG:HD3	1:B:1741:ASP:HA	1.95	0.48
1:A:1298:PHE:N	1:A:1299:PRO:HD2	2.29	0.48
1:A:1513:PHE:CE2	1:A:1514:PRO:HD2	2.48	0.48
1:B:1035:VAL:HG22	1:B:1115:PHE:HD2	1.79	0.48
1:B:1298:PHE:N	1:B:1299:PRO:HD2	2.29	0.48
1:B:1145:ASP:O	1:B:1146:LEU:CB	2.61	0.48
1:B:1200:LEU:O	1:B:1200:LEU:HG	2.12	0.48
1:A:1135:GLY:CA	1:A:1170:HIS:H	2.26	0.48
1:B:1509:THR:O	1:B:1522:HIS:HD2	1.96	0.48
1:A:1423:GLU:N	1:A:1424:PRO:CA	2.76	0.48
1:A:1461:THR:OG1	1:A:1462:LEU:N	2.45	0.48
1:B:1691:ILE:HG13	1:B:1698:LYS:HZ2	1.78	0.48
1:B:1803:GLY:H	1:B:1832:GLN:CB	2.25	0.48
1:A:1200:LEU:HG	1:A:1200:LEU:O	2.14	0.48
1:A:1432:VAL:HG13	1:A:1433:SER:N	2.29	0.48
1:B:1042:VAL:HG22	1:B:1052:PHE:HB2	1.96	0.48
1:B:1716:ILE:CG2	1:B:1738:ILE:HG23	2.43	0.48
1:B:1796:LEU:HB3	1:B:1843:ILE:HG22	1.95	0.48
1:A:1522:HIS:O	1:A:1552:THR:HA	2.14	0.48
1:A:1750:LEU:HD11	1:A:1752:TRP:HD1	1.78	0.48
1:B:1341:ILE:HG13	1:B:1382:PHE:O	2.14	0.48
1:A:1135:GLY:HA2	1:A:1170:HIS:HB2	1.94	0.48
1:A:1248:LEU:HD23	1:A:1583:ASN:HB3	1.96	0.48
1:B:1200:LEU:O	1:B:1201:PRO:C	2.50	0.48
1:A:975:ALA:HA	1:A:985:TRP:CG	2.48	0.47
1:B:1683:TYR:CD2	1:B:1739:ALA:HB1	2.49	0.47
1:A:1364:ASN:H	1:A:1376:TYR:HE1	1.62	0.47
1:A:1730:ARG:NH1	1:A:1755:GLY:HA3	2.28	0.47
1:B:1083:TYR:CD1	1:B:1083:TYR:C	2.87	0.47
1:B:1784:PHE:HD2	1:B:1785:ASN:N	2.12	0.47
1:B:1467:GLN:HE22	1:B:1475:LEU:HD13	1.79	0.47
1:B:1692:ASN:C	1:B:1698:LYS:NZ	2.65	0.47
1:B:1725:ASN:OD1	1:B:1727:HIS:HB3	2.14	0.47
1:A:1293:PRO:C	1:A:1295:PHE:H	2.17	0.47
1:A:1369:TRP:CH2	1:A:1373:VAL:HG21	2.50	0.47
1:A:1341:ILE:HG13	1:A:1382:PHE:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1467:GLN:HE22	1:A:1475:LEU:HD13	1.79	0.47
1:B:1432:VAL:HG13	1:B:1433:SER:N	2.29	0.47
1:B:1559:PHE:CE2	1:B:1586:THR:HB	2.49	0.47
1:B:1726:THR:O	1:B:1730:ARG:HG2	2.15	0.47
1:B:967:TYR:HD1	1:B:973:ALA:CA	2.26	0.47
1:A:1274:ASP:CG	1:A:1726:THR:HG23	2.35	0.47
1:B:1131:LEU:CD2	1:B:1173:TYR:CD1	2.97	0.47
1:B:1369:TRP:CH2	1:B:1373:VAL:HG21	2.50	0.47
1:A:1086:LEU:HD13	1:B:1097:ARG:NH2	2.30	0.47
1:A:1298:PHE:N	1:A:1299:PRO:CD	2.77	0.47
1:A:1575:GLY:C	1:A:1577:PHE:H	2.17	0.47
1:A:1738:ILE:HD11	1:A:1778:MET:HE2	1.96	0.47
1:B:1045:HIS:HE1	1:B:1051:GLN:NE2	2.13	0.47
1:B:1064:VAL:CG1	1:B:1066:VAL:HG13	2.44	0.47
1:B:1156:ARG:HH12	1:B:1158:GLN:HE21	1.60	0.47
1:B:1248:LEU:HD23	1:B:1583:ASN:HB3	1.96	0.47
1:B:1593:ASP:HB2	1:B:1594:PRO:HD2	1.97	0.47
1:A:1691:ILE:HG13	1:A:1698:LYS:HZ2	1.79	0.47
1:B:1313:ILE:HG23	1:B:1416:GLY:O	2.14	0.47
1:B:1223:GLU:OE1	1:B:1631:VAL:HG22	2.15	0.47
1:A:1039:ARG:HG3	1:A:1040:LEU:N	2.29	0.47
1:A:1088:LYS:HB3	1:A:1109:GLN:NE2	2.29	0.47
1:A:1489:GLN:O	1:A:1489:GLN:HG2	2.14	0.47
1:B:1750:LEU:HD11	1:B:1752:TRP:CD1	2.50	0.47
1:B:1775:GLN:O	1:B:1777:THR:HG23	2.15	0.47
1:A:1120:ILE:HG21	1:A:1212:LEU:HD21	1.96	0.47
1:A:1218:LEU:O	1:A:1219:GLY:C	2.49	0.47
1:A:1234:GLY:HA3	1:A:1518:ARG:CD	2.44	0.47
1:A:967:TYR:CD1	1:A:973:ALA:CA	2.97	0.47
1:B:1105:ILE:HG23	1:B:1183:HIS:CD2	2.50	0.47
1:B:1157:ASP:HB2	1:B:1425:SER:HB2	1.97	0.47
1:B:1836:ILE:O	1:B:1836:ILE:HG22	2.14	0.47
1:A:1035:VAL:CG2	1:A:1115:PHE:CD2	2.97	0.47
1:A:1155:SER:HB2	1:A:1482:HIS:CD2	2.49	0.47
1:A:1716:ILE:CG2	1:A:1738:ILE:HG23	2.45	0.47
1:B:1436:CYS:O	1:B:1437:ARG:CD	2.60	0.47
1:B:1441:LEU:HD13	1:B:1464:MET:H	1.77	0.47
1:A:1022:LYS:CD	1:A:1022:LYS:O	2.63	0.46
1:A:1274:ASP:OD2	1:A:1726:THR:HG23	2.15	0.46
1:A:961:GLU:C	1:A:963:LYS:N	2.69	0.46
1:B:1800:GLU:C	1:B:1801:ILE:HG13	2.36	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1036:ASN:HA	1:A:1037:PRO:HA	1.71	0.46
1:A:1329:PRO:O	1:A:1330:ALA:C	2.53	0.46
1:A:1598:ASP:OD2	1:A:1600:ALA:HB3	2.15	0.46
1:A:1097:ARG:NH1	1:B:1086:LEU:HD22	2.30	0.46
1:A:1311:ARG:NH2	1:A:1756:GLN:OE1	2.47	0.46
1:A:1741:ASP:O	1:A:1744:GLY:O	2.33	0.46
1:A:1021:LEU:HB2	1:A:1036:ASN:HD21	1.81	0.46
1:A:1165:ASN:ND2	1:A:1165:ASN:N	2.63	0.46
1:A:1333:ARG:HG3	1:A:1333:ARG:H	1.44	0.46
1:A:1437:ARG:O	1:A:1437:ARG:CG	2.63	0.46
1:A:1269:ALA:HB1	1:A:1602:VAL:CG1	2.45	0.46
1:A:1738:ILE:HD11	1:A:1778:MET:CE	2.45	0.46
1:B:1239:VAL:HB	1:B:1243:SER:OG	2.15	0.46
1:B:1249:CYS:CB	1:B:1277:TYR:HB2	2.45	0.46
1:B:1342:LYS:HB3	1:B:1349:ILE:CA	2.43	0.46
1:B:1467:GLN:HE21	1:B:1475:LEU:HD22	1.81	0.46
1:B:1484:LEU:HD12	1:B:1484:LEU:HA	1.78	0.46
1:B:1154:PHE:CZ	1:B:1464:MET:HE1	2.50	0.46
1:B:1186:LEU:HD12	1:B:1187:LEU:N	2.30	0.46
1:B:1384:ASP:C	1:B:1384:ASP:OD1	2.54	0.46
1:B:1441:LEU:HD12	1:B:1464:MET:H	1.77	0.46
1:B:1790:GLY:HA2	1:B:1846:HIS:HE1	1.80	0.46
1:A:1097:ARG:NH2	1:B:1086:LEU:HD13	2.31	0.46
1:A:1447:MET:O	1:A:1453:ARG:NH1	2.41	0.46
1:A:1223:GLU:OE1	1:A:1631:VAL:HG22	2.15	0.46
1:A:1681:ARG:HD2	1:A:1742:ASP:H	1.80	0.46
1:B:1686:TYR:CE2	1:B:1706:HIS:HE1	2.32	0.46
1:A:1441:LEU:HD12	1:A:1464:MET:H	1.74	0.46
1:A:1478:HIS:CE1	1:A:1482:HIS:ND1	2.84	0.46
1:A:1683:TYR:CD2	1:A:1739:ALA:HB1	2.51	0.46
1:B:1042:VAL:HG11	1:B:1085:VAL:HG21	1.97	0.46
1:B:1437:ARG:O	1:B:1437:ARG:HG2	2.15	0.46
1:B:1513:PHE:CE2	1:B:1514:PRO:HD2	2.51	0.46
1:B:1537:SER:O	1:B:1541:MET:HG3	2.15	0.46
1:B:1691:ILE:O	1:B:1691:ILE:HD12	2.16	0.46
1:B:1270:GLN:CA	1:B:1724:LEU:HD21	2.42	0.46
1:B:1621:THR:HG22	1:B:1751:PHE:H	1.79	0.46
1:A:1691:ILE:CD1	1:A:1698:LYS:HZ3	2.29	0.46
1:B:966:CYS:HB3	1:B:996:CYS:SG	2.55	0.46
1:A:1145:ASP:O	1:A:1146:LEU:CB	2.63	0.46
1:A:1420:ASP:CG	1:A:1421:MET:N	2.70	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1478:HIS:HE1	1:A:1482:HIS:ND1	2.13	0.46
1:B:1673:VAL:O	1:B:1673:VAL:CG2	2.64	0.46
1:B:1831:THR:O	1:B:1833:VAL:HG22	2.15	0.46
1:A:1559:PHE:CE2	1:A:1586:THR:HB	2.51	0.46
1:A:1790:GLY:HA2	1:A:1846:HIS:HE1	1.80	0.46
1:B:1315:ILE:HB	1:B:1418:TRP:CE3	2.51	0.46
1:A:1716:ILE:HG12	1:A:1748:GLY:HA3	1.98	0.45
1:A:1750:LEU:HD11	1:A:1752:TRP:CD1	2.50	0.45
1:B:1439:ALA:C	1:B:1441:LEU:H	2.19	0.45
1:B:993:VAL:HG12	1:B:1148:TRP:CZ2	2.51	0.45
1:A:1442:ASN:O	1:A:1444:PRO:N	2.49	0.45
1:B:1207:THR:HG23	1:B:1209:GLY:H	1.81	0.45
1:B:1470:LEU:HB3	1:B:1471:PRO:CD	2.46	0.45
1:B:1738:ILE:HD11	1:B:1778:MET:CE	2.47	0.45
1:B:1781:HIS:O	1:B:1783:ILE:HD12	2.16	0.45
1:A:1118:MET:HE3	1:A:1445:PRO:CG	2.47	0.45
1:A:1560:PHE:O	1:A:1561:GLN:HB2	2.16	0.45
1:A:1681:ARG:HH11	1:A:1742:ASP:N	2.12	0.45
1:A:1841:ARG:HD3	1:A:1841:ARG:N	2.31	0.45
1:B:1135:GLY:CA	1:B:1170:HIS:H	2.29	0.45
1:B:1269:ALA:HB1	1:B:1602:VAL:HG11	1.98	0.45
1:A:1188:LEU:HA	1:A:1188:LEU:HD23	1.78	0.45
1:A:1621:THR:HG22	1:A:1751:PHE:H	1.80	0.45
1:A:1837:ASP:OD1	1:A:1838:VAL:N	2.50	0.45
1:B:1079:GLU:H	1:B:1079:GLU:CD	2.20	0.45
1:A:1036:ASN:OD1	1:A:1037:PRO:HA	2.17	0.45
1:A:1156:ARG:HH11	1:A:1158:GLN:HE21	1.62	0.45
1:B:1447:MET:O	1:B:1453:ARG:NH1	2.40	0.45
1:B:1681:ARG:HD2	1:B:1742:ASP:H	1.81	0.45
1:A:1047:ASN:HD21	1:A:1076:SER:HA	1.80	0.45
1:A:1613:TYR:HA	1:A:1616:LEU:HG	1.98	0.45
1:A:1712:ARG:HD3	1:A:1715:TYR:CE2	2.52	0.45
1:A:1816:VAL:HG12	1:A:1818:GLY:H	1.82	0.45
1:B:1040:LEU:HD12	1:B:1040:LEU:C	2.37	0.45
1:B:1691:ILE:HG23	1:B:1692:ASN:N	2.32	0.45
1:A:1784:PHE:HD2	1:A:1785:ASN:N	2.15	0.45
1:A:966:CYS:HB3	1:A:996:CYS:SG	2.57	0.45
1:B:1148:TRP:NE1	1:B:1199:PRO:HG2	2.32	0.45
1:B:1489:GLN:O	1:B:1489:GLN:HG2	2.16	0.45
1:B:1803:GLY:HA2	1:B:1832:GLN:HG3	1.99	0.45
1:A:1076:SER:HB2	1:A:1081:GLN:OE1	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1586:THR:OG1	1:A:1587:ILE:N	2.50	0.45
1:A:1800:GLU:C	1:A:1801:ILE:HG13	2.37	0.45
1:A:1836:ILE:O	1:A:1838:VAL:HG23	2.17	0.45
1:B:1156:ARG:HH11	1:B:1158:GLN:HE21	1.63	0.45
1:B:1272:PRO:HB3	1:B:1723:ALA:O	2.16	0.45
1:B:1613:TYR:HA	1:B:1616:LEU:HG	1.99	0.45
1:B:1836:ILE:O	1:B:1838:VAL:HG23	2.16	0.45
1:A:1707:ILE:HG23	1:A:1707:ILE:O	2.17	0.45
1:B:1047:ASN:HD21	1:B:1076:SER:HA	1.79	0.45
1:B:1135:GLY:HA2	1:B:1170:HIS:HB2	1.99	0.45
1:B:1491:ARG:HD2	1:B:1495:GLU:OE1	2.15	0.45
1:B:1837:ASP:OD1	1:B:1838:VAL:N	2.50	0.45
1:A:1135:GLY:HA3	1:A:1170:HIS:H	1.81	0.45
1:A:1131:LEU:HD21	1:A:1173:TYR:CD1	2.52	0.45
1:A:1331:PHE:O	1:A:1335:VAL:HG23	2.17	0.45
1:A:1343:TYR:HB3	1:A:1344:PRO:CD	2.43	0.45
1:A:1593:ASP:HB2	1:A:1594:PRO:HD2	1.99	0.45
1:B:1022:LYS:O	1:B:1022:LYS:HD2	2.17	0.45
1:B:1721:GLU:OE1	1:B:1733:PHE:HB2	2.17	0.45
1:B:1753:ASP:C	1:B:1755:GLY:N	2.70	0.45
1:A:1086:LEU:HD22	1:B:1097:ARG:NH1	2.32	0.44
1:A:1239:VAL:HB	1:A:1243:SER:OG	2.17	0.44
1:A:1243:SER:HB2	1:A:1551:TYR:OH	2.17	0.44
1:A:1673:VAL:CG2	1:A:1673:VAL:O	2.64	0.44
1:B:1200:LEU:O	1:B:1202:ALA:N	2.50	0.44
1:B:1437:ARG:O	1:B:1437:ARG:CG	2.65	0.44
1:B:1635:ARG:HA	1:B:1636:PRO:HD2	1.79	0.44
1:A:1042:VAL:HG22	1:A:1052:PHE:HB2	1.99	0.44
1:A:1508:ILE:CD1	1:A:1508:ILE:N	2.80	0.44
1:A:1753:ASP:C	1:A:1755:GLY:N	2.70	0.44
1:B:998:PHE:CZ	1:B:1112:GLY:HA2	2.51	0.44
1:B:1131:LEU:HD22	1:B:1173:TYR:CD1	2.52	0.44
1:B:1446:TYR:O	1:B:1448:PRO:HD3	2.18	0.44
1:A:1040:LEU:HD11	1:A:1042:VAL:HG23	1.99	0.44
1:A:1154:PHE:HZ	1:A:1464:MET:HE1	1.78	0.44
1:A:1207:THR:HG23	1:A:1209:GLY:N	2.32	0.44
1:A:1470:LEU:HB3	1:A:1471:PRO:CD	2.48	0.44
1:A:1528:THR:CG2	1:A:1529:ALA:N	2.81	0.44
1:B:1120:ILE:HG21	1:B:1212:LEU:HD21	1.98	0.44
1:A:1484:LEU:HA	1:A:1484:LEU:HD12	1.77	0.44
1:A:1691:ILE:O	1:A:1691:ILE:HD12	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1329:PRO:O	1:B:1330:ALA:C	2.55	0.44
1:B:1508:ILE:HD13	1:B:1508:ILE:N	2.32	0.44
1:A:1401:LEU:HD22	1:A:1412:LEU:HB2	2.00	0.44
1:A:1527:ASN:HD21	1:A:1555:ASP:H	1.66	0.44
1:B:1036:ASN:HA	1:B:1037:PRO:HA	1.70	0.44
1:B:1076:SER:HB2	1:B:1081:GLN:OE1	2.18	0.44
1:B:1311:ARG:HD3	1:B:1415:ASP:OD2	2.17	0.44
1:B:1240:PRO:HD3	1:B:1505:GLY:O	2.18	0.44
1:B:1784:PHE:CD2	1:B:1785:ASN:N	2.86	0.44
1:A:1021:LEU:HD12	1:A:1036:ASN:ND2	2.33	0.44
1:A:1637:LEU:HD12	1:A:1655:LEU:HG	2.00	0.44
1:B:1007:ASP:OD1	1:B:1007:ASP:C	2.56	0.44
1:B:1219:GLY:H	1:B:1228:GLN:NE2	1.92	0.44
1:B:1470:LEU:HD11	1:B:1476:VAL:HG21	1.99	0.44
1:B:1653:GLN:HE22	1:B:1676:TYR:N	2.07	0.44
1:A:1804:VAL:HG22	1:A:1832:GLN:O	2.17	0.44
1:B:1346:ASP:N	1:B:1346:ASP:OD1	2.51	0.44
1:B:1693:ALA:N	1:B:1698:LYS:NZ	2.66	0.44
1:A:1045:HIS:HE1	1:A:1051:GLN:NE2	2.16	0.44
1:A:1745:THR:O	1:A:1746:ALA:HB2	2.18	0.44
1:A:1804:VAL:H	1:A:1832:GLN:HB3	1.83	0.44
1:B:1040:LEU:HD11	1:B:1042:VAL:HG23	1.99	0.44
1:B:1139:HIS:CG	1:B:1144:ARG:HD2	2.53	0.44
1:B:1703:PRO:HD2	1:B:1706:HIS:HB3	2.00	0.44
1:A:1272:PRO:HB3	1:A:1723:ALA:O	2.17	0.43
1:A:1614:THR:HG22	1:A:1719:TRP:HB2	2.00	0.43
1:B:1147:GLU:HA	1:B:1199:PRO:HG3	1.99	0.43
1:B:1804:VAL:HG22	1:B:1832:GLN:O	2.18	0.43
1:B:961:GLU:C	1:B:963:LYS:N	2.70	0.43
1:A:978:CYS:O	1:A:978:CYS:SG	2.76	0.43
1:B:1333:ARG:HG3	1:B:1333:ARG:H	1.45	0.43
1:B:1420:ASP:CG	1:B:1421:MET:N	2.71	0.43
1:B:1691:ILE:HG23	1:B:1692:ASN:H	1.82	0.43
1:A:1022:LYS:HA	1:A:1023:SER:HA	1.72	0.43
1:A:1200:LEU:O	1:A:1202:ALA:N	2.52	0.43
1:A:1355:TRP:N	1:A:1356:PRO:CD	2.82	0.43
1:A:1382:PHE:CD2	1:A:1462:LEU:HD21	2.52	0.43
1:A:1441:LEU:HD13	1:A:1464:MET:H	1.80	0.43
1:A:1741:ASP:CB	1:A:1744:GLY:O	2.66	0.43
1:B:1088:LYS:HB3	1:B:1109:GLN:HE22	1.83	0.43
1:B:1501:THR:C	1:B:1503:GLN:H	2.21	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1145:ASP:OD1	1:A:1147:GLU:HB2	2.19	0.43
1:A:1218:LEU:C	1:A:1219:GLY:O	2.52	0.43
1:A:1691:ILE:HG23	1:A:1692:ASN:H	1.84	0.43
1:A:1775:GLN:O	1:A:1777:THR:HG23	2.18	0.43
1:B:1022:LYS:O	1:B:1022:LYS:CD	2.67	0.43
1:B:1015:ALA:HB3	1:B:1042:VAL:HB	2.01	0.43
1:B:1035:VAL:HG22	1:B:1115:PHE:CD2	2.52	0.43
1:B:1442:ASN:O	1:B:1444:PRO:N	2.52	0.43
1:B:1683:TYR:HD2	1:B:1739:ALA:HB1	1.83	0.43
1:B:1745:THR:O	1:B:1746:ALA:HB2	2.17	0.43
1:A:1139:HIS:CG	1:A:1144:ARG:HD2	2.53	0.43
1:A:1279:ASP:O	1:A:1281:ASP:N	2.52	0.43
1:A:1421:MET:HE3	1:A:1421:MET:HB2	1.76	0.43
1:A:1724:LEU:O	1:A:1725:ASN:HB3	2.18	0.43
1:A:1838:VAL:CG1	1:A:1838:VAL:O	2.65	0.43
1:B:1274:ASP:OD2	1:B:1726:THR:HG23	2.18	0.43
1:B:1302:ILE:CD1	1:B:1312:VAL:HG21	2.48	0.43
1:B:1334:GLY:O	1:B:1339:VAL:HG22	2.18	0.43
1:B:1528:THR:HA	1:B:1560:PHE:HB2	2.01	0.43
1:A:1047:ASN:ND2	1:A:1077:THR:H	2.00	0.43
1:A:1136:GLU:OE1	1:A:1522:HIS:HE1	2.02	0.43
1:A:1841:ARG:CD	1:A:1841:ARG:N	2.81	0.43
1:B:1602:VAL:O	1:B:1606:ARG:HG3	2.19	0.43
1:A:1040:LEU:HD22	1:A:1094:ILE:HD11	2.00	0.43
1:A:993:VAL:HG12	1:A:1148:TRP:CZ2	2.53	0.43
1:A:1522:HIS:CD2	1:A:1523:TRP:O	2.71	0.43
1:B:1804:VAL:H	1:B:1832:GLN:HB3	1.84	0.43
1:A:1040:LEU:HD12	1:A:1040:LEU:C	2.39	0.43
1:A:1039:ARG:CB	1:A:1057:PRO:HG3	2.49	0.43
1:A:1121:ARG:HA	1:A:1205:TYR:O	2.18	0.43
1:A:1767:TYR:CG	1:A:1788:ILE:HD12	2.53	0.43
1:B:1124:THR:OG1	1:B:1125:ARG:N	2.52	0.43
1:B:1140:ARG:HG3	1:B:1144:ARG:CZ	2.49	0.43
1:B:1513:PHE:CG	1:B:1514:PRO:CD	3.01	0.43
1:A:1189:ASN:ND2	1:A:1207:THR:HG21	2.33	0.43
1:B:1040:LEU:HD22	1:B:1094:ILE:HD11	2.00	0.43
1:B:1274:ASP:CG	1:B:1726:THR:HG23	2.38	0.43
1:B:1653:GLN:NE2	1:B:1676:TYR:H	2.09	0.43
1:B:1621:THR:CG2	1:B:1751:PHE:H	2.32	0.43
1:A:1269:ALA:HB1	1:A:1602:VAL:HG11	2.01	0.42
1:B:1376:TYR:N	1:B:1376:TYR:CD2	2.86	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1432:VAL:CG1	1:B:1433:SER:N	2.81	0.42
1:B:1761:TYR:HA	1:B:1766:TYR:CD1	2.54	0.42
1:A:1077:THR:OG1	1:A:1079:GLU:HG2	2.19	0.42
1:A:1177:GLU:O	1:A:1179:ASP:O	2.37	0.42
1:A:1725:ASN:OD1	1:A:1727:HIS:HB3	2.20	0.42
1:A:961:GLU:O	1:A:963:LYS:N	2.52	0.42
1:B:1165:ASN:ND2	1:B:1165:ASN:N	2.61	0.42
1:B:1421:MET:HB2	1:B:1421:MET:HE3	1.83	0.42
1:B:1741:ASP:CB	1:B:1744:GLY:O	2.67	0.42
1:B:1807:VAL:O	1:B:1807:VAL:CG2	2.68	0.42
1:B:1177:GLU:O	1:B:1179:ASP:O	2.37	0.42
1:B:1303:ASN:HD21	1:B:1413:LYS:HG3	1.83	0.42
1:B:1741:ASP:N	1:B:1744:GLY:O	2.53	0.42
1:B:1841:ARG:N	1:B:1841:ARG:CD	2.83	0.42
1:A:1030:PHE:O	1:A:1031:PRO:C	2.57	0.42
1:A:1409:GLU:HG3	1:A:1409:GLU:H	1.70	0.42
1:B:1527:ASN:HD21	1:B:1555:ASP:H	1.67	0.42
1:A:1286:GLN:CD	1:A:1286:GLN:N	2.73	0.42
1:A:1529:ALA:HB1	1:A:1567:MET:HE3	2.01	0.42
1:A:1575:GLY:C	1:A:1577:PHE:N	2.72	0.42
1:A:1770:SER:O	1:A:1771:PHE:CD2	2.72	0.42
1:B:1401:LEU:HD22	1:B:1412:LEU:HB2	2.02	0.42
1:B:1141:SER:HA	1:B:1539:ILE:HD11	2.02	0.42
1:B:1637:LEU:HD12	1:B:1655:LEU:HG	2.02	0.42
1:B:1681:ARG:HH11	1:B:1742:ASP:N	2.15	0.42
1:B:960:ASP:C	1:B:961:GLU:O	2.57	0.42
1:A:1007:ASP:OD1	1:A:1007:ASP:C	2.58	0.42
1:A:1147:GLU:HA	1:A:1199:PRO:HG3	2.01	0.42
1:A:1346:ASP:N	1:A:1346:ASP:OD1	2.52	0.42
1:A:1447:MET:O	1:A:1453:ARG:HD3	2.20	0.42
1:A:1402:TYR:CD2	1:A:1500:VAL:HG13	2.54	0.42
1:A:1513:PHE:CG	1:A:1514:PRO:CD	3.02	0.42
1:B:1002:LEU:H	1:B:1002:LEU:HD23	1.83	0.42
1:B:1841:ARG:HD3	1:B:1841:ARG:N	2.34	0.42
1:A:1120:ILE:CG2	1:A:1212:LEU:HD21	2.50	0.42
1:A:1148:TRP:NE1	1:A:1199:PRO:HG2	2.35	0.42
1:A:1156:ARG:HH12	1:A:1158:GLN:HE21	1.62	0.42
1:A:1189:ASN:HD21	1:A:1207:THR:HG21	1.85	0.42
1:A:1464:MET:HG3	1:A:1479:TYR:HD2	1.84	0.42
1:A:1601:PHE:O	1:A:1602:VAL:C	2.58	0.42
1:A:1753:ASP:C	1:A:1755:GLY:H	2.23	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1821:ILE:HG13	1:A:1823:PRO:HD3	2.02	0.42
1:B:1145:ASP:OD1	1:B:1147:GLU:HB2	2.20	0.42
1:B:1286:GLN:N	1:B:1286:GLN:CD	2.73	0.42
1:B:1623:MET:HE1	1:B:1633:VAL:HG11	2.01	0.42
1:A:1384:ASP:OD1	1:A:1384:ASP:C	2.58	0.42
1:B:1406:GLN:NE2	1:B:1406:GLN:HA	2.30	0.42
1:A:1432:VAL:CG1	1:A:1433:SER:N	2.83	0.42
1:B:1304:ARG:O	1:B:1307:ALA:HB3	2.20	0.42
1:B:1716:ILE:N	1:B:1747:GLY:O	2.50	0.42
1:A:1289:PHE:CD2	1:A:1397:GLU:HG3	2.55	0.42
1:A:1442:ASN:C	1:A:1444:PRO:CD	2.88	0.42
1:A:1691:ILE:HG23	1:A:1692:ASN:N	2.35	0.42
1:B:1049:MET:HG2	1:B:1050:LEU:N	2.34	0.42
1:B:1092:PHE:CD1	1:B:1093:GLY:N	2.88	0.42
1:B:1302:ILE:HD12	1:B:1312:VAL:HG11	2.00	0.42
1:B:1478:HIS:CE1	1:B:1482:HIS:ND1	2.88	0.42
1:B:1575:GLY:C	1:B:1577:PHE:H	2.23	0.42
1:B:1796:LEU:HD23	1:B:1796:LEU:C	2.40	0.42
1:A:1166:SER:HB3	1:A:1167:TYR:H	1.54	0.41
1:A:1303:ASN:HD21	1:A:1413:LYS:HG3	1.84	0.41
1:A:1399:GLU:HG3	1:A:1400:GLU:N	2.35	0.41
1:B:1221:THR:OG1	1:B:1224:LEU:HD23	2.20	0.41
1:B:1433:SER:CB	1:B:1434:PRO:CD	2.93	0.41
1:B:1745:THR:HB	1:B:1773:ALA:O	2.20	0.41
1:A:1140:ARG:HG3	1:A:1144:ARG:CZ	2.50	0.41
1:A:1355:TRP:HE1	1:A:1421:MET:CE	2.33	0.41
1:B:1036:ASN:OD1	1:B:1037:PRO:HA	2.20	0.41
1:B:1116:SER:O	1:B:1117:ASP:C	2.58	0.41
1:B:1402:TYR:CD2	1:B:1500:VAL:HG13	2.54	0.41
1:B:1753:ASP:C	1:B:1755:GLY:H	2.22	0.41
1:B:1775:GLN:C	1:B:1777:THR:H	2.22	0.41
1:A:1037:PRO:HD2	1:A:1058:ASN:HD21	1.85	0.41
1:A:1334:GLY:O	1:A:1339:VAL:HG22	2.19	0.41
1:A:1354:VAL:HA	1:A:1427:PHE:CD2	2.55	0.41
1:B:1135:GLY:HA2	1:B:1170:HIS:H	1.85	0.41
1:B:1331:PHE:O	1:B:1335:VAL:HG23	2.20	0.41
1:B:1809:VAL:O	1:B:1809:VAL:HG13	2.20	0.41
1:A:1221:THR:OG1	1:A:1224:LEU:HD23	2.20	0.41
1:A:1252:GLY:HA3	1:A:1587:ILE:CD1	2.49	0.41
1:A:1298:PHE:CZ	1:A:1302:ILE:HD11	2.56	0.41
1:A:1154:PHE:CZ	1:A:1464:MET:HE1	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1467:GLN:HE21	1:A:1475:LEU:HD22	1.85	0.41
1:A:1683:TYR:HD2	1:A:1739:ALA:HB1	1.85	0.41
1:B:1039:ARG:CB	1:B:1057:PRO:HG3	2.50	0.41
1:B:1083:TYR:HD2	1:B:1218:LEU:HD11	1.86	0.41
1:B:1660:PHE:HZ	1:B:1709:LEU:HD13	1.84	0.41
1:A:1509:THR:O	1:A:1522:HIS:HD2	2.03	0.41
1:A:1761:TYR:HA	1:A:1766:TYR:CD1	2.55	0.41
1:B:1176:LEU:HD23	1:B:1176:LEU:HA	1.58	0.41
1:B:1247:GLN:HB2	1:B:1582:ARG:HG3	2.01	0.41
1:A:1002:LEU:HD23	1:A:1002:LEU:H	1.84	0.41
1:A:1406:GLN:NE2	1:A:1406:GLN:HA	2.29	0.41
1:A:1683:TYR:HE2	1:A:1740:LEU:O	2.04	0.41
1:A:1621:THR:CG2	1:A:1751:PHE:H	2.33	0.41
1:A:1775:GLN:C	1:A:1777:THR:H	2.24	0.41
1:B:1238:MET:HE2	1:B:1624:HIS:HA	2.01	0.41
1:B:1598:ASP:OD2	1:B:1600:ALA:HB3	2.20	0.41
1:B:961:GLU:O	1:B:963:LYS:N	2.53	0.41
1:A:1126:LEU:HD12	1:A:1126:LEU:HA	1.90	0.41
1:A:1128:SER:OG	1:A:1176:LEU:O	2.33	0.41
1:A:1407:ASN:OD1	1:A:1407:ASN:N	2.54	0.41
1:B:1069:ASN:OD1	1:B:1231:GLU:O	2.38	0.41
1:B:1229:TYR:CZ	1:B:1233:ILE:HD13	2.56	0.41
1:B:1271:ILE:HG12	1:B:1606:ARG:HG3	2.01	0.41
1:B:1442:ASN:C	1:B:1444:PRO:CD	2.89	0.41
1:B:1467:GLN:NE2	1:B:1475:LEU:HB3	2.36	0.41
1:B:1707:ILE:HG23	1:B:1707:ILE:O	2.19	0.41
1:B:1741:ASP:O	1:B:1744:GLY:O	2.38	0.41
1:A:1784:PHE:CD2	1:A:1785:ASN:N	2.89	0.41
1:B:1120:ILE:CG2	1:B:1212:LEU:HD21	2.51	0.41
1:A:1263:TYR:CD2	1:A:1263:TYR:C	2.93	0.41
1:B:1295:PHE:O	1:B:1298:PHE:HB2	2.21	0.41
1:A:1049:MET:HG2	1:A:1050:LEU:N	2.36	0.41
1:A:1288:ASP:HB3	1:A:1289:PHE:CD2	2.56	0.41
1:B:1517:GLY:CA	1:B:1549:ILE:HG12	2.47	0.41
1:B:1674:THR:HA	1:B:1698:LYS:O	2.21	0.41
1:A:1140:ARG:HG3	1:A:1140:ARG:H	1.55	0.40
1:A:1351:TRP:O	1:A:1432:VAL:HB	2.20	0.40
1:A:1270:GLN:CA	1:A:1724:LEU:HD21	2.46	0.40
1:A:1730:ARG:HB3	1:A:1752:TRP:CH2	2.52	0.40
1:B:1614:THR:HG22	1:B:1719:TRP:HB2	2.02	0.40
1:B:1616:LEU:HA	1:B:1616:LEU:HD23	1.93	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1784:PHE:CE2	1:B:1786:ASN:HB2	2.38	0.40
1:A:998:PHE:CZ	1:A:1112:GLY:HA2	2.57	0.40
1:A:1145:ASP:HB3	1:A:1149:HIS:CD2	2.57	0.40
1:A:1315:ILE:HB	1:A:1418:TRP:CE3	2.57	0.40
1:A:1528:THR:HA	1:A:1560:PHE:HB2	2.03	0.40
1:A:1770:SER:O	1:A:1771:PHE:HD2	2.04	0.40
1:A:1781:HIS:O	1:A:1783:ILE:HD12	2.21	0.40
1:B:1203:LEU:HD12	1:B:1203:LEU:C	2.41	0.40
1:B:1691:ILE:HG13	1:B:1698:LYS:NZ	2.35	0.40
1:B:1827:ASN:C	1:B:1827:ASN:OD1	2.60	0.40
1:B:1084:ASP:OD1	1:B:1084:ASP:C	2.60	0.40
1:B:1522:HIS:CD2	1:B:1523:TRP:O	2.74	0.40
1:B:1542:MET:HE3	1:B:1636:PRO:CB	2.37	0.40
1:B:1798:TYR:HE2	1:B:1839:THR:HG23	1.87	0.40
1:B:1800:GLU:O	1:B:1801:ILE:CG1	2.68	0.40
1:A:1176:LEU:HA	1:A:1176:LEU:HD23	1.50	0.40
1:A:1249:CYS:SG	1:A:1250:ARG:N	2.94	0.40
1:A:1247:GLN:HB2	1:A:1582:ARG:HG3	2.04	0.40
1:A:1741:ASP:CA	1:A:1744:GLY:O	2.70	0.40
1:A:1730:ARG:CZ	1:A:1752:TRP:CZ3	3.04	0.40
1:B:1136:GLU:OE1	1:B:1522:HIS:HE1	2.05	0.40
1:B:1593:ASP:HB2	1:B:1594:PRO:CD	2.51	0.40

There are no symmetry-related clashes.

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	888/908 (98%)	762 (86%)	100 (11%)	26 (3%)	4	21
1	B	888/908 (98%)	764 (86%)	99 (11%)	25 (3%)	5	22
All	All	1776/1816 (98%)	1526 (86%)	199 (11%)	51 (3%)	4	21

All (51) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1031	PRO
1	A	1631	VAL
1	A	1668	ARG
1	A	1692	ASN
1	A	1832	GLN
1	B	1031	PRO
1	B	1631	VAL
1	B	1668	ARG
1	B	1692	ASN
1	B	1832	GLN
1	A	961	GLU
1	A	1280	ILE
1	A	1354	VAL
1	A	1437	ARG
1	A	1445	PRO
1	A	1732	LYS
1	A	1756	GLN
1	B	961	GLU
1	B	1280	ILE
1	B	1354	VAL
1	B	1437	ARG
1	B	1445	PRO
1	B	1732	LYS
1	B	1756	GLN
1	A	1254	GLN
1	A	1559	PHE
1	A	1786	ASN
1	B	1254	GLN
1	B	1786	ASN
1	B	1799	ILE
1	A	1433	SER
1	A	1448	PRO
1	A	1799	ILE
1	B	1433	SER
1	B	1559	PHE
1	B	1589	THR
1	A	1256	ASP
1	A	1589	THR
1	B	1833	VAL
1	B	982	GLY
1	A	982	GLY
1	A	1443	HIS

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Mol	Chain	Res	Type
1	B	1074	PRO
1	B	1448	PRO
1	A	1833	VAL
1	B	1443	HIS
1	A	1349	ILE
1	A	1836	ILE
1	A	1074	PRO
1	B	1801	ILE
1	B	1836	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	772/800 (96%)	683 (88%)	89 (12%)	5	21
1	B	772/800 (96%)	683 (88%)	89 (12%)	5	21
All	All	1544/1600 (96%)	1366 (88%)	178 (12%)	5	21

All (178) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	967	TYR
1	A	999	VAL
1	A	1002	LEU
1	A	1016	THR
1	A	1020	SER
1	A	1022	LYS
1	A	1023	SER
1	A	1032	SER
1	A	1059	LYS
1	A	1103	THR
1	A	1106	TRP
1	A	1124	THR
1	A	1126	LEU
1	A	1129	LYS

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Mol	Chain	Res	Type
1	A	1140	ARG
1	A	1141	SER
1	A	1156	ARG
1	A	1158	GLN
1	A	1165	ASN
1	A	1166	SER
1	A	1187	LEU
1	A	1188	LEU
1	A	1200	LEU
1	A	1203	LEU
1	A	1207	THR
1	A	1218	LEU
1	A	1235	ARG
1	A	1273	TYR
1	A	1279	ASP
1	A	1295	PHE
1	A	1301	LEU
1	A	1323	ASN
1	A	1333	ARG
1	A	1346	ASP
1	A	1349	ILE
1	A	1354	VAL
1	A	1357	ASP
1	A	1363	VAL
1	A	1374	GLU
1	A	1389	SER
1	A	1397	GLU
1	A	1401	LEU
1	A	1406	GLN
1	A	1407	ASN
1	A	1409	GLU
1	A	1423	GLU
1	A	1432	VAL
1	A	1437	ARG
1	A	1438	ASP
1	A	1440	SER
1	A	1453	ARG
1	A	1464	MET
1	A	1484	LEU
1	A	1508	ILE
1	A	1516	SER
1	A	1528	THR

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Mol	Chain	Res	Type
1	A	1552	THR
1	A	1562	ASP
1	A	1589	THR
1	A	1590	ARG
1	A	1591	ARG
1	A	1606	ARG
1	A	1609	LEU
1	A	1631	VAL
1	A	1638	LEU
1	A	1642	VAL
1	A	1649	ASP
1	A	1663	SER
1	A	1672	ASN
1	A	1674	THR
1	A	1691	ILE
1	A	1730	ARG
1	A	1743	GLU
1	A	1745	THR
1	A	1763	LYS
1	A	1765	LEU
1	A	1775	GLN
1	A	1784	PHE
1	A	1791	THR
1	A	1792	ASN
1	A	1794	LEU
1	A	1798	TYR
1	A	1810	THR
1	A	1817	SER
1	A	1821	ILE
1	A	1841	ARG
1	A	1845	LEU
1	A	1848	PHE
1	A	1849	THR
1	B	967	TYR
1	B	999	VAL
1	B	1002	LEU
1	B	1016	THR
1	B	1020	SER
1	B	1022	LYS
1	B	1023	SER
1	B	1032	SER
1	B	1059	LYS

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Mol	Chain	Res	Type
1	B	1085	VAL
1	B	1103	THR
1	B	1106	TRP
1	B	1124	THR
1	B	1126	LEU
1	B	1129	LYS
1	B	1140	ARG
1	B	1156	ARG
1	B	1158	GLN
1	B	1165	ASN
1	B	1166	SER
1	B	1187	LEU
1	B	1188	LEU
1	B	1200	LEU
1	B	1203	LEU
1	B	1207	THR
1	B	1218	LEU
1	B	1235	ARG
1	B	1273	TYR
1	B	1279	ASP
1	B	1295	PHE
1	B	1301	LEU
1	B	1323	ASN
1	B	1333	ARG
1	B	1346	ASP
1	B	1349	ILE
1	B	1354	VAL
1	B	1357	ASP
1	B	1361	VAL
1	B	1363	VAL
1	B	1374	GLU
1	B	1389	SER
1	B	1397	GLU
1	B	1401	LEU
1	B	1406	GLN
1	B	1407	ASN
1	B	1409	GLU
1	B	1419	ILE
1	B	1423	GLU
1	B	1432	VAL
1	B	1437	ARG
1	B	1453	ARG

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Mol	Chain	Res	Type
1	B	1464	MET
1	B	1484	LEU
1	B	1508	ILE
1	B	1516	SER
1	B	1523	TRP
1	B	1528	THR
1	B	1552	THR
1	B	1562	ASP
1	B	1589	THR
1	B	1590	ARG
1	B	1591	ARG
1	B	1606	ARG
1	B	1609	LEU
1	B	1631	VAL
1	B	1638	LEU
1	B	1642	VAL
1	B	1649	ASP
1	B	1663	SER
1	B	1672	ASN
1	B	1674	THR
1	B	1691	ILE
1	B	1730	ARG
1	B	1743	GLU
1	B	1745	THR
1	B	1763	LYS
1	B	1765	LEU
1	B	1775	GLN
1	B	1784	PHE
1	B	1791	THR
1	B	1792	ASN
1	B	1794	LEU
1	B	1798	TYR
1	B	1810	THR
1	B	1817	SER
1	B	1821	ILE
1	B	1841	ARG
1	B	1845	LEU
1	B	1849	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (57) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1045	HIS
1	A	1047	ASN
1	A	1058	ASN
1	A	1069	ASN
1	A	1149	HIS
1	A	1158	GLN
1	A	1165	ASN
1	A	1191	ASN
1	A	1228	GLN
1	A	1286	GLN
1	A	1303	ASN
1	A	1372	GLN
1	A	1406	GLN
1	A	1467	GLN
1	A	1468	GLN
1	A	1478	HIS
1	A	1480	ASN
1	A	1503	GLN
1	A	1522	HIS
1	A	1585	ASN
1	A	1592	GLN
1	A	1610	GLN
1	A	1653	GLN
1	A	1672	ASN
1	A	1706	HIS
1	A	1708	ASN
1	A	1792	ASN
1	A	1846	HIS
1	B	1045	HIS
1	B	1047	ASN
1	B	1058	ASN
1	B	1069	ASN
1	B	1149	HIS
1	B	1158	GLN
1	B	1165	ASN
1	B	1191	ASN
1	B	1228	GLN
1	B	1286	GLN
1	B	1303	ASN
1	B	1372	GLN
1	B	1406	GLN
1	B	1467	GLN
1	B	1468	GLN

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Mol	Chain	Res	Type
1	B	1478	HIS
1	B	1480	ASN
1	B	1503	GLN
1	B	1522	HIS
1	B	1585	ASN
1	B	1592	GLN
1	B	1610	GLN
1	B	1653	GLN
1	B	1672	ASN
1	B	1706	HIS
1	B	1708	ASN
1	B	1786	ASN
1	B	1792	ASN
1	B	1846	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 ⓘ

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	890/908 (98%)	0.07	19 (2%)	63 46	32, 54, 96, 135	0
1	B	890/908 (98%)	0.18	51 (5%)	23 14	32, 55, 98, 136	0
All	All	1780/1816 (98%)	0.12	70 (3%)	39 25	32, 55, 98, 136	0

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	991	SER	5.8
1	B	1820	VAL	5.7
1	B	1815	SER	5.4
1	B	1843	ILE	5.2
1	B	1443	HIS	5.1
1	B	1840	ASP	5.0
1	A	1443	HIS	4.7
1	B	1823	PRO	4.5
1	A	1809	VAL	4.1
1	B	1789	THR	3.7
1	B	1825	PHE	3.6
1	B	1764	GLY	3.6
1	B	1733	PHE	3.6
1	B	1827	ASN	3.5
1	A	1346	ASP	3.5
1	A	1840	ASP	3.5
1	B	1565	TYR	3.4
1	A	1009	GLN	3.3
1	B	1829	PRO	3.3
1	A	989	ASN	3.2
1	B	1806	SER	3.2
1	B	1822	THR	3.2
1	B	1848	PHE	3.1
1	A	1511	SER	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	1346	ASP	3.0
1	B	1706	HIS	2.9
1	B	1705	ASP	2.9
1	A	1362	VAL	2.8
1	B	1765	LEU	2.8
1	A	1433	SER	2.8
1	B	1839	THR	2.8
1	B	1826	ASN	2.7
1	B	1821	ILE	2.7
1	A	1366	SER	2.6
1	B	1836	ILE	2.6
1	B	1698	LYS	2.5
1	B	1676	TYR	2.5
1	B	1847	ASN	2.5
1	A	1812	VAL	2.5
1	B	1606	ARG	2.5
1	A	1822	THR	2.5
1	B	1511	SER	2.5
1	B	990	SER	2.5
1	A	1667	GLU	2.5
1	A	1437	ARG	2.4
1	B	1641	PHE	2.4
1	B	1024	SER	2.4
1	B	1824	SER	2.4
1	A	1698	LYS	2.3
1	A	1512	THR	2.3
1	B	1809	VAL	2.3
1	B	1406	GLN	2.3
1	B	1672	ASN	2.2
1	B	1442	ASN	2.2
1	B	1588	GLY	2.2
1	A	1691	ILE	2.2
1	B	1795	LYS	2.2
1	B	1679	ARG	2.1
1	B	1841	ARG	2.1
1	B	1834	LEU	2.1
1	B	1434	PRO	2.1
1	B	1667	GLU	2.1
1	B	1697	TRP	2.1
1	B	1700	LEU	2.1
1	B	1807	VAL	2.1
1	B	1846	HIS	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	1361	VAL	2.1
1	A	1805	GLY	2.0
1	B	1759	ASP	2.0
1	B	1704	LEU	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.