



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:16 PM UTC

PDB ID : 1EWR / pdb_00001ewr
Title : CRYSTAL STRUCTURE OF TAQ MUTS
Authors : Obmolova, G.; Ban, C.; Hsieh, P.; Yang, W.
Deposited on : 2000-04-26
Resolution : 3.19 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

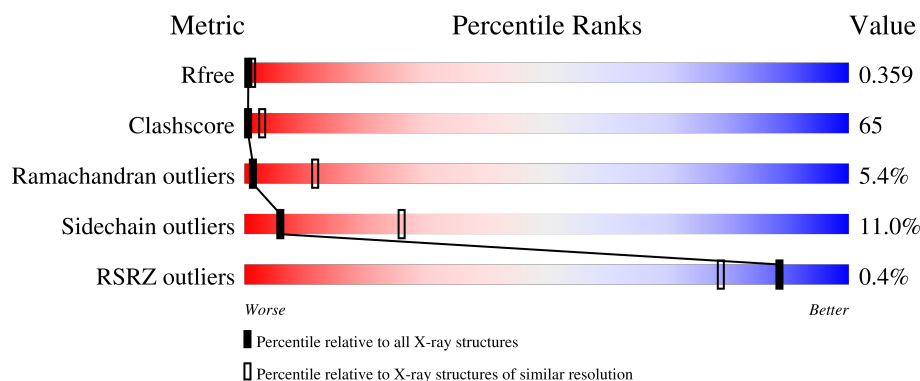
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.19 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}	180053	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

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 of 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	649	
1	B	649	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 7593 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 DNA MISMATCH REPAIR PROTEIN MUTS.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	447	Total	C	N	O	Se	0	0	0
			3468	2209	626	626	7			
1	B	529	Total	C	N	O	Se	0	0	0
			4125	2623	740	755	7			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	250	MSE	MET	modified residue	UNP Q56215
A	574	MSE	MET	modified residue	UNP Q56215
A	586	MSE	MET	modified residue	UNP Q56215
A	640	MSE	MET	modified residue	UNP Q56215
A	643	MSE	MET	modified residue	UNP Q56215
A	744	MSE	MET	modified residue	UNP Q56215
A	762	MSE	MET	modified residue	UNP Q56215
B	1250	MSE	MET	modified residue	UNP Q56215
B	1574	MSE	MET	modified residue	UNP Q56215
B	1586	MSE	MET	modified residue	UNP Q56215
B	1640	MSE	MET	modified residue	UNP Q56215
B	1643	MSE	MET	modified residue	UNP Q56215
B	1744	MSE	MET	modified residue	UNP Q56215
B	1762	MSE	MET	modified residue	UNP Q56215



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	96.73Å 96.73Å 427.13Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.94 – 3.19 19.94 – 3.20	Depositor EDS
% Data completeness (in resolution range)	93.0 (19.94-3.19) 94.3 (19.94-3.20)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.47 (at 3.22Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.331 , 0.361 0.332 , 0.359	Depositor DCC
R_{free} test set	3385 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	98.6	Xtriage
Anisotropy	0.224	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 155.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.058 for -h,-k,l	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	7593	wwPDB-VP
Average B, all atoms (Å ²)	101.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.30% 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	0.49	0/3526	1.03	15/4757 (0.3%)
1	B	0.53	0/4192	1.02	16/5662 (0.3%)
All	All	0.51	0/7718	1.03	31/10419 (0.3%)

There are no bond length outliers.

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	270	ASP	N-CA-C	7.45	119.58	110.41
1	B	1749	LYS	N-CA-C	6.93	119.71	111.33
1	B	1270	ASP	N-CA-C	6.76	119.26	110.53
1	B	1386	LEU	N-CA-C	6.70	120.08	109.50
1	B	1248	ALA	N-CA-C	-6.68	105.01	113.02
1	A	749	LYS	N-CA-C	6.52	119.22	111.33
1	B	1512	ARG	N-CA-C	-6.22	105.68	113.20
1	B	1715	ALA	N-CA-C	-6.09	100.15	109.65
1	B	1626	ILE	N-CA-C	6.02	118.03	108.89
1	A	608	PHE	N-CA-C	-5.98	100.81	110.32
1	B	1608	PHE	N-CA-C	-5.91	100.92	110.32
1	A	134	LEU	N-CA-C	-5.80	99.06	108.52
1	A	715	ALA	N-CA-C	-5.80	101.15	110.14
1	B	1696	HIS	N-CA-C	-5.72	105.64	113.30
1	B	1134	LEU	N-CA-C	-5.60	99.39	108.52
1	B	1535	GLU	N-CA-C	-5.60	104.19	111.02
1	A	731	GLY	CA-C-N	5.53	125.84	119.92
1	A	731	GLY	C-N-CA	5.53	125.84	119.92
1	A	714	ALA	N-CA-C	5.51	118.71	109.95
1	A	696	HIS	N-CA-C	-5.42	106.68	113.72
1	A	626	ILE	N-CA-C	5.41	117.17	108.85
1	B	1707	ARG	N-CA-C	5.35	118.82	112.72
1	B	1714	ALA	N-CA-C	5.29	118.34	110.14
1	A	307	ASP	N-CA-C	-5.25	105.47	111.14
1	A	613	GLU	N-CA-C	-5.24	101.39	109.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1613	GLU	N-CA-C	-5.24	101.33	109.24
1	B	1353	ARG	N-CA-C	-5.21	105.50	111.07
1	A	133	TYR	N-CA-C	5.17	117.85	109.06
1	A	707	ARG	N-CA-C	5.15	118.59	112.72
1	B	1307	ASP	N-CA-C	-5.15	105.58	111.14
1	A	535	GLU	N-CA-C	-5.03	106.65	112.89

There are no chirality outliers.

There are no planarity outliers.

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	3468	0	3513	454	0
1	B	4125	0	4200	553	0
All	All	7593	0	7713	995	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 65.

All (995) 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:292:LEU:HD23	1:A:605:VAL:HG21	1.31	1.11
1:A:272:LEU:HD11	1:A:602:LEU:HD21	1.32	1.10
1:A:209:PRO:HB2	1:A:218:ARG:HH21	1.16	1.04
1:A:557:ARG:HH21	1:A:610:PRO:HA	1.26	1.00
1:B:1557:ARG:HH21	1:B:1610:PRO:HA	1.23	0.99
1:B:1117:THR:HG22	1:B:1119:GLY:H	1.28	0.98
1:B:1698:PHE:O	1:B:1701:THR:HG22	1.63	0.97
1:B:1160:LEU:HD22	1:B:1166:LEU:HA	1.43	0.97
1:B:1129:ARG:H	1:B:1129:ARG:HE	1.11	0.96
1:A:677:ALA:HB1	1:A:700:LEU:HD11	1.47	0.95
1:A:290:SER:HA	1:A:293:ARG:HH12	1.31	0.94
1:B:1296:LEU:HD12	1:B:1302:LEU:HG	1.49	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:722:LEU:HB2	1:A:744:MSE:SE	2.18	0.94
1:B:1674:VAL:HG13	1:B:1699:GLU:HG3	1.50	0.94
1:A:698:PHE:O	1:A:701:THR:HG22	1.68	0.93
1:B:1717:GLU:HA	1:B:1722:LEU:HA	1.51	0.92
1:A:674:VAL:HG13	1:A:699:GLU:HG3	1.50	0.92
1:A:250:MSE:HE3	1:A:604:GLN:OE1	1.70	0.91
1:B:1590:SER:HA	1:B:1593:LEU:HD12	1.53	0.91
1:B:1122:LEU:HD21	1:B:1341:LEU:HD13	1.51	0.90
1:B:1354:ARG:HG2	1:B:1354:ARG:HH11	1.32	0.90
1:B:1366:LEU:HD11	1:B:1527:LEU:HD21	1.52	0.90
1:B:1674:VAL:CG1	1:B:1699:GLU:HG3	2.02	0.89
1:B:1129:ARG:HB2	1:B:1285:ARG:HD2	1.54	0.89
1:B:1677:ALA:HB1	1:B:1700:LEU:HD11	1.53	0.89
1:B:1290:SER:HA	1:B:1293:ARG:HH12	1.37	0.89
1:B:1325:LEU:HD12	1:B:1362:LEU:HD23	1.54	0.89
1:A:674:VAL:CG1	1:A:699:GLU:HG3	2.04	0.88
1:B:1129:ARG:HB3	1:B:1282:ALA:HA	1.55	0.88
1:A:263:PHE:HE2	1:A:292:LEU:HD12	1.36	0.87
1:A:590:SER:HA	1:A:593:LEU:HD12	1.53	0.87
1:B:1335:LEU:HD11	1:B:1352:LEU:HB2	1.55	0.87
1:B:1557:ARG:HH21	1:B:1610:PRO:CA	1.86	0.87
1:B:1209:PRO:HB2	1:B:1218:ARG:HH21	1.39	0.87
1:A:639:PHE:CZ	1:A:643:MSE:HE3	2.11	0.86
1:A:345:SER:HB2	1:A:346:PRO:HD2	1.55	0.86
1:A:296:LEU:HD12	1:A:302:LEU:HG	1.57	0.85
1:B:1718:GLU:HB2	1:B:1723:VAL:CG2	2.07	0.84
1:B:1639:PHE:CZ	1:B:1643:MSE:HE3	2.12	0.84
1:A:557:ARG:HH21	1:A:610:PRO:CA	1.91	0.83
1:A:160:LEU:HD22	1:A:166:LEU:HA	1.59	0.83
1:B:1161:LYS:HE2	1:B:1161:LYS:H	1.39	0.83
1:B:1280:ARG:HG3	1:B:1280:ARG:HH11	1.43	0.82
1:B:1154:GLU:HA	1:B:1239:GLN:NE2	1.95	0.81
1:A:148:LEU:HB3	1:A:224:LEU:HD13	1.60	0.81
1:B:1568:VAL:HG11	1:B:1727:GLN:HE22	1.43	0.81
1:B:1646:VAL:HA	1:B:1649:ILE:CD1	2.11	0.80
1:B:1354:ARG:HG2	1:B:1354:ARG:NH1	1.94	0.80
1:A:143:TRP:CE3	1:A:166:LEU:HD22	2.16	0.79
1:B:1563:ARG:HE	1:B:1563:ARG:HA	1.44	0.79
1:A:597:ALA:HB2	1:A:660:LEU:HD11	1.64	0.79
1:A:563:ARG:HE	1:A:563:ARG:HA	1.47	0.79
1:B:1597:ALA:HB2	1:B:1660:LEU:HD11	1.64	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:519:GLU:HA	1:A:522:ARG:NH1	1.97	0.79
1:B:1366:LEU:HD11	1:B:1527:LEU:CD2	2.14	0.78
1:B:1715:ALA:HA	1:B:1724:PHE:HA	1.64	0.78
1:A:161:LYS:HE2	1:A:161:LYS:H	1.48	0.78
1:B:1209:PRO:HB2	1:B:1218:ARG:NH2	1.99	0.78
1:A:276:LEU:HD11	1:A:602:LEU:CD2	2.14	0.77
1:A:697:TYR:HB2	1:A:700:LEU:HD12	1.66	0.77
1:B:1508:GLU:O	1:B:1512:ARG:HG3	1.84	0.77
1:B:1279:THR:HG21	1:B:1285:ARG:HB2	1.66	0.77
1:B:1352:LEU:HD12	1:B:1352:LEU:O	1.84	0.77
1:A:718:GLU:HB2	1:A:723:VAL:HG21	1.67	0.77
1:A:739:VAL:HG21	1:A:759:LEU:HD12	1.67	0.76
1:B:1331:ASP:OD2	1:B:1334:ARG:HD2	1.83	0.76
1:A:143:TRP:HE3	1:A:166:LEU:HD22	1.50	0.76
1:B:1122:LEU:CD2	1:B:1341:LEU:HD13	2.15	0.76
1:B:1544:ARG:HB2	1:B:1608:PHE:CZ	2.20	0.76
1:A:322:VAL:O	1:A:326:LEU:HG	1.86	0.76
1:A:568:VAL:HG12	1:A:727:GLN:HE22	1.51	0.76
1:B:1143:TRP:CE3	1:B:1166:LEU:HD22	2.20	0.76
1:B:1160:LEU:HD22	1:B:1166:LEU:CA	2.16	0.75
1:A:261:GLU:CG	1:A:266:LEU:HG	2.16	0.75
1:A:646:VAL:HA	1:A:649:ILE:CD1	2.15	0.75
1:A:742:ALA:HA	1:B:1643:MSE:HG3	1.66	0.75
1:B:1296:LEU:HD13	1:B:1301:PRO:HB2	1.67	0.74
1:B:1129:ARG:O	1:B:1286:ARG:HG3	1.86	0.74
1:B:1117:THR:HG22	1:B:1119:GLY:N	2.00	0.74
1:B:1298:ASP:O	1:B:1301:PRO:HD2	1.86	0.74
1:B:1718:GLU:HB2	1:B:1723:VAL:HG21	1.69	0.74
1:A:302:LEU:HD21	1:A:604:GLN:HA	1.68	0.74
1:B:1718:GLU:OE1	1:B:1723:VAL:HG21	1.87	0.74
1:A:279:THR:HG21	1:A:285:ARG:HB2	1.68	0.74
1:A:672:ASP:O	1:A:676:ILE:HG12	1.88	0.74
1:B:1143:TRP:HE3	1:B:1166:LEU:HD22	1.51	0.74
1:B:1144:GLY:HA3	1:B:1216:ALA:O	1.87	0.74
1:B:1222:GLY:HA2	1:B:1225:LEU:HD12	1.69	0.74
1:B:1118:PRO:HD2	1:B:1177:GLU:OE1	1.87	0.73
1:B:1339:LEU:O	1:B:1511:LYS:HD2	1.89	0.73
1:B:1693:PHE:HE2	1:B:1695:THR:HB	1.52	0.73
1:B:1710:ASN:O	1:B:1711:LEU:HD23	1.88	0.73
1:A:710:ASN:O	1:A:711:LEU:HD23	1.87	0.73
1:A:557:ARG:HA	1:A:567:PHE:HE2	1.52	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:568:VAL:CG1	1:A:727:GLN:HE22	2.01	0.73
1:B:1366:LEU:CD1	1:B:1527:LEU:HD21	2.18	0.73
1:B:1715:ALA:O	1:B:1716:ARG:HG2	1.87	0.72
1:A:290:SER:HA	1:A:293:ARG:NH1	2.02	0.72
1:B:1228:ALA:HB3	1:B:1236:LEU:HD11	1.72	0.72
1:B:1250:MSE:HE3	1:B:1604:GLN:OE1	1.90	0.72
1:B:1557:ARG:NH2	1:B:1610:PRO:HA	2.01	0.72
1:A:717:GLU:HA	1:A:722:LEU:HA	1.71	0.71
1:B:1708:LEU:HG	1:B:1709:LYS:H	1.54	0.71
1:B:1217:LEU:HD23	1:B:1218:ARG:N	2.05	0.71
1:B:1290:SER:HA	1:B:1293:ARG:NH1	2.05	0.71
1:A:280:ARG:HB2	1:A:528:ASP:OD1	1.90	0.71
1:B:1697:TYR:HB2	1:B:1700:LEU:HD12	1.72	0.71
1:A:572:LEU:HD13	1:A:592:PHE:HZ	1.55	0.71
1:B:1557:ARG:HA	1:B:1567:PHE:HE2	1.53	0.71
1:A:250:MSE:HB3	1:A:295:PRO:HB2	1.71	0.71
1:A:752:VAL:O	1:A:755:ALA:HB3	1.90	0.71
1:B:1261:GLU:CG	1:B:1266:LEU:HG	2.20	0.71
1:B:1161:LYS:HD2	1:B:1162:SER:H	1.56	0.71
1:B:1532:ALA:O	1:B:1535:GLU:HB3	1.90	0.71
1:B:1589:LYS:HZ2	1:B:1696:HIS:CE1	2.08	0.70
1:A:548:GLY:O	1:A:617:PRO:HA	1.91	0.70
1:A:584:PRO:HG3	1:A:715:ALA:HB2	1.72	0.70
1:A:600:ALA:HA	1:A:616:LEU:HD13	1.73	0.70
1:B:1739:VAL:HG21	1:B:1759:LEU:HD12	1.72	0.70
1:B:1122:LEU:HD12	1:B:1122:LEU:O	1.91	0.70
1:A:557:ARG:NH2	1:A:610:PRO:HA	2.05	0.70
1:A:716:ARG:O	1:A:723:VAL:N	2.24	0.70
1:B:1132:ASN:O	1:B:1149:ASP:HB2	1.90	0.70
1:A:708:LEU:HG	1:A:709:LYS:H	1.54	0.70
1:B:1717:GLU:CA	1:B:1722:LEU:HA	2.20	0.70
1:B:1563:ARG:HE	1:B:1563:ARG:CA	2.05	0.70
1:A:250:MSE:HA	1:A:620:ASP:O	1.90	0.70
1:B:1672:ASP:O	1:B:1676:ILE:HG12	1.90	0.70
1:B:1120:THR:O	1:B:1150:VAL:HG21	1.92	0.70
1:B:1646:VAL:HA	1:B:1649:ILE:HD12	1.74	0.70
1:A:698:PHE:O	1:A:701:THR:CG2	2.39	0.70
1:B:1192:ASP:O	1:B:1196:LYS:HG2	1.92	0.69
1:B:1723:VAL:HG12	1:B:1723:VAL:O	1.91	0.69
1:A:170:LEU:HD13	1:A:170:LEU:O	1.91	0.69
1:B:1161:LYS:H	1:B:1161:LYS:CE	2.04	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1716:ARG:H	1:B:1723:VAL:H	1.39	0.68
1:A:174:ARG:HH11	1:A:174:ARG:HB3	1.57	0.68
1:A:696:HIS:O	1:B:1669:SER:HB3	1.94	0.68
1:A:563:ARG:HE	1:A:563:ARG:CA	2.07	0.68
1:B:1718:GLU:HB2	1:B:1723:VAL:HG23	1.73	0.68
1:B:1171:PHE:CE2	1:B:1254:GLU:HG3	2.28	0.68
1:B:1578:LEU:C	1:B:1578:LEU:HD23	2.19	0.68
1:A:693:PHE:HE2	1:A:695:THR:HB	1.59	0.67
1:B:1322:VAL:O	1:B:1326:LEU:HG	1.94	0.67
1:B:1742:ALA:C	1:B:1747:LEU:HD12	2.19	0.67
1:A:292:LEU:CD2	1:A:605:VAL:HG21	2.20	0.67
1:A:693:PHE:CE2	1:A:695:THR:HB	2.30	0.67
1:B:1117:THR:HG23	1:B:1177:GLU:CD	2.20	0.67
1:A:161:LYS:HD2	1:A:162:SER:H	1.60	0.67
1:B:1228:ALA:O	1:B:1232:GLN:HB2	1.93	0.67
1:B:1352:LEU:HD12	1:B:1356:LEU:HG	1.76	0.67
1:A:742:ALA:HB1	1:A:747:LEU:CD1	2.25	0.67
1:B:1232:GLN:HG3	1:B:1236:LEU:HD23	1.76	0.67
1:B:1290:SER:CA	1:B:1293:ARG:HH12	2.08	0.67
1:B:1378:LEU:HG	1:B:1510:ALA:HA	1.77	0.67
1:B:1263:PHE:HE2	1:B:1292:LEU:HD12	1.60	0.66
1:B:1600:ALA:HA	1:B:1616:LEU:HD13	1.75	0.66
1:B:1332:LEU:HD12	1:B:1332:LEU:H	1.60	0.66
1:B:1367:GLY:C	1:B:1369:GLU:H	2.04	0.66
1:B:1698:PHE:O	1:B:1701:THR:CG2	2.40	0.66
1:A:625:ARG:HG3	1:A:625:ARG:HH11	1.60	0.66
1:B:1313:VAL:HG13	1:B:1538:VAL:CG2	2.24	0.66
1:B:1313:VAL:HG23	1:B:1534:ALA:HB1	1.78	0.66
1:B:1593:LEU:HD21	1:B:1694:ALA:HB2	1.78	0.66
1:A:712:HIS:ND1	1:A:731:GLY:O	2.29	0.66
1:A:750:GLU:H	1:A:750:GLU:CD	2.02	0.66
1:B:1366:LEU:HD12	1:B:1370:VAL:HG21	1.77	0.66
1:B:1522:ARG:HG2	1:B:1522:ARG:HH11	1.61	0.66
1:B:1313:VAL:HG13	1:B:1538:VAL:HG22	1.77	0.66
1:A:174:ARG:HB3	1:A:174:ARG:NH1	2.10	0.66
1:B:1536:VAL:HG12	1:B:1537:ALA:N	2.11	0.65
1:A:535:GLU:HG3	1:A:539:ARG:HH12	1.61	0.65
1:A:192:ASP:O	1:A:196:LYS:HG2	1.96	0.65
1:B:1752:VAL:O	1:B:1755:ALA:HB3	1.95	0.65
1:A:292:LEU:HD23	1:A:605:VAL:CG2	2.19	0.65
1:B:1247:GLY:HA2	1:B:1251:ARG:NH1	2.12	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:758:LEU:HB3	1:A:762:MSE:CE	2.26	0.65
1:B:1117:THR:HB	1:B:1120:THR:OG1	1.96	0.65
1:B:1174:ARG:HH11	1:B:1174:ARG:HB3	1.62	0.65
1:B:1750:GLU:CD	1:B:1750:GLU:H	2.03	0.65
1:B:1210:GLU:O	1:B:1218:ARG:HB3	1.97	0.65
1:A:293:ARG:NH1	1:A:293:ARG:HB2	2.12	0.65
1:B:1272:LEU:HD11	1:B:1602:LEU:HD21	1.77	0.64
1:A:715:ALA:HB1	1:A:722:LEU:HD22	1.78	0.64
1:A:578:LEU:HD23	1:A:578:LEU:C	2.22	0.64
1:A:260:LEU:HD21	1:A:597:ALA:HB1	1.78	0.64
1:A:625:ARG:NH2	1:A:627:GLY:O	2.30	0.64
1:A:132:ASN:O	1:A:149:ASP:HB2	1.98	0.64
1:A:589:LYS:HZ2	1:A:696:HIS:CE1	2.15	0.64
1:B:1299:ARG:NH2	1:B:1547:PHE:HB2	2.12	0.64
1:B:1693:PHE:CE2	1:B:1695:THR:HB	2.30	0.64
1:A:148:LEU:HD12	1:A:155:PHE:CD1	2.31	0.64
1:A:581:ILE:HG22	1:A:589:LYS:HG2	1.80	0.64
1:B:1315:GLU:HB3	1:B:1318:LEU:HB3	1.80	0.64
1:A:646:VAL:HA	1:A:649:ILE:HD12	1.79	0.64
1:B:1580:LEU:HA	1:B:1693:PHE:O	1.98	0.64
1:B:1742:ALA:HB1	1:B:1747:LEU:CD1	2.28	0.64
1:A:284:GLY:HA2	1:A:525:ALA:HB1	1.80	0.64
1:A:647:ALA:O	1:A:651:LYS:HG3	1.98	0.64
1:A:290:SER:CA	1:A:293:ARG:HH12	2.09	0.64
1:B:1129:ARG:HE	1:B:1129:ARG:N	1.90	0.64
1:B:1250:MSE:SE	1:B:1622:ILE:HG13	2.47	0.64
1:B:1280:ARG:HG3	1:B:1280:ARG:NH1	2.11	0.63
1:A:518:ARG:HB3	1:A:522:ARG:NH2	2.14	0.63
1:B:1313:VAL:CG2	1:B:1534:ALA:HB1	2.28	0.63
1:A:263:PHE:HE2	1:A:292:LEU:CD1	2.08	0.63
1:A:579:VAL:HB	1:A:692:LEU:HD23	1.79	0.63
1:B:1625:ARG:HH11	1:B:1625:ARG:HG3	1.63	0.63
1:B:1647:ALA:O	1:B:1651:LYS:HG3	1.99	0.63
1:A:319:ARG:HD2	1:A:534:ALA:HB3	1.80	0.63
1:A:342:GLY:O	1:A:343:ARG:HG3	1.99	0.63
1:A:742:ALA:C	1:A:747:LEU:HD12	2.23	0.63
1:B:1534:ALA:O	1:B:1538:VAL:HG23	1.98	0.63
1:A:237:SER:HB2	1:A:341:LEU:HG	1.81	0.63
1:B:1581:ILE:O	1:B:1589:LYS:HD3	1.99	0.63
1:A:743:ALA:HB2	1:A:752:VAL:HG11	1.79	0.62
1:A:148:LEU:CB	1:A:224:LEU:HD13	2.29	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:574:MSE:HE3	1:A:579:VAL:HG23	1.81	0.62
1:B:1717:GLU:N	1:B:1722:LEU:HD23	2.13	0.62
1:B:1722:LEU:HB2	1:B:1744:MSE:SE	2.49	0.62
1:B:1568:VAL:CG1	1:B:1727:GLN:HE22	2.11	0.62
1:A:539:ARG:NH1	1:A:539:ARG:HB2	2.14	0.62
1:B:1130:GLU:HG3	1:B:1285:ARG:HD3	1.80	0.62
1:B:1346:PRO:HG3	1:B:1503:PHE:CZ	2.35	0.62
1:B:1712:HIS:ND1	1:B:1731:GLY:O	2.32	0.62
1:A:181:ALA:O	1:A:185:LEU:HG	1.98	0.62
1:A:305:ARG:O	1:A:309:VAL:HG23	1.99	0.62
1:B:1743:ALA:HB2	1:B:1752:VAL:CG1	2.29	0.62
1:A:743:ALA:HB2	1:A:752:VAL:CG1	2.29	0.62
1:B:1717:GLU:HA	1:B:1722:LEU:CA	2.29	0.62
1:A:161:LYS:H	1:A:161:LYS:CE	2.13	0.62
1:A:297:LEU:O	1:A:618:LEU:HD13	2.00	0.62
1:B:1698:PHE:O	1:B:1701:THR:N	2.33	0.62
1:B:1743:ALA:HB2	1:B:1752:VAL:HG11	1.82	0.61
1:B:1129:ARG:CZ	1:B:1285:ARG:NH1	2.63	0.61
1:B:1373:PRO:HG2	1:B:1519:GLU:HG2	1.82	0.61
1:B:1609:VAL:HB	1:B:1610:PRO:HD2	1.82	0.61
1:B:1292:LEU:HD23	1:B:1605:VAL:HG21	1.82	0.61
1:A:654:THR:O	1:A:689:ALA:HB2	2.01	0.61
1:B:1261:GLU:HG3	1:B:1266:LEU:HG	1.81	0.61
1:B:1250:MSE:HB3	1:B:1295:PRO:HB2	1.82	0.61
1:B:1129:ARG:H	1:B:1129:ARG:NE	1.91	0.61
1:A:581:ILE:O	1:A:589:LYS:HD3	2.00	0.61
1:B:1211:GLY:O	1:B:1218:ARG:HD2	2.01	0.61
1:B:1587:ALA:HB3	1:B:1713:VAL:HG21	1.83	0.61
1:B:1174:ARG:HB3	1:B:1174:ARG:NH1	2.16	0.61
1:B:1572:LEU:HD13	1:B:1592:PHE:HZ	1.65	0.61
1:B:1178:VAL:O	1:B:1202:LEU:HA	2.01	0.60
1:B:1170:LEU:HD13	1:B:1170:LEU:O	2.01	0.60
1:B:1574:MSE:HE3	1:B:1579:VAL:HG23	1.82	0.60
1:A:581:ILE:CG2	1:A:589:LYS:HG2	2.31	0.60
1:A:586:MSE:HB2	1:A:724:PHE:CE2	2.36	0.60
1:B:1722:LEU:HD12	1:B:1744:MSE:SE	2.51	0.60
1:A:580:LEU:HA	1:A:693:PHE:O	2.00	0.60
1:B:1581:ILE:HG22	1:B:1589:LYS:HG2	1.83	0.60
1:B:1654:THR:O	1:B:1689:ALA:HB2	2.02	0.60
1:A:221:ARG:HD3	1:A:241:PHE:CE1	2.37	0.60
1:A:280:ARG:HG3	1:A:280:ARG:HH11	1.67	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1710:ASN:C	1:B:1711:LEU:HD23	2.27	0.60
1:A:578:LEU:HD22	1:A:708:LEU:HD12	1.83	0.60
1:B:1674:VAL:HG11	1:B:1699:GLU:HG3	1.83	0.60
1:B:1685:HIS:CD2	1:B:1705:LEU:HD13	2.37	0.60
1:A:209:PRO:HB2	1:A:218:ARG:NH2	2.01	0.59
1:A:698:PHE:O	1:A:701:THR:N	2.35	0.59
1:B:1698:PHE:O	1:B:1699:GLU:C	2.44	0.59
1:A:171:PHE:CE2	1:A:254:GLU:HG3	2.37	0.59
1:A:315:GLU:HB3	1:A:318:LEU:HB3	1.83	0.59
1:A:302:LEU:HD22	1:A:547:PHE:CZ	2.37	0.59
1:A:710:ASN:C	1:A:711:LEU:HD23	2.28	0.59
1:B:1716:ARG:O	1:B:1723:VAL:N	2.35	0.59
1:A:160:LEU:HD13	1:A:166:LEU:HD12	1.84	0.59
1:B:1578:LEU:HD22	1:B:1708:LEU:HD12	1.84	0.59
1:A:283:PRO:HB2	1:A:525:ALA:HB2	1.84	0.59
1:B:1161:LYS:H	1:B:1161:LYS:CD	2.15	0.59
1:B:1579:VAL:HB	1:B:1692:LEU:HD23	1.84	0.59
1:B:1599:ILE:HG23	1:B:1609:VAL:HG21	1.85	0.59
1:A:221:ARG:NH1	1:A:241:PHE:CD2	2.71	0.59
1:B:1117:THR:HG23	1:B:1177:GLU:OE1	2.03	0.59
1:B:1166:LEU:HD23	1:B:1167:TYR:CD1	2.38	0.59
1:A:578:LEU:HD22	1:A:708:LEU:CD1	2.33	0.58
1:B:1602:LEU:O	1:B:1605:VAL:HG12	2.03	0.58
1:A:278:GLU:C	1:A:532:ALA:HB1	2.28	0.58
1:A:321:GLY:O	1:A:325:LEU:HG	2.03	0.58
1:B:1342:GLY:O	1:B:1343:ARG:HG3	2.02	0.58
1:A:148:LEU:HD12	1:A:155:PHE:CE1	2.37	0.58
1:B:1291:TRP:CZ3	1:B:1305:ARG:HD3	2.37	0.58
1:B:1312:PHE:HD2	1:B:1319:ARG:HA	1.69	0.58
1:A:552:GLN:HG2	1:A:573:GLU:HG2	1.85	0.58
1:A:685:HIS:CD2	1:A:705:LEU:HD13	2.38	0.58
1:B:1578:LEU:HD22	1:B:1708:LEU:CD1	2.34	0.58
1:A:302:LEU:CD2	1:A:604:GLN:HA	2.34	0.58
1:A:572:LEU:HD13	1:A:592:PHE:CZ	2.38	0.58
1:A:685:HIS:CE1	1:A:707:ARG:HB2	2.39	0.58
1:B:1172:ARG:O	1:B:1293:ARG:HD2	2.03	0.58
1:A:261:GLU:HG2	1:A:266:LEU:HG	1.86	0.58
1:B:1352:LEU:HD12	1:B:1352:LEU:C	2.28	0.58
1:B:1715:ALA:HB1	1:B:1722:LEU:HD22	1.86	0.58
1:A:587:ALA:HB3	1:A:713:VAL:HG21	1.85	0.57
1:B:1716:ARG:N	1:B:1723:VAL:H	2.01	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:558:HIS:HD2	1:A:561:VAL:HG23	1.69	0.57
1:A:551:LEU:HA	1:A:615:HIS:O	2.04	0.57
1:A:593:LEU:HD21	1:A:694:ALA:HB2	1.84	0.57
1:A:722:LEU:HB2	1:A:744:MSE:CE	2.34	0.57
1:B:1658:LEU:HD12	1:B:1659:VAL:N	2.19	0.57
1:B:1716:ARG:O	1:B:1718:GLU:N	2.38	0.57
1:B:1120:THR:HG21	1:B:1231:THR:OG1	2.04	0.57
1:B:1321:GLY:O	1:B:1325:LEU:HG	2.04	0.57
1:B:1581:ILE:CG2	1:B:1589:LYS:HG2	2.35	0.57
1:A:715:ALA:HA	1:A:724:PHE:HA	1.85	0.57
1:B:1551:LEU:HA	1:B:1615:HIS:O	2.04	0.57
1:A:284:GLY:CA	1:A:525:ALA:HB1	2.35	0.57
1:A:663:GLU:HB3	1:A:666:ARG:HD3	1.86	0.57
1:B:1150:VAL:HG23	1:B:1151:SER:N	2.18	0.57
1:B:1356:LEU:O	1:B:1360:PRO:HD3	2.05	0.57
1:B:1716:ARG:CB	1:B:1723:VAL:HB	2.33	0.57
1:A:263:PHE:CE2	1:A:292:LEU:HD12	2.28	0.57
1:B:1533:LEU:O	1:B:1536:VAL:N	2.38	0.57
1:B:1564:ARG:O	1:B:1565:THR:HG23	2.05	0.57
1:B:1698:PHE:C	1:B:1701:THR:HG22	2.27	0.57
1:A:137:ILE:HA	1:A:144:GLY:O	2.05	0.57
1:A:263:PHE:HE1	1:A:293:ARG:HG3	1.69	0.57
1:A:273:PHE:O	1:A:277:ASP:N	2.37	0.57
1:A:564:ARG:O	1:A:565:THR:HG23	2.04	0.57
1:A:680:VAL:O	1:A:683:ALA:HB3	2.04	0.57
1:A:713:VAL:HG12	1:A:728:VAL:HG22	1.86	0.57
1:B:1183:GLU:CD	1:B:1219:ARG:HH22	2.13	0.57
1:B:1354:ARG:HH11	1:B:1354:ARG:CG	2.08	0.57
1:A:282:ALA:N	1:A:283:PRO:CD	2.68	0.56
1:A:150:VAL:HG23	1:A:151:SER:N	2.20	0.56
1:B:1317:ALA:O	1:B:1320:GLU:HB2	2.05	0.56
1:B:1716:ARG:HB2	1:B:1723:VAL:HB	1.86	0.56
1:B:1589:LYS:O	1:B:1592:PHE:HB3	2.06	0.56
1:A:261:GLU:HG3	1:A:266:LEU:HG	1.86	0.56
1:A:604:GLN:HE22	1:A:618:LEU:HA	1.70	0.56
1:B:1309:VAL:HG13	1:B:1534:ALA:HB2	1.88	0.56
1:B:1501:GLU:O	1:B:1505:GLU:HG3	2.05	0.56
1:B:1685:HIS:CE1	1:B:1707:ARG:HB2	2.40	0.56
1:A:232:GLN:HG3	1:A:236:LEU:HD23	1.87	0.56
1:A:281:THR:HB	1:A:283:PRO:HD2	1.87	0.56
1:A:284:GLY:N	1:A:525:ALA:HB1	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1282:ALA:N	1:B:1283:PRO:CD	2.69	0.56
1:B:1357:GLN:O	1:B:1360:PRO:HD2	2.06	0.56
1:B:1379:LYS:O	1:B:1383:GLU:HG3	2.05	0.56
1:B:1680:VAL:O	1:B:1683:ALA:HB3	2.06	0.56
1:A:581:ILE:HD13	1:A:711:LEU:HB2	1.88	0.56
1:B:1376:SER:OG	1:B:1377:PRO:HD3	2.06	0.56
1:B:1542:TYR:CE1	1:B:1610:PRO:HB3	2.41	0.56
1:B:1581:ILE:HD13	1:B:1711:LEU:HB2	1.87	0.56
1:B:1263:PHE:O	1:B:1271:THR:HG21	2.06	0.56
1:B:1282:ALA:HB3	1:B:1283:PRO:HD3	1.88	0.56
1:B:1520:ALA:O	1:B:1524:LEU:HG	2.06	0.56
1:B:1533:LEU:O	1:B:1536:VAL:HB	2.05	0.56
1:B:1587:ALA:HB3	1:B:1713:VAL:CG2	2.36	0.56
1:A:674:VAL:HG11	1:A:699:GLU:HG3	1.87	0.55
1:B:1205:ALA:HB2	1:B:1227:TYR:HD1	1.71	0.55
1:A:171:PHE:O	1:A:174:ARG:HG2	2.07	0.55
1:A:698:PHE:HA	1:A:701:THR:HG22	1.88	0.55
1:A:160:LEU:HD22	1:A:166:LEU:CA	2.31	0.55
1:A:211:GLY:O	1:A:218:ARG:HD2	2.05	0.55
1:A:281:THR:HG23	1:A:528:ASP:CG	2.31	0.55
1:A:625:ARG:HG3	1:A:625:ARG:NH1	2.18	0.55
1:A:518:ARG:HH11	1:A:518:ARG:HG2	1.70	0.55
1:A:602:LEU:O	1:A:605:VAL:HG12	2.06	0.55
1:B:1551:LEU:O	1:B:1573:GLU:HA	2.07	0.55
1:B:1552:GLN:HG2	1:B:1573:GLU:HG2	1.89	0.55
1:A:609:VAL:HB	1:A:610:PRO:HD2	1.88	0.55
1:A:713:VAL:CG1	1:A:728:VAL:HG22	2.36	0.55
1:B:1139:THR:C	1:B:1216:ALA:HB2	2.32	0.55
1:B:1296:LEU:HB2	1:B:1302:LEU:HD11	1.88	0.55
1:A:306:LEU:HB3	1:A:544:ARG:NE	2.22	0.55
1:A:540:TYR:CE2	1:A:563:ARG:HD3	2.41	0.55
1:A:698:PHE:O	1:A:699:GLU:C	2.49	0.55
1:B:1137:ILE:HA	1:B:1144:GLY:O	2.06	0.55
1:A:139:THR:C	1:A:216:ALA:HB2	2.32	0.55
1:A:643:MSE:HG3	1:B:1742:ALA:HA	1.87	0.55
1:B:1131:ALA:HB2	1:B:1286:ARG:HD2	1.89	0.55
1:B:1182:PRO:O	1:B:1186:GLU:HG3	2.07	0.55
1:B:1625:ARG:HA	1:B:1645:GLU:OE1	2.07	0.55
1:A:712:HIS:CD2	1:A:733:ALA:HA	2.42	0.55
1:B:1643:MSE:HE1	1:B:1665:GLY:HA2	1.89	0.55
1:B:1712:HIS:CD2	1:B:1733:ALA:HA	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:625:ARG:HG3	1:A:625:ARG:O	2.07	0.54
1:A:717:GLU:N	1:A:722:LEU:HD23	2.22	0.54
1:A:166:LEU:O	1:A:168:ASP:N	2.41	0.54
1:A:237:SER:OG	1:A:340:GLU:HB2	2.07	0.54
1:A:658:LEU:HD12	1:A:659:VAL:N	2.22	0.54
1:A:587:ALA:HB3	1:A:713:VAL:CG2	2.38	0.54
1:A:599:ILE:HG23	1:A:609:VAL:HG21	1.89	0.54
1:A:551:LEU:O	1:A:573:GLU:HA	2.07	0.54
1:A:651:LYS:HE2	1:B:1748:PRO:HG3	1.88	0.54
1:A:685:HIS:NE2	1:A:705:LEU:HB3	2.22	0.54
1:B:1148:LEU:C	1:B:1148:LEU:HD23	2.33	0.54
1:A:161:LYS:H	1:A:161:LYS:CD	2.21	0.54
1:A:589:LYS:O	1:A:592:PHE:HB3	2.07	0.54
1:B:1120:THR:C	1:B:1150:VAL:HG21	2.32	0.54
1:B:1298:ASP:O	1:B:1302:LEU:HD12	2.07	0.54
1:B:1721:GLY:O	1:B:1722:LEU:HG	2.08	0.54
1:B:1270:ASP:HB2	1:B:1564:ARG:HH12	1.73	0.54
1:B:1503:PHE:CD2	1:B:1504:LEU:HD12	2.43	0.54
1:B:1619:PHE:CE1	1:B:1658:LEU:HD22	2.43	0.54
1:A:276:LEU:HD11	1:A:602:LEU:HD21	1.89	0.54
1:A:604:GLN:NE2	1:A:618:LEU:HA	2.23	0.54
1:B:1171:PHE:CD2	1:B:1254:GLU:HG3	2.42	0.54
1:B:1663:GLU:HB3	1:B:1666:ARG:HD3	1.90	0.54
1:A:674:VAL:HA	1:A:697:TYR:CE1	2.43	0.54
1:B:1166:LEU:C	1:B:1168:ASP:N	2.65	0.54
1:B:1354:ARG:HH12	1:B:1358:ILE:CD1	2.21	0.54
1:B:1625:ARG:HG3	1:B:1625:ARG:O	2.08	0.54
1:A:148:LEU:C	1:A:148:LEU:HD23	2.33	0.53
1:A:252:LEU:HD22	1:A:257:LEU:HG	1.89	0.53
1:A:753:ALA:C	1:A:755:ALA:N	2.66	0.53
1:B:1143:TRP:CH2	1:B:1163:LYS:HD3	2.42	0.53
1:B:1356:LEU:HA	1:B:1359:LEU:HD22	1.90	0.53
1:B:1597:ALA:O	1:B:1600:ALA:HB3	2.08	0.53
1:B:1698:PHE:HA	1:B:1701:THR:HG22	1.89	0.53
1:A:143:TRP:N	1:A:160:LEU:O	2.41	0.53
1:A:180:LEU:HD22	1:A:184:LEU:HD13	1.90	0.53
1:A:748:PRO:HB2	1:A:751:VAL:HG23	1.90	0.53
1:B:1760:GLN:C	1:B:1762:MSE:H	2.15	0.53
1:A:524:LEU:O	1:A:528:ASP:N	2.37	0.53
1:A:696:HIS:CD2	1:B:1668:THR:HA	2.43	0.53
1:A:722:LEU:N	1:A:744:MSE:HE3	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1320:GLU:O	1:B:1324:ARG:HG3	2.08	0.53
1:B:1625:ARG:NH2	1:B:1627:GLY:O	2.41	0.53
1:A:237:SER:O	1:A:238:LEU:HD23	2.08	0.53
1:A:299:ARG:HA	1:A:618:LEU:HD11	1.90	0.53
1:B:1322:VAL:HG13	1:B:1362:LEU:HD22	1.90	0.53
1:B:1595:GLN:O	1:B:1599:ILE:HG13	2.07	0.53
1:B:1625:ARG:HG3	1:B:1625:ARG:NH1	2.21	0.53
1:A:143:TRP:CH2	1:A:163:LYS:HD3	2.43	0.53
1:B:1247:GLY:HA2	1:B:1251:ARG:HH12	1.70	0.53
1:B:1327:TYR:O	1:B:1328:ARG:HB2	2.07	0.53
1:B:1353:ARG:O	1:B:1357:GLN:HG3	2.09	0.53
1:B:1319:ARG:NH1	1:B:1319:ARG:HB3	2.24	0.53
1:B:1685:HIS:NE2	1:B:1705:LEU:HB3	2.23	0.53
1:B:1693:PHE:C	1:B:1693:PHE:CD2	2.86	0.53
1:A:171:PHE:CD2	1:A:254:GLU:HG3	2.44	0.53
1:B:1129:ARG:CB	1:B:1285:ARG:HD2	2.35	0.53
1:B:1693:PHE:C	1:B:1693:PHE:HD2	2.15	0.53
1:A:228:ALA:HB3	1:A:236:LEU:HD11	1.90	0.53
1:A:718:GLU:HB2	1:A:723:VAL:CG2	2.37	0.53
1:B:1352:LEU:HD11	1:B:1356:LEU:HD11	1.91	0.53
1:B:1703:LEU:O	1:B:1704:GLY:C	2.51	0.53
1:B:1148:LEU:HD12	1:B:1155:PHE:CD1	2.44	0.53
1:B:1716:ARG:C	1:B:1722:LEU:HA	2.34	0.53
1:A:139:THR:CG2	1:A:184:LEU:HD21	2.38	0.53
1:A:552:GLN:O	1:A:614:ALA:HA	2.09	0.53
1:B:1542:TYR:HA	1:B:1609:VAL:O	2.08	0.53
1:A:249:PHE:HA	1:A:297:LEU:HG	1.90	0.52
1:A:646:VAL:O	1:A:650:LEU:HG	2.09	0.52
1:A:323:ARG:CG	1:A:531:ALA:HB1	2.38	0.52
1:B:1273:PHE:HE1	1:B:1288:LEU:HD23	1.75	0.52
1:B:1323:ARG:HG2	1:B:1323:ARG:HH11	1.73	0.52
1:B:1552:GLN:O	1:B:1614:ALA:HA	2.10	0.52
1:A:250:MSE:HG2	1:A:621:GLY:HA2	1.90	0.52
1:A:296:LEU:HD21	1:A:305:ARG:NH2	2.24	0.52
1:B:1604:GLN:HE22	1:B:1618:LEU:HA	1.73	0.52
1:B:1723:VAL:HG12	1:B:1725:TYR:CE1	2.44	0.52
1:A:166:LEU:C	1:A:168:ASP:N	2.65	0.52
1:A:299:ARG:CA	1:A:618:LEU:HD11	2.40	0.52
1:A:619:PHE:CE1	1:A:658:LEU:HD22	2.43	0.52
1:B:1166:LEU:O	1:B:1168:ASP:N	2.43	0.52
1:B:1557:ARG:CA	1:B:1567:PHE:HE2	2.21	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1646:VAL:O	1:B:1650:LEU:HG	2.10	0.52
1:A:228:ALA:O	1:A:232:GLN:HB2	2.10	0.52
1:B:1273:PHE:CE1	1:B:1288:LEU:HD23	2.45	0.52
1:B:1284:GLY:HA2	1:B:1525:ALA:HB1	1.92	0.52
1:A:251:ARG:HG2	1:A:251:ARG:HH11	1.75	0.52
1:A:166:LEU:HD23	1:A:167:TYR:CD1	2.45	0.52
1:A:557:ARG:CA	1:A:567:PHE:HE2	2.19	0.52
1:A:698:PHE:C	1:A:701:THR:HG22	2.32	0.52
1:B:1245:ASP:C	1:B:1247:GLY:H	2.18	0.52
1:B:1620:ASP:OD1	1:B:1657:SER:HA	2.09	0.52
1:B:1674:VAL:HA	1:B:1697:TYR:CE1	2.45	0.52
1:B:1578:LEU:C	1:B:1578:LEU:CD2	2.83	0.52
1:A:276:LEU:HD11	1:A:602:LEU:HD23	1.92	0.51
1:B:1250:MSE:HA	1:B:1297:LEU:HD21	1.92	0.51
1:B:1753:ALA:C	1:B:1755:ALA:N	2.68	0.51
1:A:625:ARG:NE	1:A:642:GLU:HG2	2.24	0.51
1:A:740:GLU:O	1:A:741:VAL:C	2.53	0.51
1:A:758:LEU:O	1:A:762:MSE:HE3	2.11	0.51
1:B:1217:LEU:HD23	1:B:1217:LEU:C	2.36	0.51
1:B:1270:ASP:HB2	1:B:1564:ARG:NH1	2.25	0.51
1:B:1604:GLN:NE2	1:B:1618:LEU:HA	2.24	0.51
1:A:250:MSE:SE	1:A:622:ILE:HG13	2.61	0.51
1:A:760:GLN:O	1:A:763:ALA:HB3	2.10	0.51
1:B:1335:LEU:CD1	1:B:1352:LEU:HB2	2.32	0.51
1:A:317:ALA:O	1:A:320:GLU:HB2	2.10	0.51
1:B:1718:GLU:CB	1:B:1723:VAL:HG21	2.38	0.51
1:A:263:PHE:CE1	1:A:293:ARG:HG3	2.44	0.51
1:A:625:ARG:HA	1:A:645:GLU:OE1	2.10	0.51
1:A:742:ALA:HB1	1:A:747:LEU:HD12	1.93	0.51
1:B:1151:SER:O	1:B:1337:THR:HG21	2.09	0.51
1:B:1505:GLU:O	1:B:1509:ARG:HG3	2.11	0.51
1:A:228:ALA:HA	1:A:231:THR:OG1	2.10	0.51
1:A:298:ASP:O	1:A:302:LEU:HD12	2.11	0.51
1:B:1366:LEU:HD12	1:B:1370:VAL:CG2	2.41	0.51
1:B:1654:THR:HG23	1:B:1656:ASN:H	1.76	0.51
1:B:1202:LEU:N	1:B:1202:LEU:HD12	2.26	0.51
1:B:1544:ARG:HD3	1:B:1546:ARG:NH2	2.25	0.51
1:B:1558:HIS:CE1	1:B:1598:LEU:HD11	2.45	0.51
1:A:281:THR:N	1:A:528:ASP:OD2	2.44	0.51
1:A:287:LEU:HD23	1:A:526:GLU:HA	1.92	0.51
1:A:518:ARG:HB3	1:A:522:ARG:CZ	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1228:ALA:HB3	1:B:1236:LEU:CD1	2.40	0.51
1:B:1331:ASP:OD1	1:B:1331:ASP:O	2.29	0.51
1:A:224:LEU:O	1:A:225:LEU:C	2.53	0.51
1:B:1542:TYR:HB3	1:B:1608:PHE:C	2.35	0.51
1:B:1645:GLU:O	1:B:1649:ILE:HG13	2.11	0.51
1:B:1722:LEU:HB2	1:B:1744:MSE:CE	2.40	0.51
1:A:182:PRO:O	1:A:186:GLU:HG3	2.11	0.51
1:A:574:MSE:SE	1:A:692:LEU:HD21	2.60	0.51
1:B:1129:ARG:HB2	1:B:1285:ARG:CD	2.32	0.51
1:B:1143:TRP:N	1:B:1160:LEU:O	2.42	0.51
1:B:1558:HIS:HD2	1:B:1561:VAL:HG23	1.76	0.51
1:A:135:ALA:HA	1:A:146:ALA:O	2.11	0.50
1:A:244:TYR:CD1	1:A:246:PRO:HD3	2.46	0.50
1:A:556:GLY:O	1:A:557:ARG:HG3	2.11	0.50
1:A:523:ILE:O	1:A:527:LEU:HG	2.11	0.50
1:A:643:MSE:HE1	1:A:665:GLY:HA2	1.92	0.50
1:A:758:LEU:HB3	1:A:762:MSE:HE3	1.94	0.50
1:B:1148:LEU:HB3	1:B:1224:LEU:HD13	1.94	0.50
1:B:1716:ARG:O	1:B:1722:LEU:C	2.54	0.50
1:A:322:VAL:HG12	1:A:326:LEU:HD11	1.94	0.50
1:B:1127:LEU:HD13	1:B:1151:SER:HB2	1.93	0.50
1:B:1214:PRO:O	1:B:1217:LEU:HB3	2.12	0.50
1:A:581:ILE:HG22	1:A:589:LYS:HD3	1.94	0.50
1:B:1263:PHE:CE2	1:B:1292:LEU:HD12	2.43	0.50
1:B:1270:ASP:OD2	1:B:1564:ARG:NH1	2.44	0.50
1:A:213:GLY:O	1:A:218:ARG:HD3	2.11	0.50
1:A:240:PRO:O	1:A:241:PHE:C	2.55	0.50
1:A:557:ARG:HA	1:A:567:PHE:CE2	2.41	0.50
1:A:723:VAL:O	1:A:725:TYR:CD1	2.64	0.50
1:B:1624:THR:HB	1:B:1626:ILE:HG13	1.94	0.50
1:A:715:ALA:CB	1:A:722:LEU:HD22	2.41	0.50
1:B:1145:LEU:O	1:B:1158:THR:N	2.42	0.50
1:B:1279:THR:HG21	1:B:1285:ARG:CB	2.40	0.50
1:B:1642:GLU:O	1:B:1645:GLU:HB2	2.11	0.50
1:B:1717:GLU:N	1:B:1722:LEU:HA	2.26	0.50
1:A:170:LEU:HD13	1:A:170:LEU:C	2.36	0.50
1:A:540:TYR:CD2	1:A:563:ARG:NH1	2.79	0.50
1:A:558:HIS:HD2	1:A:561:VAL:CG2	2.25	0.50
1:A:578:LEU:C	1:A:578:LEU:CD2	2.85	0.50
1:A:693:PHE:HD2	1:A:693:PHE:C	2.20	0.50
1:B:1332:LEU:H	1:B:1332:LEU:CD1	2.25	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1577:GLU:OE1	1:B:1709:LYS:HE3	2.12	0.50
1:B:1298:ASP:C	1:B:1301:PRO:HD2	2.37	0.49
1:B:1299:ARG:O	1:B:1303:GLU:HG2	2.12	0.49
1:A:273:PHE:CE1	1:A:288:LEU:HD23	2.47	0.49
1:A:279:THR:HG21	1:A:285:ARG:CB	2.39	0.49
1:A:319:ARG:CD	1:A:534:ALA:HB3	2.41	0.49
1:B:1123:GLN:H	1:B:1123:GLN:NE2	2.11	0.49
1:A:518:ARG:CB	1:A:522:ARG:NH2	2.75	0.49
1:B:1325:LEU:HB2	1:B:1362:LEU:HD21	1.93	0.49
1:B:1676:ILE:O	1:B:1680:VAL:HG23	2.12	0.49
1:A:210:GLU:O	1:A:218:ARG:HB3	2.13	0.49
1:A:703:LEU:O	1:A:704:GLY:C	2.55	0.49
1:B:1171:PHE:CZ	1:B:1254:GLU:HG3	2.46	0.49
1:B:1273:PHE:O	1:B:1277:ASP:N	2.40	0.49
1:B:1340:GLU:OE2	1:B:1515:GLU:OE2	2.30	0.49
1:A:737:TYR:O	1:A:740:GLU:HB2	2.13	0.49
1:B:1332:LEU:HD12	1:B:1332:LEU:N	2.27	0.49
1:B:1572:LEU:HD13	1:B:1592:PHE:CZ	2.46	0.49
1:A:556:GLY:C	1:A:557:ARG:HG3	2.37	0.49
1:B:1182:PRO:HG2	1:B:1183:GLU:OE1	2.13	0.49
1:B:1568:VAL:HG11	1:B:1727:GLN:NE2	2.21	0.49
1:A:263:PHE:O	1:A:271:THR:HG21	2.11	0.49
1:A:574:MSE:HG2	1:A:579:VAL:HG21	1.95	0.49
1:A:693:PHE:C	1:A:693:PHE:CD2	2.91	0.49
1:A:155:PHE:O	1:A:241:PHE:HA	2.13	0.49
1:A:214:PRO:O	1:A:217:LEU:HB3	2.13	0.49
1:A:250:MSE:HE2	1:A:619:PHE:HB2	1.95	0.49
1:A:279:THR:HA	1:A:532:ALA:HB2	1.93	0.49
1:A:558:HIS:CD2	1:A:561:VAL:HG23	2.47	0.49
1:A:663:GLU:CB	1:A:666:ARG:HD3	2.42	0.49
1:B:1638:THR:HG22	1:B:1642:GLU:OE2	2.13	0.49
1:A:159:VAL:CG2	1:A:217:LEU:HB2	2.42	0.49
1:A:539:ARG:HB2	1:A:539:ARG:CZ	2.43	0.49
1:A:699:GLU:CD	1:A:699:GLU:H	2.20	0.49
1:B:1117:THR:C	1:B:1119:GLY:N	2.71	0.49
1:B:1117:THR:CG2	1:B:1119:GLY:H	2.13	0.49
1:A:586:MSE:HB2	1:A:724:PHE:CD2	2.48	0.48
1:B:1535:GLU:O	1:B:1536:VAL:C	2.55	0.48
1:B:1584:PRO:HG3	1:B:1715:ALA:HB2	1.94	0.48
1:A:586:MSE:HE1	1:B:1640:MSE:CE	2.42	0.48
1:A:716:ARG:H	1:A:723:VAL:H	1.60	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1209:PRO:CB	1:B:1218:ARG:HH21	2.18	0.48
1:B:1698:PHE:CA	1:B:1701:THR:HG22	2.43	0.48
1:A:279:THR:CG2	1:A:285:ARG:HB2	2.41	0.48
1:A:654:THR:HG23	1:A:656:ASN:H	1.78	0.48
1:A:697:TYR:CB	1:A:700:LEU:HD12	2.41	0.48
1:B:1558:HIS:CE1	1:B:1598:LEU:CD1	2.97	0.48
1:A:753:ALA:C	1:A:755:ALA:H	2.20	0.48
1:A:754:ARG:NH2	1:A:758:LEU:HD21	2.28	0.48
1:B:1352:LEU:CD1	1:B:1356:LEU:HG	2.43	0.48
1:A:620:ASP:OD1	1:A:657:SER:HA	2.13	0.48
1:A:638:THR:HG22	1:A:642:GLU:OE2	2.13	0.48
1:B:1293:ARG:HG3	1:B:1293:ARG:HH11	1.78	0.48
1:A:322:VAL:HG12	1:A:326:LEU:CD1	2.43	0.48
1:A:708:LEU:HG	1:A:709:LYS:N	2.25	0.48
1:B:1378:LEU:HD23	1:B:1378:LEU:O	2.13	0.48
1:B:1574:MSE:HG2	1:B:1579:VAL:HG21	1.95	0.48
1:B:1685:HIS:HE1	1:B:1707:ARG:HB2	1.79	0.48
1:B:1753:ALA:C	1:B:1755:ALA:H	2.21	0.48
1:A:645:GLU:O	1:A:649:ILE:HG13	2.13	0.48
1:A:685:HIS:HE1	1:A:707:ARG:H	1.62	0.48
1:A:723:VAL:O	1:A:723:VAL:HG12	2.13	0.48
1:B:1169:GLU:OE2	1:B:1246:PRO:HB3	2.14	0.48
1:B:1351:ALA:O	1:B:1354:ARG:HB3	2.14	0.48
1:B:1553:ILE:HD13	1:B:1599:ILE:HD12	1.96	0.48
1:B:1659:VAL:C	1:B:1660:LEU:HD23	2.39	0.48
1:B:1289:GLN:O	1:B:1293:ARG:NH1	2.46	0.48
1:A:654:THR:H	1:A:657:SER:HB2	1.79	0.48
1:A:659:VAL:C	1:A:660:LEU:HD23	2.39	0.48
1:B:1247:GLY:HA2	1:B:1251:ARG:CZ	2.44	0.48
1:B:1697:TYR:CB	1:B:1700:LEU:HD12	2.43	0.48
1:A:180:LEU:HB2	1:A:185:LEU:HD21	1.96	0.47
1:A:306:LEU:HD12	1:A:547:PHE:HE1	1.77	0.47
1:B:1367:GLY:C	1:B:1369:GLU:N	2.71	0.47
1:A:302:LEU:HD22	1:A:547:PHE:HZ	1.79	0.47
1:B:1146:ALA:HB1	1:B:1224:LEU:HD11	1.96	0.47
1:B:1754:ARG:NH2	1:B:1758:LEU:HD21	2.28	0.47
1:A:221:ARG:HD3	1:A:241:PHE:CD1	2.49	0.47
1:A:270:ASP:OD2	1:A:564:ARG:NH1	2.47	0.47
1:A:580:LEU:CD1	1:A:701:THR:HA	2.44	0.47
1:A:642:GLU:O	1:A:645:GLU:HB2	2.15	0.47
1:B:1129:ARG:CZ	1:B:1285:ARG:HH12	2.25	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1528:ASP:O	1:B:1532:ALA:HB2	2.14	0.47
1:B:1148:LEU:HD12	1:B:1155:PHE:CE1	2.48	0.47
1:B:1171:PHE:O	1:B:1174:ARG:HG2	2.15	0.47
1:B:1519:GLU:OE1	1:B:1522:ARG:NH2	2.47	0.47
1:B:1376:SER:N	1:B:1377:PRO:CD	2.77	0.47
1:A:145:LEU:O	1:A:158:THR:N	2.40	0.47
1:A:345:SER:CB	1:A:346:PRO:HD2	2.36	0.47
1:A:625:ARG:CZ	1:A:642:GLU:HG2	2.44	0.47
1:A:639:PHE:CE1	1:A:643:MSE:HE3	2.49	0.47
1:A:703:LEU:O	1:A:705:LEU:HG	2.15	0.47
1:A:716:ARG:O	1:A:722:LEU:C	2.57	0.47
1:B:1135:ALA:HA	1:B:1146:ALA:O	2.14	0.47
1:B:1302:LEU:HD21	1:B:1604:GLN:HA	1.97	0.47
1:B:1355:SER:C	1:B:1357:GLN:N	2.73	0.47
1:B:1563:ARG:CA	1:B:1563:ARG:NE	2.77	0.47
1:B:1580:LEU:CD1	1:B:1701:THR:HA	2.45	0.47
1:B:1625:ARG:NE	1:B:1642:GLU:HG2	2.29	0.47
1:A:237:SER:C	1:A:238:LEU:HD23	2.40	0.47
1:A:542:TYR:HB3	1:A:609:VAL:O	2.15	0.47
1:B:1161:LYS:HD2	1:B:1162:SER:N	2.28	0.47
1:B:1363:ARG:HG2	1:B:1363:ARG:HH11	1.79	0.47
1:B:1757:ALA:O	1:B:1758:LEU:C	2.57	0.47
1:A:303:GLU:HA	1:A:303:GLU:OE2	2.14	0.47
1:B:1542:TYR:C	1:B:1608:PHE:HB3	2.40	0.47
1:B:1556:GLY:C	1:B:1557:ARG:HG3	2.40	0.47
1:A:273:PHE:HE1	1:A:288:LEU:HD23	1.79	0.47
1:A:588:GLY:O	1:A:592:PHE:N	2.45	0.47
1:A:599:ILE:HG22	1:A:616:LEU:HD11	1.98	0.47
1:A:760:GLN:O	1:A:761:ALA:C	2.56	0.47
1:B:1303:GLU:OE2	1:B:1303:GLU:HA	2.15	0.47
1:A:323:ARG:HH11	1:A:323:ARG:HG2	1.81	0.46
1:A:577:GLU:OE1	1:A:709:LYS:HE3	2.14	0.46
1:A:678:THR:O	1:A:682:GLU:HG3	2.14	0.46
1:B:1533:LEU:O	1:B:1534:ALA:C	2.58	0.46
1:B:1537:ALA:O	1:B:1541:GLY:N	2.48	0.46
1:B:1723:VAL:O	1:B:1725:TYR:CD1	2.68	0.46
1:B:1737:TYR:O	1:B:1740:GLU:HB2	2.14	0.46
1:A:237:SER:CB	1:A:341:LEU:HG	2.44	0.46
1:A:312:PHE:HD2	1:A:319:ARG:HA	1.79	0.46
1:A:654:THR:HG22	1:A:657:SER:OG	2.14	0.46
1:A:685:HIS:HE1	1:A:707:ARG:HB2	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1338:ARG:NH2	1:B:1348:ASP:OD2	2.48	0.46
1:B:1553:ILE:O	1:B:1571:ASP:HA	2.15	0.46
1:A:243:PHE:CD2	1:A:243:PHE:C	2.93	0.46
1:B:1748:PRO:HB2	1:B:1751:VAL:HG23	1.97	0.46
1:A:637:SER:O	1:A:638:THR:C	2.57	0.46
1:B:1258:ARG:O	1:B:1266:LEU:HD21	2.15	0.46
1:B:1293:ARG:HH11	1:B:1293:ARG:CG	2.28	0.46
1:B:1355:SER:O	1:B:1357:GLN:N	2.49	0.46
1:B:1544:ARG:HB2	1:B:1608:PHE:CE2	2.50	0.46
1:B:1699:GLU:H	1:B:1699:GLU:CD	2.22	0.46
1:A:190:PHE:C	1:A:190:PHE:CD2	2.93	0.46
1:A:554:ARG:HB3	1:A:613:GLU:H	1.80	0.46
1:A:682:GLU:HA	1:A:685:HIS:HB3	1.98	0.46
1:B:1117:THR:HG21	1:B:1134:LEU:HD13	1.98	0.46
1:A:287:LEU:CD2	1:A:526:GLU:HA	2.46	0.46
1:A:586:MSE:SE	1:B:1640:MSE:SE	3.33	0.46
1:A:716:ARG:C	1:A:722:LEU:HD23	2.40	0.46
1:A:757:ALA:O	1:A:758:LEU:C	2.57	0.46
1:B:1313:VAL:HG13	1:B:1538:VAL:HG21	1.97	0.46
1:B:1625:ARG:CZ	1:B:1642:GLU:HG2	2.46	0.46
1:B:1637:SER:O	1:B:1638:THR:C	2.58	0.46
1:B:1715:ALA:CB	1:B:1722:LEU:HD22	2.45	0.46
1:B:1743:ALA:CB	1:B:1752:VAL:HG11	2.45	0.46
1:A:597:ALA:O	1:A:600:ALA:HB3	2.16	0.46
1:A:698:PHE:CA	1:A:701:THR:HG22	2.46	0.46
1:B:1117:THR:C	1:B:1119:GLY:H	2.22	0.46
1:B:1181:ALA:H	1:B:1184:LEU:HD12	1.81	0.46
1:B:1262:VAL:HG12	1:B:1263:PHE:N	2.31	0.46
1:A:207:PHE:CD2	1:A:220:ALA:HA	2.51	0.46
1:A:696:HIS:O	1:B:1669:SER:CB	2.62	0.46
1:A:743:ALA:CB	1:A:752:VAL:HG11	2.45	0.46
1:B:1574:MSE:HE3	1:B:1579:VAL:CG2	2.46	0.46
1:B:1740:GLU:O	1:B:1741:VAL:C	2.58	0.46
1:A:182:PRO:HD2	1:A:183:GLU:OE1	2.16	0.46
1:A:574:MSE:HE3	1:A:579:VAL:CG2	2.43	0.46
1:A:558:HIS:N	1:A:567:PHE:CE2	2.78	0.46
1:B:1279:THR:CG2	1:B:1285:ARG:HB2	2.42	0.46
1:B:1715:ALA:HA	1:B:1724:PHE:CA	2.41	0.46
1:A:207:PHE:HB3	1:A:219:ARG:HB3	1.97	0.45
1:A:624:THR:HB	1:A:626:ILE:HG13	1.97	0.45
1:A:718:GLU:OE1	1:A:723:VAL:HG11	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1126:LEU:O	1:B:1127:LEU:HD23	2.15	0.45
1:B:1313:VAL:CG1	1:B:1538:VAL:HG22	2.44	0.45
1:B:1546:ARG:O	1:B:1615:HIS:HA	2.16	0.45
1:B:1558:HIS:HD2	1:B:1561:VAL:CG2	2.28	0.45
1:B:1581:ILE:HA	1:B:1711:LEU:O	2.16	0.45
1:A:718:GLU:O	1:A:719:ALA:C	2.60	0.45
1:B:1184:LEU:HB3	1:B:1190:PHE:CE2	2.52	0.45
1:B:1544:ARG:HD3	1:B:1546:ARG:HH21	1.80	0.45
1:B:1557:ARG:HA	1:B:1567:PHE:CE2	2.43	0.45
1:B:1580:LEU:HD12	1:B:1701:THR:HA	1.96	0.45
1:B:1639:PHE:O	1:B:1640:MSE:C	2.58	0.45
1:B:1703:LEU:O	1:B:1705:LEU:HG	2.16	0.45
1:A:167:TYR:CD2	1:A:197:ARG:HD3	2.52	0.45
1:A:558:HIS:CE1	1:A:598:LEU:HD11	2.50	0.45
1:A:725:TYR:C	1:A:727:GLN:H	2.24	0.45
1:A:758:LEU:C	1:A:762:MSE:HE3	2.40	0.45
1:A:278:GLU:OE1	1:A:536:VAL:HG22	2.16	0.45
1:B:1120:THR:HA	1:B:1150:VAL:CG1	2.47	0.45
1:B:1380:GLU:HA	1:B:1383:GLU:OE1	2.17	0.45
1:B:1522:ARG:HG2	1:B:1522:ARG:NH1	2.28	0.45
1:B:1623:TYR:N	1:B:1623:TYR:CD1	2.84	0.45
1:B:1711:LEU:HD22	1:B:1730:PRO:HA	1.98	0.45
1:A:260:LEU:N	1:A:260:LEU:HD12	2.32	0.45
1:A:534:ALA:O	1:A:538:VAL:HG23	2.16	0.45
1:A:544:ARG:HB2	1:A:608:PHE:CZ	2.51	0.45
1:A:692:LEU:HD23	1:A:692:LEU:HA	1.79	0.45
1:B:1318:LEU:HD11	1:B:1366:LEU:HD23	1.99	0.45
1:B:1387:VAL:O	1:B:1389:ASP:N	2.49	0.45
1:A:280:ARG:HG3	1:A:280:ARG:NH1	2.30	0.45
1:B:1232:GLN:C	1:B:1234:GLY:H	2.25	0.45
1:B:1710:ASN:O	1:B:1731:GLY:N	2.46	0.45
1:A:581:ILE:HB	1:A:694:ALA:HA	1.98	0.45
1:B:1161:LYS:HE2	1:B:1161:LYS:N	2.19	0.45
1:B:1250:MSE:CE	1:B:1604:GLN:OE1	2.63	0.45
1:B:1281:THR:HB	1:B:1283:PRO:HD2	1.99	0.45
1:B:1537:ALA:HA	1:B:1542:TYR:HB2	1.98	0.45
1:B:1555:ALA:HA	1:B:1570:ASN:O	2.17	0.45
1:B:1563:ARG:HA	1:B:1563:ARG:NE	2.23	0.45
1:B:1301:PRO:O	1:B:1304:ALA:HB3	2.17	0.45
1:B:1574:MSE:SE	1:B:1692:LEU:HD21	2.67	0.45
1:B:1692:LEU:HD23	1:B:1692:LEU:HA	1.77	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:166:LEU:C	1:A:168:ASP:H	2.24	0.45
1:A:232:GLN:HG3	1:A:236:LEU:CD2	2.46	0.45
1:A:250:MSE:HE1	1:A:622:ILE:HD11	2.00	0.45
1:A:296:LEU:HB2	1:A:302:LEU:HD11	1.98	0.45
1:A:518:ARG:HD2	1:A:522:ARG:HH21	1.82	0.45
1:B:1207:PHE:CD2	1:B:1220:ALA:HA	2.51	0.45
1:B:1515:GLU:C	1:B:1517:LEU:N	2.73	0.45
1:B:1678:THR:O	1:B:1682:GLU:HG3	2.17	0.45
1:B:1708:LEU:HG	1:B:1709:LYS:N	2.26	0.45
1:A:138:ALA:HB3	1:A:216:ALA:O	2.16	0.44
1:A:215:LEU:HD13	1:A:215:LEU:C	2.42	0.44
1:A:590:SER:HA	1:A:593:LEU:CD1	2.38	0.44
1:B:1180:LEU:HD11	1:B:1194:PHE:CD2	2.52	0.44
1:B:1263:PHE:HE1	1:B:1293:ARG:HG2	1.82	0.44
1:B:1722:LEU:O	1:B:1723:VAL:HG23	2.17	0.44
1:A:247:GLY:HA2	1:A:251:ARG:NH2	2.31	0.44
1:A:654:THR:H	1:A:657:SER:CB	2.31	0.44
1:B:1291:TRP:HH2	1:B:1530:TYR:CE2	2.35	0.44
1:B:1558:HIS:N	1:B:1567:PHE:CE2	2.78	0.44
1:B:1589:LYS:NZ	1:B:1696:HIS:HD1	2.15	0.44
1:A:746:GLY:O	1:B:1651:LYS:NZ	2.44	0.44
1:B:1117:THR:HB	1:B:1120:THR:HG1	1.81	0.44
1:B:1183:GLU:CD	1:B:1183:GLU:H	2.26	0.44
1:B:1557:ARG:HB2	1:B:1610:PRO:HB2	1.99	0.44
1:A:553:ILE:HD13	1:A:599:ILE:HD12	1.98	0.44
1:A:623:TYR:CD1	1:A:623:TYR:N	2.85	0.44
1:A:748:PRO:O	1:A:752:VAL:HG23	2.18	0.44
1:A:750:GLU:O	1:A:753:ALA:HB3	2.17	0.44
1:A:757:ALA:C	1:A:759:LEU:N	2.73	0.44
1:B:1540:TYR:CD1	1:B:1563:ARG:NH1	2.85	0.44
1:B:1639:PHE:CE1	1:B:1643:MSE:HE3	2.51	0.44
1:A:671:LEU:O	1:A:672:ASP:C	2.60	0.44
1:B:1120:THR:HA	1:B:1150:VAL:HG13	2.00	0.44
1:B:1179:LEU:HD22	1:B:1203:SER:O	2.18	0.44
1:B:1373:PRO:CG	1:B:1519:GLU:HG2	2.45	0.44
1:A:251:ARG:HG2	1:A:251:ARG:NH1	2.33	0.44
1:B:1581:ILE:HB	1:B:1694:ALA:HA	1.98	0.44
1:A:191:LEU:HD21	1:A:195:ARG:NH2	2.33	0.44
1:A:739:VAL:HA	1:B:1676:ILE:HD11	2.00	0.44
1:B:1143:TRP:HH2	1:B:1163:LYS:HD3	1.80	0.44
1:B:1220:ALA:O	1:B:1223:ALA:HB3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1363:ARG:NH2	1:B:1368:GLU:HG3	2.33	0.44
1:B:1682:GLU:HA	1:B:1685:HIS:HB3	1.98	0.44
1:B:1742:ALA:O	1:B:1747:LEU:HD12	2.16	0.44
1:A:281:THR:CB	1:A:283:PRO:HD2	2.47	0.44
1:A:282:ALA:HB3	1:A:283:PRO:HD3	2.00	0.44
1:B:1554:ARG:HB3	1:B:1613:GLU:H	1.81	0.44
1:B:1640:MSE:O	1:B:1641:VAL:C	2.60	0.44
1:A:171:PHE:CZ	1:A:254:GLU:HG3	2.52	0.44
1:A:262:VAL:HG12	1:A:263:PHE:CD2	2.53	0.44
1:A:557:ARG:C	1:A:595:GLN:HG3	2.42	0.44
1:A:580:LEU:HD12	1:A:701:THR:HA	2.00	0.44
1:B:1148:LEU:CB	1:B:1224:LEU:HD13	2.48	0.44
1:B:1302:LEU:HD21	1:B:1604:GLN:C	2.43	0.44
1:B:1654:THR:HG22	1:B:1657:SER:OG	2.18	0.44
1:A:162:SER:C	1:A:164:SER:N	2.74	0.43
1:A:557:ARG:CZ	1:A:562:GLU:OE2	2.65	0.43
1:A:581:ILE:HA	1:A:711:LEU:O	2.18	0.43
1:A:589:LYS:HZ2	1:A:696:HIS:HD1	1.66	0.43
1:A:595:GLN:O	1:A:599:ILE:HG13	2.18	0.43
1:B:1166:LEU:O	1:B:1167:TYR:C	2.61	0.43
1:B:1558:HIS:CD2	1:B:1561:VAL:HG23	2.51	0.43
1:A:143:TRP:HH2	1:A:163:LYS:HD3	1.82	0.43
1:A:230:ARG:HD2	1:A:230:ARG:O	2.19	0.43
1:A:559:PRO:HB3	1:A:610:PRO:HG3	2.00	0.43
1:A:724:PHE:H	1:A:724:PHE:HD1	1.64	0.43
1:B:1181:ALA:HB1	1:B:1219:ARG:NH2	2.33	0.43
1:B:1252:LEU:HD23	1:B:1252:LEU:HA	1.80	0.43
1:B:1359:LEU:CB	1:B:1360:PRO:HD3	2.48	0.43
1:B:1557:ARG:C	1:B:1595:GLN:HG3	2.43	0.43
1:B:1685:HIS:HE1	1:B:1707:ARG:H	1.66	0.43
1:A:540:TYR:CD2	1:A:563:ARG:HD3	2.53	0.43
1:B:1578:LEU:HD23	1:B:1579:VAL:N	2.33	0.43
1:B:1599:ILE:HG22	1:B:1616:LEU:HD11	1.99	0.43
1:B:1663:GLU:CB	1:B:1666:ARG:HD3	2.47	0.43
1:B:1718:GLU:CG	1:B:1723:VAL:HG21	2.48	0.43
1:A:553:ILE:O	1:A:571:ASP:HA	2.18	0.43
1:A:563:ARG:HA	1:A:563:ARG:NE	2.26	0.43
1:A:639:PHE:O	1:A:640:MSE:C	2.61	0.43
1:B:1128:PRO:C	1:B:1130:GLU:N	2.75	0.43
1:B:1579:VAL:HG13	1:B:1709:LYS:HG2	2.00	0.43
1:A:581:ILE:HG22	1:A:589:LYS:CG	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:757:ALA:O	1:A:759:LEU:N	2.52	0.43
1:B:1125:SER:O	1:B:1126:LEU:HD23	2.19	0.43
1:B:1138:ALA:O	1:B:1216:ALA:HB1	2.18	0.43
1:B:1244:TYR:CE1	1:B:1246:PRO:HG3	2.53	0.43
1:B:1345:SER:HB2	1:B:1346:PRO:CD	2.48	0.43
1:B:1673:GLY:HA3	1:B:1697:TYR:OH	2.18	0.43
1:B:1717:GLU:HA	1:B:1721:GLY:O	2.18	0.43
1:B:1743:ALA:HB2	1:B:1752:VAL:HG13	1.99	0.43
1:A:296:LEU:O	1:A:297:LEU:HD23	2.18	0.43
1:A:558:HIS:CE1	1:A:598:LEU:CD1	3.02	0.43
1:B:1170:LEU:HD13	1:B:1170:LEU:C	2.43	0.43
1:B:1252:LEU:HD21	1:B:1256:THR:CG2	2.48	0.43
1:B:1331:ASP:O	1:B:1333:GLU:N	2.52	0.43
1:B:1592:PHE:CD1	1:B:1728:VAL:HG21	2.53	0.43
1:B:1152:THR:O	1:B:1239:GLN:OE1	2.37	0.43
1:B:1166:LEU:C	1:B:1168:ASP:H	2.27	0.43
1:B:1594:ARG:O	1:B:1595:GLN:C	2.61	0.43
1:B:1714:ALA:O	1:B:1724:PHE:HA	2.19	0.43
1:A:299:ARG:O	1:A:303:GLU:HG2	2.19	0.43
1:A:578:LEU:HD23	1:A:579:VAL:N	2.33	0.43
1:A:594:ARG:C	1:A:596:THR:N	2.77	0.43
1:A:759:LEU:O	1:A:760:GLN:C	2.61	0.43
1:A:681:ALA:O	1:A:682:GLU:C	2.61	0.43
1:A:722:LEU:C	1:A:723:VAL:HG23	2.44	0.43
1:B:1130:GLU:HG2	1:B:1289:GLN:NE2	2.33	0.43
1:B:1150:VAL:CG2	1:B:1151:SER:N	2.82	0.43
1:B:1354:ARG:HH12	1:B:1358:ILE:HD12	1.83	0.43
1:A:263:PHE:CE2	1:A:292:LEU:CD1	2.96	0.43
1:B:1183:GLU:OE2	1:B:1219:ARG:NH1	2.51	0.43
1:B:1371:GLY:O	1:B:1372:LEU:C	2.61	0.43
1:B:1557:ARG:CZ	1:B:1562:GLU:OE2	2.66	0.43
1:B:1654:THR:H	1:B:1657:SER:HB2	1.83	0.43
1:B:1717:GLU:H	1:B:1717:GLU:HG3	1.63	0.43
1:A:547:PHE:CD2	1:A:618:LEU:HD21	2.54	0.42
1:B:1123:GLN:H	1:B:1123:GLN:CD	2.27	0.42
1:A:138:ALA:HB2	1:A:207:PHE:CD2	2.54	0.42
1:A:180:LEU:HD22	1:A:184:LEU:CD1	2.48	0.42
1:A:743:ALA:HB2	1:A:752:VAL:HG13	2.01	0.42
1:B:1127:LEU:HD13	1:B:1151:SER:CB	2.49	0.42
1:B:1518:ARG:HG2	1:B:1518:ARG:HH11	1.84	0.42
1:B:1568:VAL:CG1	1:B:1727:GLN:NE2	2.79	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:256:THR:HA	1:A:624:THR:OG1	2.18	0.42
1:A:586:MSE:HE1	1:B:1640:MSE:HE1	2.00	0.42
1:A:669:SER:HB3	1:B:1696:HIS:O	2.18	0.42
1:B:1748:PRO:O	1:B:1752:VAL:HG23	2.19	0.42
1:A:236:LEU:HB3	1:A:238:LEU:HD21	2.02	0.42
1:A:278:GLU:HB2	1:A:536:VAL:CG2	2.49	0.42
1:A:289:GLN:O	1:A:293:ARG:NH1	2.52	0.42
1:B:1367:GLY:O	1:B:1369:GLU:N	2.51	0.42
1:B:1552:GLN:HA	1:B:1572:LEU:O	2.19	0.42
1:B:1588:GLY:O	1:B:1592:PHE:N	2.44	0.42
1:B:1671:LEU:O	1:B:1672:ASP:C	2.61	0.42
1:A:299:ARG:HB2	1:A:618:LEU:HD11	2.01	0.42
1:A:518:ARG:O	1:A:519:GLU:C	2.62	0.42
1:A:765:ARG:HH11	1:A:765:ARG:HG2	1.84	0.42
1:A:143:TRP:CZ3	1:A:166:LEU:HD22	2.53	0.42
1:A:150:VAL:CG2	1:A:151:SER:N	2.83	0.42
1:A:166:LEU:O	1:A:167:TYR:C	2.62	0.42
1:B:1296:LEU:CD1	1:B:1301:PRO:HB2	2.42	0.42
1:B:1315:GLU:O	1:B:1316:GLY:C	2.62	0.42
1:B:1750:GLU:O	1:B:1753:ALA:HB3	2.19	0.42
1:A:299:ARG:NH2	1:A:547:PHE:O	2.52	0.42
1:A:676:ILE:O	1:A:680:VAL:HG23	2.20	0.42
1:B:1117:THR:HG22	1:B:1119:GLY:CA	2.49	0.42
1:B:1135:ALA:O	1:B:1178:VAL:HA	2.20	0.42
1:B:1222:GLY:HA2	1:B:1225:LEU:CD1	2.44	0.42
1:B:1738:GLY:O	1:B:1739:VAL:C	2.62	0.42
1:A:345:SER:HB2	1:A:346:PRO:CD	2.39	0.42
1:A:598:LEU:O	1:A:599:ILE:C	2.62	0.42
1:A:710:ASN:HB2	1:A:732:PRO:HD3	2.02	0.42
1:B:1603:ALA:CB	1:B:1616:LEU:HD12	2.50	0.42
1:B:1625:ARG:CZ	1:B:1625:ARG:C	2.93	0.42
1:B:1742:ALA:HB1	1:B:1747:LEU:HD12	1.99	0.42
1:A:236:LEU:CB	1:A:238:LEU:HD21	2.50	0.42
1:B:1250:MSE:CA	1:B:1297:LEU:HD21	2.49	0.42
1:B:1261:GLU:HG2	1:B:1266:LEU:HG	1.98	0.42
1:B:1354:ARG:HA	1:B:1357:GLN:OE1	2.19	0.42
1:B:1725:TYR:C	1:B:1727:GLN:H	2.27	0.42
1:A:135:ALA:HB2	1:A:147:PHE:CE2	2.55	0.42
1:A:244:TYR:CD1	1:A:244:TYR:C	2.98	0.42
1:A:600:ALA:HA	1:A:616:LEU:CD1	2.47	0.42
1:A:663:GLU:OE1	1:A:666:ARG:HD3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:133:TYR:CD2	1:A:147:PHE:HB3	2.55	0.41
1:A:315:GLU:O	1:A:316:GLY:C	2.63	0.41
1:A:563:ARG:CA	1:A:563:ARG:NE	2.79	0.41
1:B:1312:PHE:HB3	1:B:1319:ARG:HB2	2.02	0.41
1:B:1710:ASN:HB2	1:B:1732:PRO:HD3	2.02	0.41
1:B:1722:LEU:C	1:B:1723:VAL:HG23	2.44	0.41
1:A:555:ALA:HA	1:A:570:ASN:O	2.20	0.41
1:B:1293:ARG:NH1	1:B:1293:ARG:HB2	2.35	0.41
1:B:1581:ILE:HG22	1:B:1589:LYS:HD3	2.02	0.41
1:B:1589:LYS:HZ2	1:B:1696:HIS:HD1	1.66	0.41
1:B:1659:VAL:O	1:B:1691:THR:HA	2.19	0.41
1:A:262:VAL:HG12	1:A:263:PHE:N	2.35	0.41
1:A:265:PRO:HB3	1:A:270:ASP:O	2.21	0.41
1:A:279:THR:HG21	1:A:285:ARG:CA	2.50	0.41
1:A:685:HIS:CE1	1:A:707:ARG:H	2.39	0.41
1:A:710:ASN:O	1:A:731:GLY:N	2.49	0.41
1:B:1124:GLU:HB2	1:B:1338:ARG:NH1	2.35	0.41
1:B:1215:LEU:HD13	1:B:1215:LEU:C	2.45	0.41
1:B:1291:TRP:CH2	1:B:1530:TYR:CE2	3.09	0.41
1:B:1345:SER:HB2	1:B:1346:PRO:HD2	2.03	0.41
1:B:1537:ALA:CB	1:B:1542:TYR:HB2	2.50	0.41
1:B:1554:ARG:HB3	1:B:1613:GLU:HB3	2.01	0.41
1:B:1578:LEU:HD21	1:B:1580:LEU:CD2	2.51	0.41
1:B:1620:ASP:OD1	1:B:1657:SER:CA	2.68	0.41
1:B:1658:LEU:HD12	1:B:1659:VAL:H	1.83	0.41
1:A:253:PRO:HD2	1:A:256:THR:OG1	2.20	0.41
1:B:1685:HIS:CE1	1:B:1707:ARG:CZ	3.03	0.41
1:A:161:LYS:HD2	1:A:162:SER:N	2.32	0.41
1:A:557:ARG:HB2	1:A:610:PRO:HB2	2.03	0.41
1:A:575:ALA:O	1:A:576:HIS:HB2	2.19	0.41
1:A:663:GLU:O	1:A:664:VAL:C	2.64	0.41
1:A:711:LEU:HD22	1:A:730:PRO:HA	2.02	0.41
1:A:716:ARG:HB2	1:A:725:TYR:HE1	1.86	0.41
1:B:1129:ARG:HA	1:B:1282:ALA:HB1	2.02	0.41
1:B:1618:LEU:HA	1:B:1618:LEU:HD23	1.83	0.41
1:A:222:GLY:HA2	1:A:225:LEU:HD12	2.03	0.41
1:A:589:LYS:NZ	1:A:696:HIS:HD1	2.19	0.41
1:A:603:ALA:CB	1:A:616:LEU:HD12	2.50	0.41
1:A:693:PHE:HD2	1:A:694:ALA:N	2.19	0.41
1:B:1140:GLY:N	1:B:1216:ALA:HB2	2.35	0.41
1:B:1160:LEU:HD22	1:B:1166:LEU:N	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1261:GLU:HG2	1:B:1266:LEU:H	1.86	0.41
1:B:1287:LEU:O	1:B:1290:SER:HB3	2.20	0.41
1:B:1387:VAL:C	1:B:1389:ASP:N	2.79	0.41
1:B:1387:VAL:HG12	1:B:1389:ASP:H	1.86	0.41
1:B:1520:ALA:O	1:B:1521:ALA:C	2.64	0.41
1:B:1588:GLY:O	1:B:1589:LYS:C	2.64	0.41
1:B:1594:ARG:C	1:B:1596:THR:N	2.77	0.41
1:B:1666:ARG:O	1:B:1667:GLY:C	2.64	0.41
1:B:1718:GLU:HB3	1:B:1719:ALA:H	1.46	0.41
1:B:1510:ALA:C	1:B:1512:ARG:H	2.29	0.41
1:B:1594:ARG:O	1:B:1596:THR:N	2.54	0.41
1:B:1693:PHE:HD2	1:B:1694:ALA:N	2.19	0.41
1:A:326:LEU:CD1	1:A:528:ASP:HA	2.50	0.40
1:A:552:GLN:HA	1:A:572:LEU:O	2.21	0.40
1:B:1232:GLN:HE22	1:B:1343:ARG:CZ	2.34	0.40
1:A:135:ALA:O	1:A:178:VAL:HA	2.22	0.40
1:A:320:GLU:O	1:A:324:ARG:HG3	2.20	0.40
1:A:518:ARG:CD	1:A:522:ARG:HH21	2.35	0.40
1:B:1145:LEU:HD22	1:B:1147:PHE:CE1	2.56	0.40
1:B:1685:HIS:CE1	1:B:1707:ARG:NH2	2.90	0.40
1:B:1759:LEU:O	1:B:1760:GLN:C	2.64	0.40
1:A:250:MSE:HE3	1:A:604:GLN:CD	2.40	0.40
1:A:301:PRO:O	1:A:304:ALA:HB3	2.21	0.40
1:A:554:ARG:HB3	1:A:613:GLU:HB3	2.02	0.40
1:B:1168:ASP:OD2	1:B:1253:PRO:HA	2.21	0.40
1:B:1250:MSE:HE1	1:B:1622:ILE:HD11	2.03	0.40
1:B:1547:PHE:HA	1:B:1616:LEU:O	2.21	0.40
1:A:152:THR:O	1:A:239:GLN:OE1	2.39	0.40
1:A:184:LEU:H	1:A:184:LEU:HG	1.66	0.40
1:A:220:ALA:O	1:A:223:ALA:HB3	2.21	0.40
1:A:225:LEU:O	1:A:227:TYR:N	2.55	0.40
1:A:312:PHE:HB3	1:A:319:ARG:HG3	2.03	0.40
1:B:1744:MSE:O	1:B:1745:ALA:C	2.65	0.40
1:A:291:TRP:C	1:A:605:VAL:HG23	2.46	0.40
1:B:1246:PRO:O	1:B:1251:ARG:CZ	2.70	0.40
1:B:1247:GLY:HA2	1:B:1251:ARG:NH2	2.37	0.40
1:B:1339:LEU:HD22	1:B:1511:LYS:HB2	2.03	0.40
1:B:1382:LEU:HD23	1:B:1506:VAL:CG1	2.52	0.40
1:B:1556:GLY:O	1:B:1557:ARG:HG3	2.21	0.40
1:B:1575:ALA:O	1:B:1576:HIS:HB2	2.20	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	437/649 (67%)	344 (79%)	69 (16%)	24 (6%)	1	11
1	B	521/649 (80%)	406 (78%)	87 (17%)	28 (5%)	1	12
All	All	958/1298 (74%)	750 (78%)	156 (16%)	52 (5%)	1	12

All (52) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	187	ASN
1	A	235	ALA
1	A	519	GLU
1	A	670	SER
1	A	704	GLY
1	A	719	ALA
1	B	1670	SER
1	B	1717	GLU
1	A	167	TYR
1	A	226	ALA
1	A	277	ASP
1	A	625	ARG
1	A	738	GLY
1	B	1167	TYR
1	B	1277	ASP
1	B	1332	LEU
1	B	1388	GLU
1	B	1625	ARG
1	B	1704	GLY
1	B	1738	GLY
1	B	1761	ALA
1	A	215	LEU
1	A	225	LEU
1	A	721	GLY
1	A	761	ALA

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Mol	Chain	Res	Type
1	B	1187	ASN
1	B	1356	LEU
1	B	1368	GLU
1	B	1385	ALA
1	B	1718	GLU
1	A	166	LEU
1	A	183	GLU
1	A	681	ALA
1	B	1589	LYS
1	B	1681	ALA
1	B	1723	VAL
1	A	589	LYS
1	A	723	VAL
1	B	1124	GLU
1	B	1166	LEU
1	B	1343	ARG
1	B	1511	LYS
1	B	1536	VAL
1	B	1675	ALA
1	B	1532	ALA
1	B	1740	GLU
1	B	1627	GLY
1	A	345	SER
1	A	627	GLY
1	A	240	PRO
1	B	1209	PRO
1	A	209	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	346/515 (67%)	308 (89%)	38 (11%)	6	26
1	B	419/515 (81%)	373 (89%)	46 (11%)	6	26
All	All	765/1030 (74%)	681 (89%)	84 (11%)	6	26

All (84) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	141	ASP
1	A	145	LEU
1	A	148	LEU
1	A	161	LYS
1	A	168	ASP
1	A	170	LEU
1	A	174	ARG
1	A	195	ARG
1	A	230	ARG
1	A	232	GLN
1	A	242	ARG
1	A	250	MSE
1	A	252	LEU
1	A	278	GLU
1	A	293	ARG
1	A	302	LEU
1	A	315	GLU
1	A	549	ASP
1	A	551	LEU
1	A	560	VAL
1	A	563	ARG
1	A	564	ARG
1	A	565	THR
1	A	578	LEU
1	A	596	THR
1	A	625	ARG
1	A	636	LYS
1	A	649	ILE
1	A	655	GLU
1	A	660	LEU
1	A	662	ASP
1	A	670	SER
1	A	693	PHE
1	A	699	GLU
1	A	739	VAL
1	A	750	GLU
1	A	759	LEU
1	A	760	GLN
1	B	1124	GLU
1	B	1129	ARG
1	B	1141	ASP
1	B	1145	LEU

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Mol	Chain	Res	Type
1	B	1148	LEU
1	B	1161	LYS
1	B	1168	ASP
1	B	1174	ARG
1	B	1202	LEU
1	B	1217	LEU
1	B	1230	ARG
1	B	1232	GLN
1	B	1252	LEU
1	B	1278	GLU
1	B	1302	LEU
1	B	1315	GLU
1	B	1335	LEU
1	B	1352	LEU
1	B	1354	ARG
1	B	1359	LEU
1	B	1370	VAL
1	B	1378	LEU
1	B	1519	GLU
1	B	1536	VAL
1	B	1546	ARG
1	B	1551	LEU
1	B	1560	VAL
1	B	1563	ARG
1	B	1564	ARG
1	B	1565	THR
1	B	1578	LEU
1	B	1596	THR
1	B	1625	ARG
1	B	1626	ILE
1	B	1636	LYS
1	B	1649	ILE
1	B	1655	GLU
1	B	1660	LEU
1	B	1662	ASP
1	B	1670	SER
1	B	1693	PHE
1	B	1699	GLU
1	B	1739	VAL
1	B	1750	GLU
1	B	1759	LEU
1	B	1760	GLN

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

Mol	Chain	Res	Type
1	A	173	HIS
1	A	229	GLN
1	A	232	GLN
1	A	239	GLN
1	A	558	HIS
1	A	585	ASN
1	A	595	GLN
1	A	604	GLN
1	A	685	HIS
1	A	727	GLN
1	B	1123	GLN
1	B	1173	HIS
1	B	1232	GLN
1	B	1239	GLN
1	B	1269	GLN
1	B	1513	GLN
1	B	1558	HIS
1	B	1585	ASN
1	B	1595	GLN
1	B	1685	HIS
1	B	1727	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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	A	440/649 (67%)	-0.78	1 (0%) 91 85	34, 104, 154, 181	0
1	B	522/649 (80%)	-0.82	3 (0%) 85 73	14, 98, 158, 188	0
All	All	962/1298 (74%)	-0.80	4 (0%) 88 79	14, 102, 156, 188	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	549	ASP	2.5
1	B	1268	GLY	2.4
1	B	1142	GLY	2.3
1	B	1635	GLY	2.2

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 oligosaccharides 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.