Full wwPDB X-ray Structure Validation Report (i)

Jun 12, 2024 – 07:37 PM EDT

PDB ID	:	1EWR
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 (i) 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 (1)) were used in the production of this report:

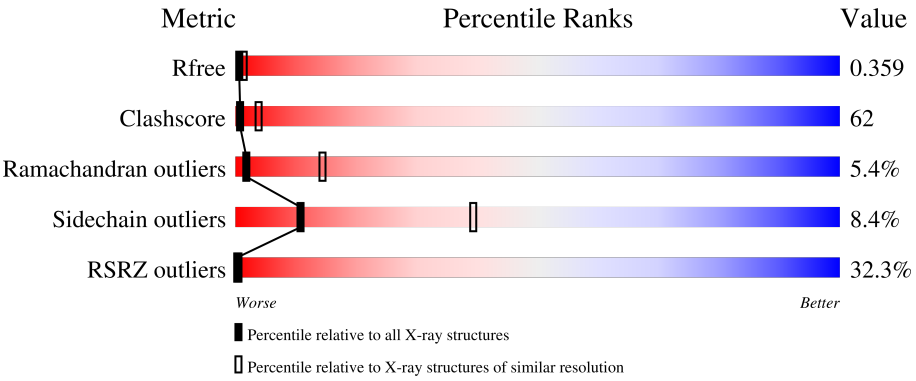
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

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}	130704	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (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 <=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	24% 19% 44% 6% 31%
1	B	649	24% 22% 52% 7% 18%

2 Entry composition (i)

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:

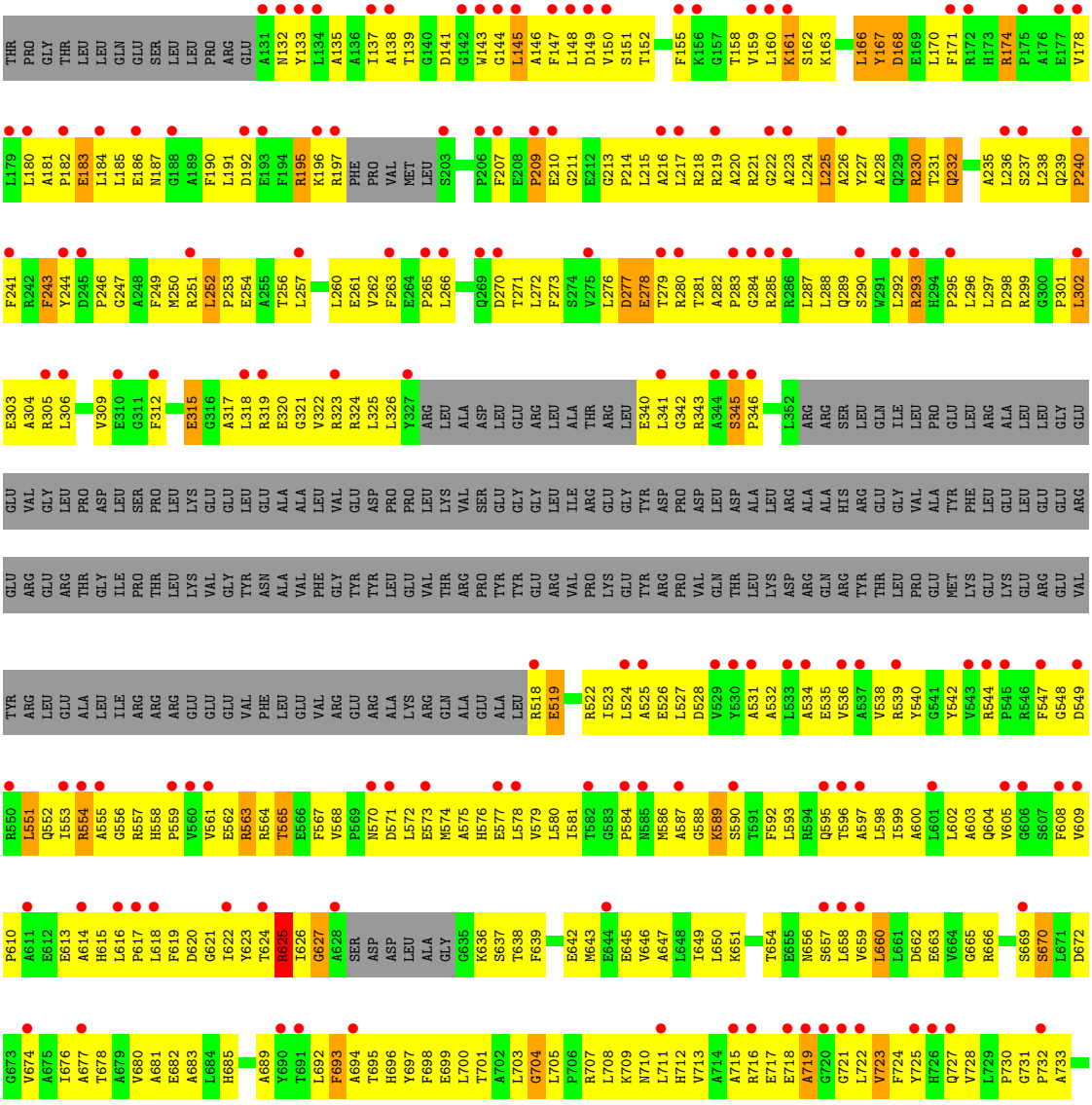
Chain	Residue	Modelled	Actual	Comment	Reference
A	250	MSE	MET	modified residue	UNP Q56215
A	574	MSE	MET	modified residue	UNP Q56215
A	586	MSE	MET	modified residue	UNP Q56215
A	640	MSE	MET	modified residue	UNP Q56215
A	643	MSE	MET	modified residue	UNP Q56215
A	744	MSE	MET	modified residue	UNP Q56215
A	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

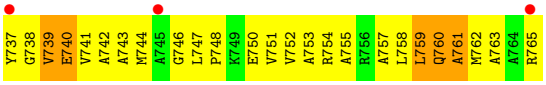
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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: DNA MISMATCH REPAIR PROTEIN MUTS

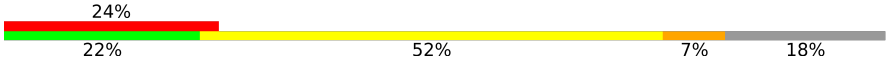
Chain A:

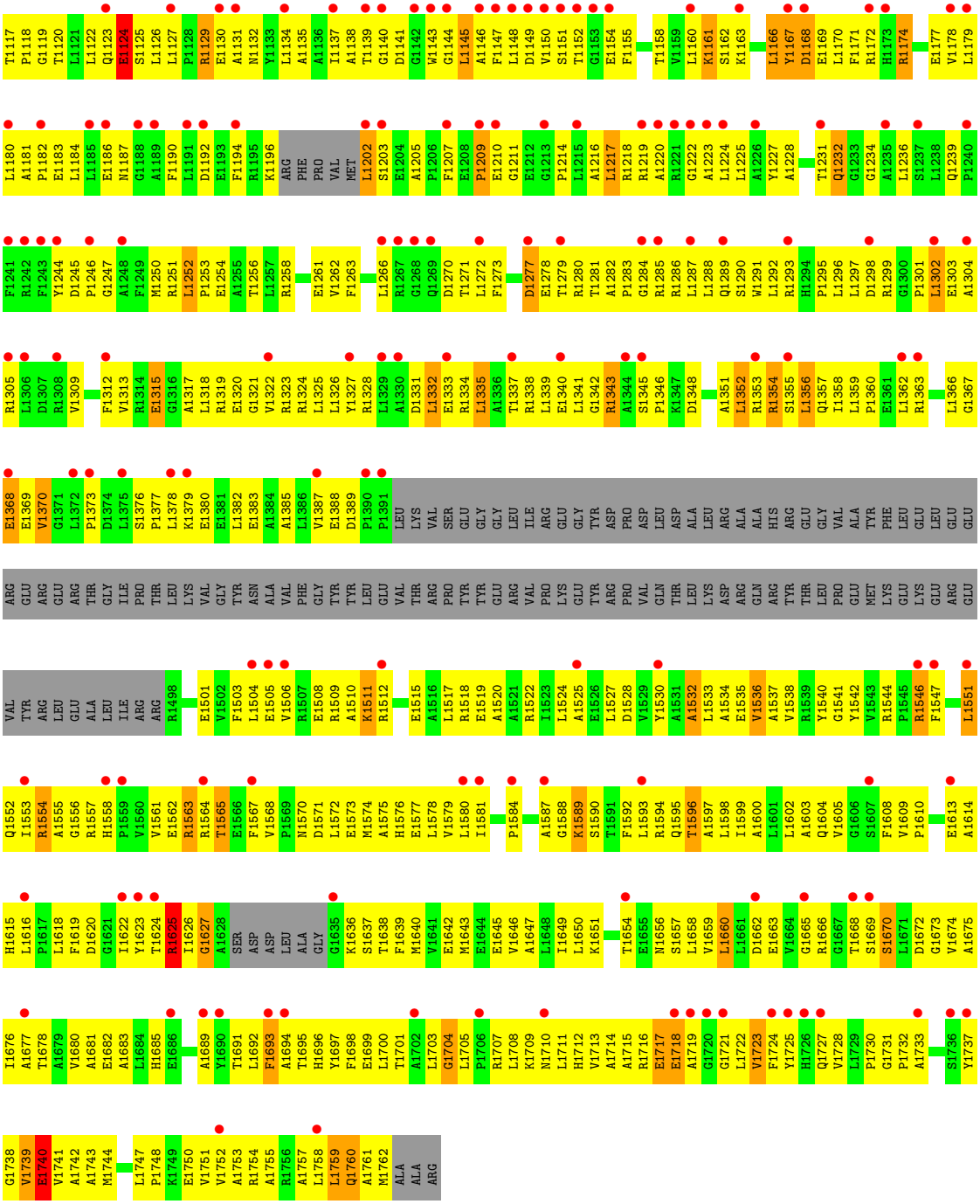




• Molecule 1: DNA MISMATCH REPAIR PROTEIN MUTS

Chain B:





4 Data and refinement statistics (i)

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) 94.2 (19.94-3.20)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [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)	0.31 , 52.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.43$, $< L^2 > = 0.25$	Xtriage
Estimated twinning fraction	0.058 for -h,-k,l	Xtriage
F_o,F_c correlation	0.84	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0/3526	0.67	0/4757
1	B	0.51	0/4192	0.69	0/5662
All	All	0.50	0/7718	0.68	0/10419

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	435	0
1	B	4125	0	4200	526	0
All	All	7593	0	7713	949	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 62.

All (949) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1589:LYS:HZ2	1:B:1696:HIS:CE1	2.09	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:B:1723:VAL:HG12	1:B:1723:VAL:O	1.91	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: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
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: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: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: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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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: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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1742:ALA:C	1:B:1747:LEU:HD12	2.19	0.62
1:A:148:LEU:CB	1:A:224:LEU:HD13	2.29	0.62
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:1117:THR:HG23	1:B:1177:GLU:CD	2.20	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:A:750:GLU:H	1:A:750:GLU:CD	2.02	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:1367:GLY:C	1:B:1369:GLU:H	2.04	0.61
1:B:1578:LEU:C	1:B:1578:LEU:HD23	2.19	0.61
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:A:589:LYS:HZ2	1:A:696:HIS:CE1	2.19	0.60
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1750:GLU:CD	1:B:1750:GLU:H	2.03	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
1:A:578:LEU:HD22	1:A:708:LEU:HD12	1.83	0.60
1:A:578:LEU:HD23	1:A:578:LEU:C	2.22	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: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: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: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:742:ALA:C	1:A:747:LEU:HD12	2.23	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:B:1710:ASN:C	1:B:1711:LEU:HD23	2.27	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: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:B:1137:ILE:HA	1:B:1144:GLY:O	2.06	0.55
1:A:643:MSE:HG3	1:B:1742:ALA:HA	1.87	0.55
1:B:1698:PHE:O	1:B:1699:GLU:C	2.44	0.55
1:B:1131:ALA:HB2	1:B:1286:ARG:HD2	1.89	0.55
1:A:710:ASN:C	1:A:711:LEU:HD23	2.28	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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: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:A:278:GLU:C	1:A:532:ALA:HB1	2.28	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: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:252:LEU:HD22	1:A:257:LEU:HG	1.89	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:1352:LEU:HD12	1:B:1352:LEU:C	2.28	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:1148:LEU:HD12	1:B:1155:PHE:CD1	2.44	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: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:1698:PHE:C	1:B:1701:THR:HG22	2.27	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
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:1183:GLU:CD	1:B:1219:ARG:HH22	2.13	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:A:625:ARG:NE	1:A:642:GLU:HG2	2.24	0.51
1:A:758:LEU:O	1:A:762:MSE:HE3	2.11	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
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: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:281:THR:HG23	1:A:528:ASP:CG	2.31	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:B:1139:THR:C	1:B:1216:ALA:HB2	2.32	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:698:PHE:O	1:A:699:GLU:C	2.49	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:A:139:THR:C	1:A:216:ALA:HB2	2.32	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: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:1760:GLN:C	1:B:1762:MSE:H	2.15	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: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:B:1332:LEU:H	1:B:1332:LEU:CD1	2.25	0.50
1:B:1577:GLU:OE1	1:B:1709:LYS:HE3	2.12	0.50
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:B:1148:LEU:C	1:B:1148:LEU:HD23	2.33	0.49
1:A:518:ARG:CB	1:A:522:ARG:NH2	2.75	0.49
1:B:1120:THR:C	1:B:1150:VAL:HG21	2.32	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:B:1171:PHE:CZ	1:B:1254:GLU:HG3	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:166:LEU:C	1:A:168:ASP:N	2.65	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:B:1166:LEU:C	1:B:1168:ASP:N	2.65	0.49
1:A:148:LEU:C	1:A:148:LEU:HD23	2.33	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: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: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
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:A:753:ALA:C	1:A:755:ALA:N	2.66	0.48
1:B:1558:HIS:CE1	1:B:1598:LEU:CD1	2.97	0.48
1:B:1693:PHE:C	1:B:1693:PHE:CD2	2.86	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:B:1693:PHE:C	1:B:1693:PHE:HD2	2.15	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:B:1703:LEU:O	1:B:1704:GLY:C	2.51	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1716:ARG:C	1:B:1722:LEU:HA	2.34	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: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: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: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
1:B:1528:ASP:O	1:B:1532:ALA:HB2	2.14	0.47
1:B:1753:ALA:C	1:B:1755:ALA:N	2.68	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:A:698:PHE:C	1:A:701:THR:HG22	2.32	0.47
1:B:1245:ASP:C	1:B:1247:GLY:H	2.18	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1542:TYR:HB3	1:B:1608:PHE:C	2.35	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: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:A:303:GLU:HA	1:A:303:GLU:OE2	2.14	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:740:GLU:O	1:A:741:VAL:C	2.53	0.47
1:B:1217:LEU:HD23	1:B:1217:LEU:C	2.36	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: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
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:B:1748:PRO:HB2	1:B:1751:VAL:HG23	1.97	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: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:224:LEU:O	1:A:225:LEU:C	2.53	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:B:1716:ARG:O	1:B:1722:LEU:C	2.54	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
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: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: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:240:PRO:O	1:A:241:PHE:C	2.55	0.45
1:A:558:HIS:CE1	1:A:598:LEU:HD11	2.50	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1387:VAL:O	1:B:1389:ASP:N	2.49	0.45
1:A:693:PHE:HD2	1:A:693:PHE:C	2.20	0.45
1:A:170:LEU:HD13	1:A:170:LEU:C	2.36	0.45
1:A:280:ARG:HG3	1:A:280:ARG:NH1	2.30	0.45
1:A:556:GLY:C	1:A:557:ARG:HG3	2.37	0.45
1:A:578:LEU:C	1:A:578:LEU:CD2	2.85	0.45
1:B:1298:ASP:C	1:B:1301:PRO:HD2	2.37	0.45
1:B:1578:LEU:C	1:B:1578:LEU:CD2	2.83	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
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:A:703:LEU:O	1:A:704:GLY:C	2.55	0.45
1:B:1207:PHE:CD2	1:B:1220:ALA:HA	2.51	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:693:PHE:C	1:A:693:PHE:CD2	2.91	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:B:1536:VAL:CG1	1:B:1537:ALA:N	2.80	0.44
1:A:251:ARG:HG2	1:A:251:ARG:NH1	2.33	0.44
1:B:1117:THR:C	1:B:1119:GLY:N	2.71	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
1:B:1363:ARG:NH2	1:B:1368:GLU:HG3	2.33	0.44
1:B:1535:GLU:O	1:B:1536:VAL:C	2.55	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: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:580:LEU:HD12	1:A:701:THR:HA	2.00	0.44
1:A:753:ALA:C	1:A:755:ALA:H	2.20	0.44
1:B:1148:LEU:CB	1:B:1224:LEU:HD13	2.48	0.44
1:B:1654:THR:HG22	1:B:1657:SER:OG	2.18	0.44
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:595:GLN:O	1:A:599:ILE:HG13	2.18	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:1659:VAL:C	1:B:1660:LEU:HD23	2.39	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:1579:VAL:HG13	1:B:1709:LYS:HG2	2.00	0.43
1:B:1753:ALA:C	1:B:1755:ALA:H	2.21	0.43
1:A:581:ILE:HG22	1:A:589:LYS:CG	2.47	0.43
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: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:A:699:GLU:CD	1:A:699:GLU:H	2.20	0.43
1:A:760:GLN:O	1:A:761:ALA:C	2.56	0.43
1:B:1152:THR:O	1:B:1239:GLN:OE1	2.37	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:659:VAL:C	1:A:660:LEU:HD23	2.39	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:B:1367:GLY:C	1:B:1369:GLU:N	2.71	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:A:716:ARG:O	1:A:722:LEU:C	2.57	0.42
1:B:1355:SER:C	1:B:1357:GLN:N	2.73	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:A:299:ARG:HB2	1:A:618:LEU:HD11	2.01	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:237:SER:C	1:A:238:LEU:HD23	2.40	0.42
1:B:1296:LEU:CD1	1:B:1301:PRO:HB2	2.42	0.42
1:B:1750:GLU:O	1:B:1753:ALA:HB3	2.19	0.42
1:B:1757:ALA:O	1:B:1758:LEU:C	2.57	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:1542:TYR:C	1:B:1608:PHE:HB3	2.40	0.42
1:B:1556:GLY:C	1:B:1557:ARG:HG3	2.40	0.42
1:A:345:SER:HB2	1:A:346:PRO:CD	2.39	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1533:LEU:O	1:B:1534:ALA:C	2.58	0.42
1:A:135:ALA:HB2	1:A:147:PHE:CE2	2.55	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
1:B:1515:GLU:C	1:B:1517:LEU:N	2.73	0.42
1:A:133:TYR:CD2	1:A:147:PHE:HB3	2.55	0.41
1:A:243:PHE:CD2	1:A:243:PHE:C	2.93	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:1699:GLU:H	1:B:1699:GLU:CD	2.22	0.41
1:B:1710:ASN:HB2	1:B:1732:PRO:HD3	2.02	0.41
1:A:190:PHE:CD2	1:A:190:PHE:C	2.93	0.41
1:A:637:SER:O	1:A:638:THR:C	2.57	0.41
1:B:1117:THR:C	1:B:1119:GLY:H	2.22	0.41
1:A:555:ALA:HA	1:A:570:ASN:O	2.20	0.41
1:A:757:ALA:O	1:A:758:LEU:C	2.57	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:1637:SER:O	1:B:1638:THR:C	2.58	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:A:716:ARG:C	1:A:722:LEU:HD23	2.40	0.41
1:B:1124:GLU:HB2	1:B:1338:ARG:NH1	2.35	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:1740:GLU:O	1:B:1741:VAL:C	2.58	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:711:LEU:HD22	1:A:730:PRO:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:718:GLU:O	1:A:719:ALA:C	2.60	0.41
1:A:758:LEU:C	1:A:762:MSE:HE3	2.40	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
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:HG12	1:B:1389:ASP:H	1.86	0.41
1:B:1639:PHE:O	1:B:1640:MSE:C	2.58	0.41
1:B:1718:GLU:HB3	1:B:1719:ALA:H	1.46	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:A:725:TYR:C	1:A:727:GLN:H	2.24	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: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:A:589:LYS:HZ2	1:A:696:HIS:HD1	1.70	0.40
1:B:1232:GLN:C	1:B:1234:GLY:H	2.25	0.40
1:B:1575:ALA:O	1:B:1576:HIS:HB2	2.20	0.40
1:B:1246:PRO:O	1:B:1251:ARG:CZ	2.70	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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

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	437/649 (67%)	344 (79%)	69 (16%)	24 (6%)	2 14
1	B	521/649 (80%)	406 (78%)	87 (17%)	28 (5%)	2 14
All	All	958/1298 (74%)	750 (78%)	156 (16%)	52 (5%)	2 14

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

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Mol	Chain	Res	Type
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
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 (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	346/515 (67%)	316 (91%)	30 (9%)	10	37
1	B	419/515 (81%)	385 (92%)	34 (8%)	11	42
All	All	765/1030 (74%)	701 (92%)	64 (8%)	11	39

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	141	ASP
1	A	145	LEU
1	A	161	LYS
1	A	168	ASP
1	A	174	ARG
1	A	195	ARG
1	A	230	ARG
1	A	232	GLN
1	A	243	PHE
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	554	ARG
1	A	563	ARG
1	A	565	THR
1	A	596	THR
1	A	625	ARG
1	A	636	LYS
1	A	660	LEU
1	A	662	ASP
1	A	670	SER
1	A	693	PHE
1	A	739	VAL

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Mol	Chain	Res	Type
1	A	740	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
1	B	1161	LYS
1	B	1168	ASP
1	B	1174	ARG
1	B	1202	LEU
1	B	1217	LEU
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	1370	VAL
1	B	1546	ARG
1	B	1551	LEU
1	B	1554	ARG
1	B	1563	ARG
1	B	1565	THR
1	B	1596	THR
1	B	1625	ARG
1	B	1636	LYS
1	B	1660	LEU
1	B	1662	ASP
1	B	1670	SER
1	B	1693	PHE
1	B	1739	VAL
1	B	1740	GLU
1	B	1759	LEU
1	B	1760	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	173	HIS

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Mol	Chain	Res	Type
1	A	232	GLN
1	A	239	GLN
1	A	558	HIS
1	A	585	ASN
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	1558	HIS
1	B	1585	ASN
1	B	1604	GLN
1	B	1615	HIS
1	B	1685	HIS
1	B	1727	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

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, 95^{th} 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%)	1.82	156 (35%)	0	0	34, 104, 154, 181	0
1	B	522/649 (80%)	1.68	155 (29%)	0	0	14, 98, 158, 188	0
All	All	962/1298 (74%)	1.74	311 (32%)	0	0	14, 102, 156, 188	0

All (311) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1142	GLY	13.3
1	A	530	TYR	8.5
1	A	216	ALA	8.2
1	B	1726	HIS	8.1
1	B	1719	ALA	8.0
1	A	279	THR	7.8
1	A	726	HIS	7.5
1	A	725	TYR	7.3
1	A	549	ASP	7.1
1	A	236	LEU	7.0
1	A	533	LEU	6.9
1	B	1267	ARG	6.9
1	A	550	ARG	6.7
1	B	1235	ALA	6.6
1	A	280	ARG	6.4
1	B	1362	LEU	6.2
1	A	720	GLY	6.2
1	B	1140	GLY	6.1
1	B	1223	ALA	6.1
1	B	1143	TRP	6.0
1	B	1344	ALA	6.0
1	A	525	ALA	5.9
1	B	1231	THR	5.9
1	B	1718	GLU	5.9

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Mol	Chain	Res	Type	RSRZ
1	B	1337	THR	5.8
1	B	1720	GLY	5.7
1	A	192	ASP	5.7
1	B	1241	PHE	5.7
1	B	1149	ASP	5.7
1	B	1220	ALA	5.7
1	A	188	GLY	5.6
1	B	1378	LEU	5.5
1	B	1737	TYR	5.4
1	A	719	ALA	5.4
1	A	210	GLU	5.3
1	A	302	LEU	5.2
1	A	544	ARG	5.1
1	B	1148	LEU	5.0
1	A	240	PRO	4.8
1	A	690	TYR	4.8
1	B	1345	SER	4.8
1	B	1191	LEU	4.8
1	B	1244	TYR	4.7
1	B	1725	TYR	4.7
1	B	1188	GLY	4.7
1	A	179	LEU	4.6
1	B	1178	VAL	4.6
1	B	1192	ASP	4.6
1	A	159	VAL	4.6
1	A	571	ASP	4.6
1	A	283	PRO	4.5
1	B	1180	LEU	4.5
1	B	1152	THR	4.5
1	B	1269	GLN	4.5
1	B	1224	LEU	4.5
1	A	284	GLY	4.5
1	B	1373	PRO	4.4
1	A	223	ALA	4.4
1	B	1173	HIS	4.4
1	B	1635	GLY	4.4
1	B	1363	ARG	4.4
1	B	1330	ALA	4.4
1	B	1587	ALA	4.4
1	A	133	TYR	4.3
1	B	1379	LYS	4.3
1	B	1277	ASP	4.3

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Mol	Chain	Res	Type	RSRZ
1	B	1202	LEU	4.2
1	B	1134	LEU	4.2
1	A	716	ARG	4.2
1	B	1203	SER	4.1
1	A	345	SER	4.1
1	A	310	GLU	4.1
1	A	149	ASP	4.1
1	A	265	PRO	4.1
1	A	584	PRO	4.0
1	A	178	VAL	4.0
1	B	1146	ALA	4.0
1	B	1139	THR	4.0
1	A	570	ASN	4.0
1	A	290	SER	3.9
1	A	721	GLY	3.8
1	A	617	PRO	3.8
1	A	524	LEU	3.8
1	A	206	PRO	3.8
1	A	715	ALA	3.8
1	A	160	LEU	3.8
1	B	1215	LEU	3.8
1	A	295	PRO	3.8
1	A	177	GLU	3.8
1	B	1189	ALA	3.8
1	A	722	LEU	3.8
1	B	1243	PHE	3.8
1	B	1505	GLU	3.7
1	A	241	PHE	3.7
1	A	614	ALA	3.7
1	A	244	TYR	3.7
1	B	1375	LEU	3.7
1	B	1185	LEU	3.7
1	B	1721	GLY	3.6
1	A	143	TRP	3.6
1	B	1525	ALA	3.6
1	B	1368	GLU	3.6
1	B	1553	ILE	3.6
1	B	1153	GLY	3.6
1	B	1504	LEU	3.6
1	A	275	VAL	3.5
1	B	1662	ASP	3.5
1	A	323	ARG	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	1279	THR	3.5
1	A	545	PRO	3.5
1	A	217	LEU	3.5
1	A	727	GLN	3.5
1	B	1186	GLU	3.5
1	A	534	ALA	3.4
1	A	605	VAL	3.4
1	B	1327	TYR	3.4
1	B	1221	ARG	3.4
1	A	237	SER	3.4
1	B	1150	VAL	3.4
1	A	677	ALA	3.3
1	B	1172	ARG	3.3
1	A	175	PRO	3.3
1	A	186	GLU	3.3
1	A	737	TYR	3.3
1	A	207	PHE	3.2
1	A	745	ALA	3.2
1	A	203	SER	3.2
1	A	344	ALA	3.2
1	B	1580	LEU	3.1
1	B	1144	GLY	3.1
1	A	138	ALA	3.1
1	A	292	LEU	3.1
1	A	536	VAL	3.1
1	A	142	GLY	3.1
1	A	547	PHE	3.1
1	A	618	LEU	3.1
1	A	155	PHE	3.1
1	A	611	ALA	3.1
1	A	765	ARG	3.0
1	B	1736	SER	3.0
1	A	529	VAL	3.0
1	A	184	LEU	3.0
1	B	1390	PRO	3.0
1	B	1160	LEU	3.0
1	A	582	THR	3.0
1	B	1677	ALA	3.0
1	B	1151	SER	3.0
1	A	312	PHE	3.0
1	B	1289	GLN	3.0
1	B	1506	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	1207	PHE	2.9
1	A	606	GLY	2.9
1	A	341	LEU	2.9
1	B	1752	VAL	2.9
1	B	1372	LEU	2.9
1	A	596	THR	2.9
1	A	156	LYS	2.9
1	B	1210	GLU	2.9
1	A	616	LEU	2.9
1	B	1690	TYR	2.9
1	B	1622	ILE	2.9
1	A	555	ALA	2.9
1	A	577	GLU	2.9
1	A	718	GLU	2.9
1	A	561	VAL	2.9
1	B	1123	GLN	2.9
1	A	286	ARG	2.8
1	B	1727	GLN	2.8
1	A	193	GLU	2.8
1	A	131	ALA	2.8
1	A	251	ARG	2.8
1	B	1127	LEU	2.8
1	A	608	PHE	2.8
1	A	624	THR	2.8
1	B	1182	PRO	2.8
1	A	209	PRO	2.8
1	B	1147	PHE	2.8
1	B	1558	HIS	2.8
1	A	560	VAL	2.7
1	A	327	TYR	2.7
1	A	293	ARG	2.7
1	A	669	SER	2.7
1	A	587	ALA	2.7
1	B	1237	SER	2.7
1	A	180	LEU	2.7
1	A	628	ALA	2.7
1	A	134	LEU	2.7
1	A	196	LYS	2.7
1	B	1669	SER	2.7
1	B	1219	ARG	2.7
1	A	543	VAL	2.7
1	B	1272	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	1168	ASP	2.6
1	A	145	LEU	2.6
1	A	554	ARG	2.6
1	B	1167	TYR	2.6
1	A	601	LEU	2.6
1	B	1213	GLY	2.6
1	B	1242	ARG	2.6
1	A	585	ASN	2.6
1	B	1179	LEU	2.6
1	B	1530	TYR	2.6
1	A	573	GLU	2.6
1	A	518	ARG	2.6
1	B	1226	ALA	2.6
1	B	1306	LEU	2.6
1	A	172	ARG	2.6
1	A	711	LEU	2.6
1	B	1581	ILE	2.6
1	B	1607	SER	2.6
1	A	622	ILE	2.6
1	B	1689	ALA	2.5
1	A	559	PRO	2.5
1	B	1131	ALA	2.5
1	A	144	GLY	2.5
1	B	1512	ARG	2.5
1	B	1564	ARG	2.5
1	B	1724	PHE	2.5
1	A	657	SER	2.5
1	A	137	ILE	2.5
1	B	1686	GLU	2.5
1	B	1668	THR	2.5
1	B	1702	ALA	2.5
1	A	222	GLY	2.4
1	B	1130	GLU	2.4
1	B	1287	LEU	2.4
1	A	285	ARG	2.4
1	B	1353	ARG	2.4
1	A	150	VAL	2.4
1	B	1268	GLY	2.4
1	A	269	GLN	2.4
1	B	1387	VAL	2.4
1	B	1209	PRO	2.4
1	B	1546	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	182	PRO	2.4
1	A	245	ASP	2.3
1	B	1137	ILE	2.3
1	B	1308	ARG	2.3
1	B	1584	PRO	2.3
1	A	539	ARG	2.3
1	B	1240	PRO	2.3
1	B	1305	ARG	2.3
1	A	346	PRO	2.3
1	B	1547	PHE	2.3
1	A	197	ARG	2.3
1	B	1624	THR	2.3
1	B	1163	LYS	2.3
1	B	1293	ARG	2.3
1	B	1551	LEU	2.3
1	A	609	VAL	2.3
1	A	658	LEU	2.3
1	A	659	VAL	2.3
1	B	1322	VAL	2.3
1	A	132	ASN	2.3
1	B	1266	LEU	2.3
1	A	161	LYS	2.3
1	B	1285	ARG	2.2
1	A	597	ALA	2.2
1	B	1613	GLU	2.2
1	B	1616	LEU	2.2
1	B	1194	PHE	2.2
1	B	1333	GLU	2.2
1	A	257	LEU	2.2
1	B	1593	LEU	2.2
1	A	270	ASP	2.2
1	A	732	PRO	2.2
1	B	1623	TYR	2.2
1	B	1733	ALA	2.2
1	A	318	LEU	2.2
1	B	1298	ASP	2.2
1	B	1758	LEU	2.2
1	B	1665	GLY	2.2
1	A	553	ILE	2.2
1	B	1340	GLU	2.2
1	A	306	LEU	2.2
1	B	1248	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	1391	PRO	2.2
1	A	319	ARG	2.2
1	B	1329	LEU	2.1
1	B	1154	GLU	2.1
1	A	691	THR	2.1
1	B	1304	ALA	2.1
1	B	1312	PHE	2.1
1	A	263	PHE	2.1
1	A	147	PHE	2.1
1	A	226	ALA	2.1
1	A	674	VAL	2.1
1	B	1559	PRO	2.1
1	A	537	ALA	2.1
1	A	595	GLN	2.1
1	B	1246	PRO	2.1
1	B	1706	PRO	2.1
1	B	1222	GLY	2.1
1	B	1284	GLY	2.1
1	B	1567	PHE	2.1
1	A	148	LEU	2.1
1	A	578	LEU	2.1
1	A	694	ALA	2.1
1	A	590	SER	2.1
1	B	1355	SER	2.1
1	A	644	GLU	2.0
1	B	1694	ALA	2.0
1	B	1710	ASN	2.0
1	B	1302	LEU	2.0
1	A	171	PHE	2.0
1	B	1693	PHE	2.0
1	A	305	ARG	2.0
1	A	531	ALA	2.0
1	A	219	ARG	2.0
1	B	1654	THR	2.0
1	A	266	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 monosaccharides 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.