Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 07:17 PM GMT

PDB ID	:	1EWR
Title	:	CRYSTAL STRUCTURE OF TAQ MUTS
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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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

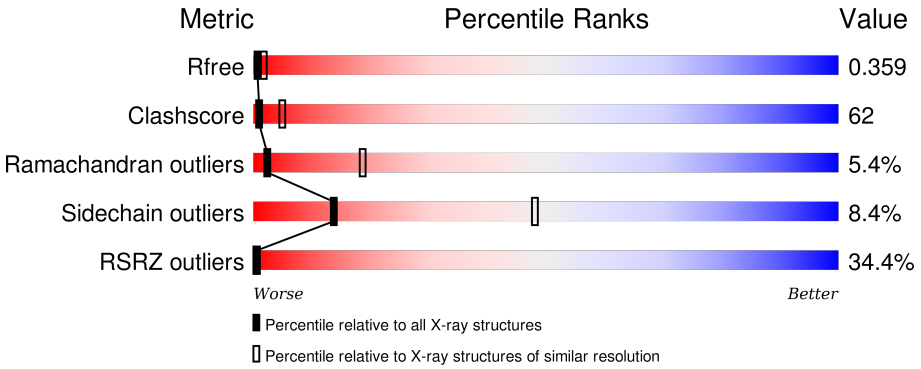
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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}	91344	1124 (3.24-3.16)
Clashscore	102246	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (3.22-3.18)
RSRZ outliers	91569	1129 (3.24-3.16)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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	26% 19% 44% 6% 31%
1	B	649	25% 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:

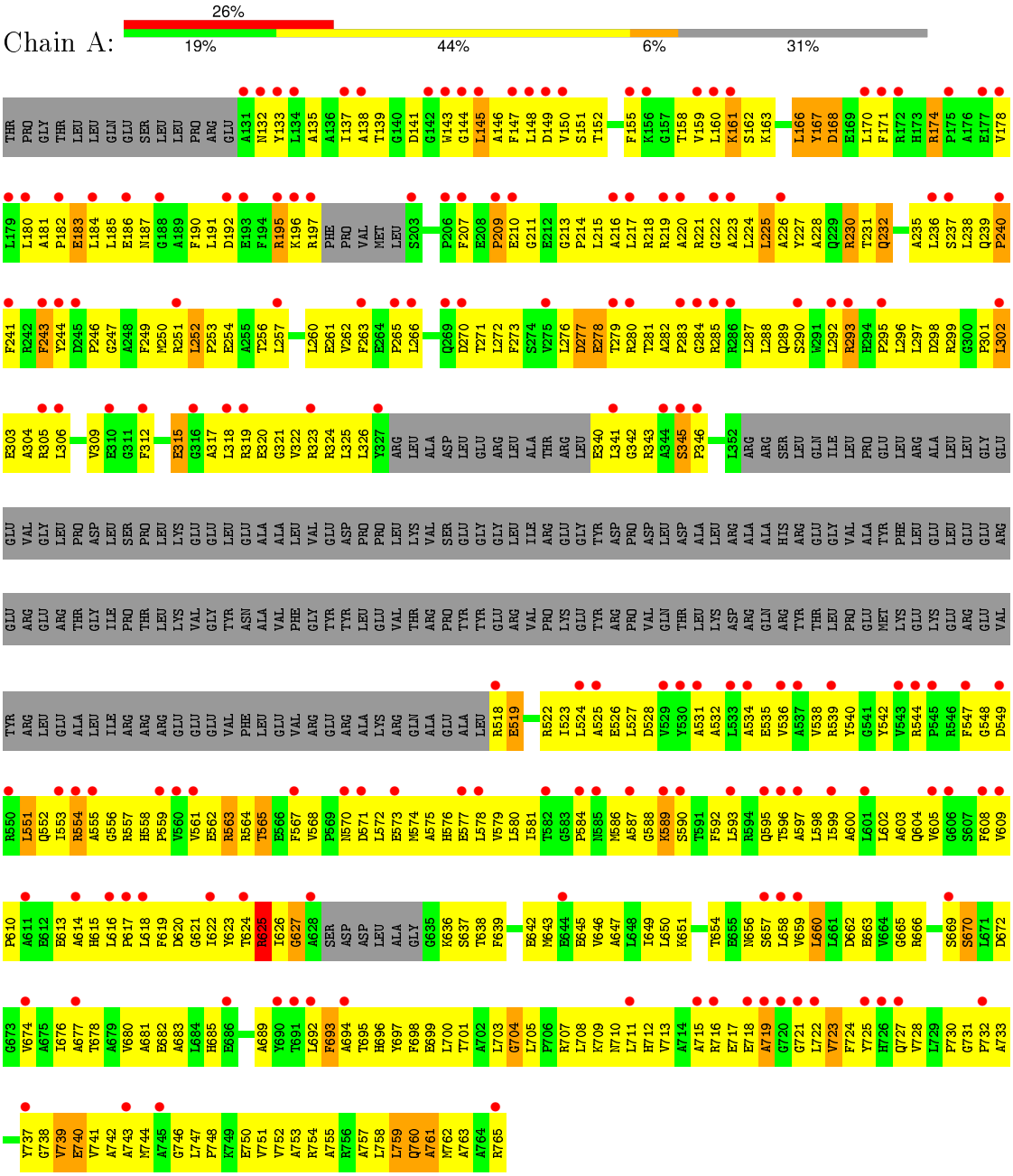
Chain	Residue	Modelled	Actual	Comment	Reference
A	250	MSE	MET	MODIFIED	UNP Q56215
A	574	MSE	MET	MODIFIED	UNP Q56215
A	586	MSE	MET	MODIFIED	UNP Q56215
A	640	MSE	MET	MODIFIED	UNP Q56215
A	643	MSE	MET	MODIFIED	UNP Q56215
A	744	MSE	MET	MODIFIED	UNP Q56215
A	762	MSE	MET	MODIFIED	UNP Q56215
B	1250	MSE	MET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

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

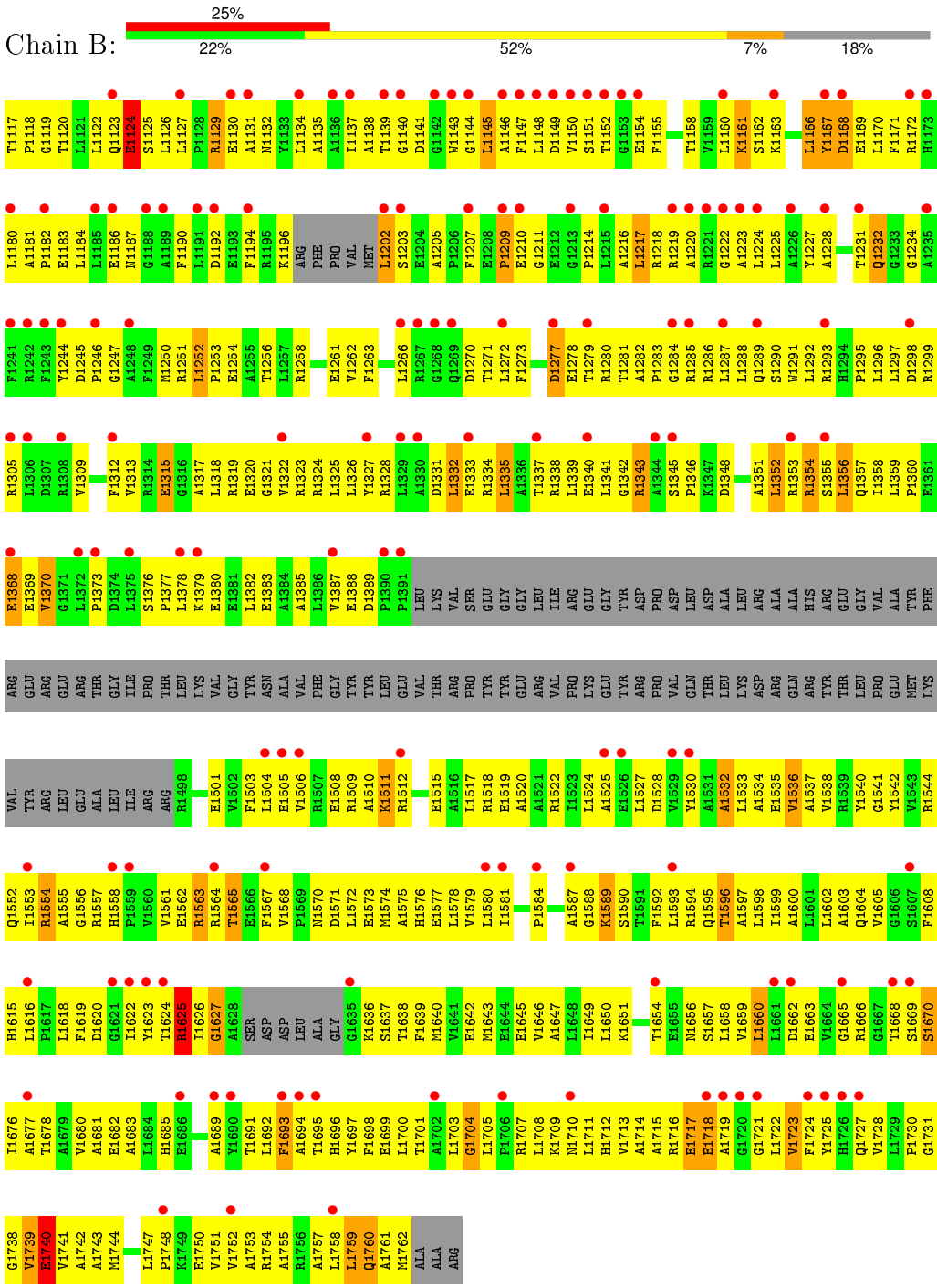
- Molecule 1: DNA MISMATCH REPAIR PROTEIN MUTS

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 0.9	Depositor
R, R_{free}	0.331 , 0.361 0.332 , 0.359	Depositor DCC
R_{free} test set	1813 reflections (4.87%)	DCC
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
Estimated twinning fraction	0.058 for -h,-k,l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.43$, $< L^2 > = 0.25$	Xtriage
Outliers	0 of 68672 reflections	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, 0.375 respectively for untwinned datasets, and 0.333, 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:HH11	1:B:1354:ARG:HG2	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:H	1:B:1161:LYS:HE2	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:B:1568:VAL:HG11	1:B:1727:GLN:HE22	1.43	0.81
1:A:148:LEU:HB3	1:A:224:LEU:HD13	1.60	0.81
1:B:1646:VAL:HA	1:B:1649:ILE:CD1	2.11	0.80
1:B:1354:ARG:NH1	1:B:1354:ARG:HG2	1.94	0.80
1:A:143:TRP:CE3	1:A:166:LEU:HD22	2.16	0.79
1:B:1563:ARG:HA	1:B:1563:ARG:HE	1.44	0.79
1:A:597:ALA:HB2	1:A:660:LEU:HD11	1.64	0.79
1:A:563:ARG:HA	1:A:563:ARG:HE	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:O	1:B:1352:LEU:HD12	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:B:1544:ARG:HB2	1:B:1608:PHE:CZ	2.20	0.76
1:B:1122:LEU:CD2	1:B:1341:LEU:HD13	2.15	0.76
1:A:143:TRP:HE3	1:A:166:LEU:HD22	1.50	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:B:1143:TRP:HE3	1:B:1166:LEU:HD22	1.51	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:1557:ARG:NH2	1:B:1610:PRO:HA	2.01	0.72
1:B:1250:MSE:HE3	1:B:1604:GLN:OE1	1.90	0.72
1:B:1708:LEU:HG	1:B:1709:LYS:H	1.54	0.71
1:A:717:GLU:HA	1:A:722:LEU:HA	1.71	0.71
1:B:1290:SER:HA	1:B:1293:ARG:NH1	2.05	0.71
1:B:1217:LEU:HD23	1:B:1218:ARG:N	2.05	0.71
1:B:1697:TYR:HB2	1:B:1700:LEU:HD12	1.72	0.71
1:A:280:ARG:HB2	1:A:528:ASP:OD1	1.90	0.71
1:B:1557:ARG:HA	1:B:1567:PHE:HE2	1.53	0.71
1:A:572:LEU:HD13	1:A:592:PHE:HZ	1.55	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:600:ALA:HA	1:A:616:LEU:HD13	1.73	0.70
1:A:584:PRO:HG3	1:A:715:ALA:HB2	1.72	0.70
1:B:1739:VAL:HG21	1:B:1759:LEU:HD12	1.72	0.70
1:A:548:GLY:O	1:A:617:PRO:HA	1.91	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:1589:LYS:HZ2	1:B:1696:HIS:CE1	2.09	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1563:ARG:CA	1:B:1563:ARG:HE	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:1723:VAL:O	1:B:1723:VAL:HG12	1.91	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:1161:LYS:CE	1:B:1161:LYS:H	2.04	0.69
1:A:170:LEU:O	1:A:170:LEU:HD13	1.91	0.69
1:B:1716:ARG:H	1:B:1723:VAL:H	1.39	0.68
1:A:696:HIS:O	1:B:1669:SER:HB3	1.94	0.68
1:A:174:ARG:HH11	1:A:174:ARG:HB3	1.57	0.68
1:A:563:ARG:CA	1:A:563:ARG:HE	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:B:1352:LEU:HD12	1:B:1356:LEU:HG	1.76	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:1290:SER:CA	1:B:1293:ARG:HH12	2.08	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:1378:LEU:HG	1:B:1510:ALA:HA	1.77	0.67
1:B:1600:ALA:HA	1:B:1616:LEU:HD13	1.75	0.66
1:B:1263:PHE:HE2	1:B:1292:LEU:HD12	1.60	0.66
1:B:1332:LEU:H	1:B:1332:LEU:HD12	1.60	0.66
1:B:1698:PHE:O	1:B:1701:THR:CG2	2.40	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:625:ARG:HG3	1:A:625:ARG:HH11	1.60	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:HH11	1:B:1522:ARG:HG2	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:B:1117:THR:HB	1:B:1120:THR:OG1	1.96	0.65
1:A:758:LEU:HB3	1:A:762:MSE:CE	2.26	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: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:132:ASN:O	1:A:149:ASP:HB2	1.98	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:148:LEU:HD12	1:A:155:PHE:CD1	2.31	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:646:VAL:HA	1:A:649:ILE:HD12	1.79	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:N	1:B:1129:ARG:HE	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:B:1625:ARG:HG3	1:B:1625:ARG:HH11	1.63	0.63
1:A:579:VAL:HB	1:A:692:LEU:HD23	1.79	0.63
1:B:1647:ALA:O	1:B:1651:LYS:HG3	1.99	0.63
1:B:1534:ALA:O	1:B:1538:VAL:HG23	1.98	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:1581:ILE:O	1:B:1589:LYS:HD3	1.99	0.63
1:A:237:SER:HB2	1:A:341:LEU:HG	1.81	0.63
1:B:1742:ALA:C	1:B:1747:LEU:HD12	2.19	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:743:ALA:HB2	1:A:752:VAL:HG11	1.79	0.62
1:B:1722:LEU:HB2	1:B:1744:MSE:SE	2.49	0.62
1:B:1717:GLU:N	1:B:1722:LEU:HD23	2.13	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:1568:VAL:CG1	1:B:1727:GLN:HE22	2.11	0.62
1:B:1117:THR:HG23	1:B:1177:GLU:CD	2.20	0.62
1:A:539:ARG:HB2	1:A:539:ARG:NH1	2.14	0.62
1:B:1712:HIS:ND1	1:B:1731:GLY:O	2.32	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: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:181:ALA:O	1:A:185:LEU:HG	1.98	0.62
1:B:1717:GLU:HA	1:B:1722:LEU:CA	2.29	0.62
1:A:750:GLU:CD	1:A:750:GLU:H	2.02	0.62
1:A:743:ALA:HB2	1:A:752:VAL:CG1	2.29	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:A:161:LYS:CE	1:A:161:LYS:H	2.13	0.62
1:B:1578:LEU:HD23	1:B:1578:LEU:C	2.19	0.61
1:B:1743:ALA:HB2	1:B:1752:VAL:HG11	1.82	0.61
1:B:1367:GLY:C	1:B:1369:GLU:H	2.04	0.61
1:B:1129:ARG:CZ	1:B:1285:ARG:NH1	2.63	0.61
1:B:1609:VAL:HB	1:B:1610:PRO:HD2	1.82	0.61
1:B:1373:PRO:HG2	1:B:1519:GLU:HG2	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:1572:LEU:HD13	1:B:1592:PHE:HZ	1.65	0.61
1:B:1174:ARG:HB3	1:B:1174:ARG:NH1	2.16	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:1574:MSE:HE3	1:B:1579:VAL:HG23	1.82	0.60
1:B:1170:LEU:HD13	1:B:1170:LEU:O	2.01	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:H	1:B:1750:GLU:CD	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:B:1674:VAL:HG11	1:B:1699:GLU:HG3	1.83	0.60
1:A:578:LEU:HD23	1:A:578:LEU:C	2.22	0.60
1:A:578:LEU:HD22	1:A:708:LEU:HD12	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:B:1578:LEU:HD22	1:B:1708:LEU:HD12	1.84	0.59
1:A:160:LEU:HD13	1:A:166:LEU:HD12	1.84	0.59
1:B:1599:ILE:HG23	1:B:1609:VAL:HG21	1.85	0.59
1:B:1579:VAL:HB	1:B:1692:LEU:HD23	1.84	0.59
1:B:1161:LYS:CD	1:B:1161:LYS:H	2.15	0.59
1:A:283:PRO:HB2	1:A:525:ALA:HB2	1.84	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:B:1602:LEU:O	1:B:1605:VAL:HG12	2.03	0.58
1:A:578:LEU:HD22	1:A:708:LEU:CD1	2.33	0.58
1:B:1342:GLY:O	1:B:1343:ARG:HG3	2.02	0.58
1:A:321:GLY:O	1:A:325:LEU:HG	2.03	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:B:1578:LEU:HD22	1:B:1708:LEU:CD1	2.34	0.58
1:A:685:HIS:CD2	1:A:705:LEU:HD13	2.38	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:B:1172:ARG:O	1:B:1293:ARG:HD2	2.03	0.58
1:A:572:LEU:HD13	1:A:592:PHE:CZ	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:685:HIS:CE1	1:A:707:ARG:HB2	2.39	0.58
1:B:1715:ALA:HB1	1:B:1722:LEU:HD22	1.86	0.58
1:A:261:GLU:HG2	1:A:266:LEU:HG	1.86	0.58
1:B:1716:ARG:N	1:B:1723:VAL:H	2.01	0.57
1:A:587:ALA:HB3	1:A:713:VAL:HG21	1.85	0.57
1:A:558:HIS:HD2	1:A:561:VAL:HG23	1.69	0.57
1:B:1658:LEU:HD12	1:B:1659:VAL:N	2.19	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:1716:ARG:O	1:B:1718:GLU:N	2.38	0.57
1:B:1581:ILE:CG2	1:B:1589:LYS:HG2	2.35	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:1551:LEU:HA	1:B:1615:HIS:O	2.04	0.57
1:A:715:ALA:HA	1:A:724:PHE:HA	1.85	0.57
1:B:1150:VAL:HG23	1:B:1151:SER:N	2.18	0.57
1:B:1716:ARG:CB	1:B:1723:VAL:HB	2.33	0.57
1:B:1356:LEU:O	1:B:1360:PRO:HD3	2.05	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: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:263:PHE:HE1	1:A:293:ARG:HG3	1.69	0.57
1:A:137:ILE:HA	1:A:144:GLY:O	2.05	0.57
1:A:273:PHE:O	1:A:277:ASP:N	2.37	0.57
1:B:1354:ARG:HH11	1:B:1354:ARG:CG	2.08	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:A:564:ARG:O	1:A:565:THR:HG23	2.04	0.57
1:A:282:ALA:N	1:A:283:PRO:CD	2.68	0.56
1:B:1317:ALA:O	1:B:1320:GLU:HB2	2.05	0.56
1:A:150:VAL:HG23	1:A:151:SER:N	2.20	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: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:A:261:GLU:HG3	1:A:266:LEU:HG	1.86	0.56
1:B:1685:HIS:CE1	1:B:1707:ARG:HB2	2.40	0.56
1:B:1501:GLU:O	1:B:1505:GLU:HG3	2.05	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: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:A:232:GLN:HG3	1:A:236:LEU:HD23	1.87	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:B:1581:ILE:HD13	1:B:1711:LEU:HB2	1.87	0.56
1:B:1542:TYR:CE1	1:B:1610:PRO:HB3	2.41	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:1533:LEU:O	1:B:1536:VAL:HB	2.05	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:1587:ALA:HB3	1:B:1713:VAL:CG2	2.36	0.56
1:B:1520:ALA:O	1:B:1524:LEU:HG	2.06	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:698:PHE:HA	1:A:701:THR:HG22	1.88	0.55
1:A:171:PHE:O	1:A:174:ARG:HG2	2.07	0.55
1:A:211:GLY:O	1:A:218:ARG:HD2	2.05	0.55
1:A:160:LEU:HD22	1:A:166:LEU:CA	2.31	0.55
1:A:625:ARG:HG3	1:A:625:ARG:NH1	2.18	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:518:ARG:HG2	1:A:518:ARG:HH11	1.70	0.55
1:A:609:VAL:HB	1:A:610:PRO:HD2	1.88	0.55
1:B:1296:LEU:HB2	1:B:1302:LEU:HD11	1.88	0.55
1:A:713:VAL:CG1	1:A:728:VAL:HG22	2.36	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:B:1698:PHE:O	1:B:1699:GLU:C	2.44	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:A:710:ASN:C	1:A:711:LEU:HD23	2.28	0.55
1:B:1625:ARG:HA	1:B:1645:GLU:OE1	2.07	0.55
1:B:1182:PRO:O	1:B:1186:GLU:HG3	2.07	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: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:A:717:GLU:N	1:A:722:LEU:HD23	2.22	0.54
1:A:625:ARG:HG3	1:A:625:ARG:O	2.07	0.54
1:A:658:LEU:HD12	1:A:659:VAL:N	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:599:ILE:HG23	1:A:609:VAL:HG21	1.89	0.54
1:A:587:ALA:HB3	1:A:713:VAL:CG2	2.38	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: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:A:161:LYS:H	1:A:161:LYS:CD	2.21	0.54
1:B:1503:PHE:CD2	1:B:1504:LEU:HD12	2.43	0.54
1:B:1270:ASP:HB2	1:B:1564:ARG:HH12	1.73	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:O	1:B:1625:ARG:HG3	2.08	0.54
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: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:A:252:LEU:HD22	1:A:257:LEU:HG	1.89	0.53
1:A:143:TRP:N	1:A:160:LEU:O	2.41	0.53
1:A:748:PRO:HB2	1:A:751:VAL:HG23	1.90	0.53
1:A:180:LEU:HD22	1:A:184:LEU:HD13	1.90	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:1625:ARG:NH2	1:B:1627:GLY:O	2.41	0.53
1:A:524:LEU:O	1:A:528:ASP:N	2.37	0.53
1:B:1320:GLU:O	1:B:1324:ARG:HG3	2.08	0.53
1:A:299:ARG:HA	1:A:618:LEU:HD11	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1595:GLN:O	1:B:1599:ILE:HG13	2.07	0.53
1:B:1322:VAL:HG13	1:B:1362:LEU:HD22	1.90	0.53
1:B:1625:ARG:NH1	1:B:1625:ARG:HG3	2.21	0.53
1:A:237:SER:O	1:A:238:LEU:HD23	2.08	0.53
1:B:1353:ARG:O	1:B:1357:GLN:HG3	2.09	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:1685:HIS:NE2	1:B:1705:LEU:HB3	2.23	0.53
1:B:1319:ARG:NH1	1:B:1319:ARG:HB3	2.24	0.53
1:B:1129:ARG:CB	1:B:1285:ARG:HD2	2.35	0.53
1:B:1352:LEU:C	1:B:1352:LEU:HD12	2.28	0.53
1:A:171:PHE:CD2	1:A:254:GLU:HG3	2.44	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:A:228:ALA:HB3	1:A:236:LEU:HD11	1.90	0.53
1:B:1148:LEU:HD12	1:B:1155:PHE:CD1	2.44	0.53
1:B:1542:TYR:HA	1:B:1609:VAL:O	2.08	0.53
1:A:552:GLN:O	1:A:614:ALA:HA	2.09	0.53
1:A:139:THR:CG2	1:A:184:LEU:HD21	2.38	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:B:1552:GLN:O	1:B:1614:ALA:HA	2.10	0.52
1:B:1273:PHE:HE1	1:B:1288:LEU:HD23	1.75	0.52
1:B:1323:ARG:HH11	1:B:1323:ARG:HG2	1.73	0.52
1:A:323:ARG:CG	1:A:531:ALA:HB1	2.38	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:1557:ARG:CA	1:B:1567:PHE:HE2	2.21	0.52
1:B:1166:LEU:O	1:B:1168:ASP:N	2.43	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:557:ARG:CA	1:A:567:PHE:HE2	2.19	0.52
1:A:166:LEU:HD23	1:A:167:TYR:CD1	2.45	0.52
1:B:1674:VAL:HA	1:B:1697:TYR:CE1	2.45	0.52
1:B:1620:ASP:OD1	1:B:1657:SER:HA	2.09	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:1604:GLN:NE2	1:B:1618:LEU:HA	2.24	0.51
1:A:758:LEU:O	1:A:762:MSE:HE3	2.11	0.51
1:A:625:ARG:NE	1:A:642:GLU:HG2	2.24	0.51
1:B:1270:ASP:HB2	1:B:1564:ARG:NH1	2.25	0.51
1:A:250:MSE:SE	1:A:622:ILE:HG13	2.61	0.51
1:B:1335:LEU:CD1	1:B:1352:LEU:HB2	2.32	0.51
1:A:760:GLN:O	1:A:763:ALA:HB3	2.10	0.51
1:B:1718:GLU:CB	1:B:1723:VAL:HG21	2.38	0.51
1:A:317:ALA:O	1:A:320:GLU:HB2	2.10	0.51
1:A:263:PHE:CE1	1:A:293:ARG:HG3	2.44	0.51
1:B:1151:SER:O	1:B:1337:THR:HG21	2.09	0.51
1:A:742:ALA:HB1	1:A:747:LEU:HD12	1.93	0.51
1:A:625:ARG:HA	1:A:645:GLU:OE1	2.10	0.51
1:B:1505:GLU:O	1:B:1509:ARG:HG3	2.11	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:A:228:ALA:HA	1:A:231:THR:OG1	2.10	0.51
1:B:1654:THR:HG23	1:B:1656:ASN:H	1.76	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:B:1202:LEU:N	1:B:1202:LEU:HD12	2.26	0.51
1:A:518:ARG:HB3	1:A:522:ARG:CZ	2.41	0.51
1:B:1331:ASP:O	1:B:1331:ASP:OD1	2.29	0.51
1:A:281:THR:N	1:A:528:ASP:OD2	2.44	0.51
1:B:1228:ALA:HB3	1:B:1236:LEU:CD1	2.40	0.51
1:A:287:LEU:HD23	1:A:526:GLU:HA	1.92	0.51
1:B:1722:LEU:HB2	1:B:1744:MSE:CE	2.40	0.51
1:B:1645:GLU:O	1:B:1649:ILE:HG13	2.11	0.51
1:B:1558:HIS:HD2	1:B:1561:VAL:HG23	1.76	0.51
1:B:1143:TRP:N	1:B:1160:LEU:O	2.42	0.51
1:B:1129:ARG:HB2	1:B:1285:ARG:CD	2.32	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:A:182:PRO:O	1:A:186:GLU:HG3	2.11	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:556:GLY:O	1:A:557:ARG:HG3	2.11	0.50
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:698:PHE:O	1:A:699:GLU:C	2.49	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:A:523:ILE:O	1:A:527:LEU:HG	2.11	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:322:VAL:HG12	1:A:326:LEU:HD11	1.94	0.50
1:A:139:THR:C	1:A:216:ALA:HB2	2.32	0.50
1:B:1263:PHE:CE2	1:B:1292:LEU:HD12	2.43	0.50
1:A:581:ILE:HG22	1:A:589:LYS:HD3	1.94	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:B:1279:THR:HG21	1:B:1285:ARG:CB	2.40	0.50
1:A:715:ALA:CB	1:A:722:LEU:HD22	2.41	0.50
1:B:1760:GLN:C	1:B:1762:MSE:H	2.15	0.50
1:B:1145:LEU:O	1:B:1158:THR:N	2.42	0.50
1:B:1717:GLU:N	1:B:1722:LEU:HA	2.26	0.50
1:B:1642:GLU:O	1:B:1645:GLU:HB2	2.11	0.50
1:A:558:HIS:HD2	1:A:561:VAL:CG2	2.25	0.50
1:B:1577:GLU:OE1	1:B:1709:LYS:HE3	2.12	0.50
1:A:540:TYR:CD2	1:A:563:ARG:NH1	2.79	0.50
1:B:1332:LEU:H	1:B:1332:LEU:CD1	2.25	0.50
1:B:1299:ARG:O	1:B:1303:GLU:HG2	2.12	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:1148:LEU:C	1:B:1148:LEU:HD23	2.33	0.49
1:A:273:PHE:CE1	1:A:288:LEU:HD23	2.47	0.49
1:B:1123:GLN:NE2	1:B:1123:GLN:H	2.11	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:A:518:ARG:CB	1:A:522:ARG:NH2	2.75	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:B:1572:LEU:HD13	1:B:1592:PHE:CZ	2.46	0.49
1:B:1332:LEU:HD12	1:B:1332:LEU:N	2.27	0.49
1:A:737:TYR:O	1:A:740:GLU:HB2	2.13	0.49
1:A:166:LEU:C	1:A:168:ASP:N	2.65	0.49
1:B:1568:VAL:HG11	1:B:1727:GLN:NE2	2.21	0.49
1:B:1182:PRO:HG2	1:B:1183:GLU:OE1	2.13	0.49
1:A:263:PHE:O	1:A:271:THR:HG21	2.11	0.49
1:B:1166:LEU:C	1:B:1168:ASP:N	2.65	0.49
1:A:574:MSE:HG2	1:A:579:VAL:HG21	1.95	0.49
1:A:250:MSE:HE2	1:A:619:PHE:HB2	1.95	0.49
1:A:558:HIS:CD2	1:A:561:VAL:HG23	2.47	0.49
1:A:148:LEU:HD23	1:A:148:LEU:C	2.33	0.49
1:A:155:PHE:O	1:A:241:PHE:HA	2.13	0.49
1:B:1638:THR:HG22	1:B:1642:GLU:OE2	2.13	0.49
1:A:279:THR:HA	1:A:532:ALA:HB2	1.93	0.49
1:A:663:GLU:CB	1:A:666:ARG:HD3	2.42	0.49
1:A:214:PRO:O	1:A:217:LEU:HB3	2.13	0.49
1:B:1117:THR:CG2	1:B:1119:GLY:H	2.13	0.49
1:A:539:ARG:CZ	1:A:539:ARG:HB2	2.43	0.49
1:A:159:VAL:CG2	1:A:217:LEU:HB2	2.42	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:B:1698:PHE:CA	1:B:1701:THR:HG22	2.43	0.48
1:A:716:ARG:H	1:A:723:VAL:H	1.60	0.48
1:A:586:MSE:HE1	1:B:1640:MSE:CE	2.42	0.48
1:B:1209:PRO:CB	1:B:1218:ARG:HH21	2.18	0.48
1:A:654:THR:HG23	1:A:656:ASN:H	1.78	0.48
1:A:279:THR:CG2	1:A:285:ARG:HB2	2.41	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: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:1693:PHE:HD2	1:B:1693:PHE:C	2.15	0.48
1:B:1352:LEU:CD1	1:B:1356:LEU:HG	2.43	0.48
1:A:754:ARG:NH2	1:A:758:LEU:HD21	2.28	0.48
1:A:620:ASP:OD1	1:A:657:SER:HA	2.13	0.48
1:B:1293:ARG:HH11	1:B:1293:ARG:HG3	1.78	0.48
1:A:638:THR:HG22	1:A:642:GLU:OE2	2.13	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:B:1574:MSE:HG2	1:B:1579:VAL:HG21	1.95	0.48
1:B:1716:ARG:C	1:B:1722:LEU:HA	2.34	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:O	1:B:1378:LEU:HD23	2.13	0.48
1:B:1685:HIS:HE1	1:B:1707:ARG:HB2	1.79	0.48
1:B:1553:ILE:HD13	1:B:1599:ILE:HD12	1.96	0.48
1:A:723:VAL:HG12	1:A:723:VAL:O	2.13	0.48
1:B:1351:ALA:O	1:B:1354:ARG:HB3	2.14	0.48
1:A:645:GLU:O	1:A:649:ILE:HG13	2.13	0.48
1:B:1169:GLU:OE2	1:B:1246:PRO:HB3	2.14	0.48
1:A:685:HIS:HE1	1:A:707:ARG:H	1.62	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:1697:TYR:CB	1:B:1700:LEU:HD12	2.43	0.48
1:B:1247:GLY:HA2	1:B:1251:ARG:CZ	2.44	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:B:1528:ASP:O	1:B:1532:ALA:HB2	2.14	0.47
1:B:1129:ARG:CZ	1:B:1285:ARG:HH12	2.25	0.47
1:A:580:LEU:CD1	1:A:701:THR:HA	2.44	0.47
1:A:221:ARG:HD3	1:A:241:PHE:CD1	2.49	0.47
1:A:642:GLU:O	1:A:645:GLU:HB2	2.15	0.47
1:B:1753:ALA:C	1:B:1755:ALA:N	2.68	0.47
1:A:270:ASP:OD2	1:A:564:ARG:NH1	2.47	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:1148:LEU:HD12	1:B:1155:PHE:CE1	2.48	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:B:1542:TYR:HB3	1:B:1608:PHE:C	2.35	0.47
1:B:1580:LEU:CD1	1:B:1701:THR:HA	2.45	0.47
1:B:1302:LEU:HD21	1:B:1604:GLN:HA	1.97	0.47
1:A:639:PHE:CE1	1:A:643:MSE:HE3	2.49	0.47
1:A:345:SER:CB	1:A:346:PRO:HD2	2.36	0.47
1:B:1625:ARG:NE	1:B:1642:GLU:HG2	2.29	0.47
1:B:1563:ARG:CA	1:B:1563:ARG:NE	2.77	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:625:ARG:CZ	1:A:642:GLU:HG2	2.44	0.47
1:B:1135:ALA:HA	1:B:1146:ALA:O	2.14	0.47
1:A:703:LEU:O	1:A:705:LEU:HG	2.15	0.47
1:A:145:LEU:O	1:A:158:THR:N	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:HH11	1:B:1363:ARG:HG2	1.79	0.47
1:A:303:GLU:OE2	1:A:303:GLU:HA	2.14	0.47
1:A:599:ILE:HG22	1:A:616:LEU:HD11	1.98	0.47
1:B:1303:GLU:HA	1:B:1303:GLU:OE2	2.15	0.47
1:A:588:GLY:O	1:A:592:PHE:N	2.45	0.47
1:B:1217:LEU:HD23	1:B:1217:LEU:C	2.36	0.47
1:A:273:PHE:HE1	1:A:288:LEU:HD23	1.79	0.47
1:A:740:GLU:O	1:A:741:VAL:C	2.53	0.47
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: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:A:323:ARG:HH11	1:A:323:ARG:HG2	1.81	0.46
1:B:1737:TYR:O	1:B:1740:GLU:HB2	2.14	0.46
1:A:654:THR:HG22	1:A:657:SER:OG	2.14	0.46
1:B:1553:ILE:O	1:B:1571:ASP:HA	2.15	0.46
1:A:312:PHE:HD2	1:A:319:ARG:HA	1.79	0.46
1:A:237:SER:CB	1:A:341:LEU:HG	2.44	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:1748:PRO:HB2	1:B:1751:VAL:HG23	1.97	0.46
1:B:1544:ARG:HB2	1:B:1608:PHE:CE2	2.50	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:1258:ARG:O	1:B:1266:LEU:HD21	2.15	0.46
1:B:1117:THR:HG21	1:B:1134:LEU:HD13	1.98	0.46
1:A:682:GLU:HA	1:A:685:HIS:HB3	1.98	0.46
1:A:554:ARG:HB3	1:A:613:GLU:H	1.80	0.46
1:B:1313:VAL:HG13	1:B:1538:VAL:HG21	1.97	0.46
1:A:586:MSE:SE	1:B:1640:MSE:SE	3.33	0.46
1:B:1715:ALA:CB	1:B:1722:LEU:HD22	2.45	0.46
1:A:224:LEU:O	1:A:225:LEU:C	2.53	0.46
1:B:1625:ARG:CZ	1:B:1642:GLU:HG2	2.46	0.46
1:B:1743:ALA:CB	1:B:1752:VAL:HG11	2.45	0.46
1:A:287:LEU:CD2	1:A:526:GLU:HA	2.46	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:B:1262:VAL:HG12	1:B:1263:PHE:N	2.31	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:1574:MSE:HE3	1:B:1579:VAL:CG2	2.46	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:A:207:PHE:CD2	1:A:220:ALA:HA	2.51	0.46
1:A:574:MSE:HE3	1:A:579:VAL:CG2	2.43	0.46
1:A:182:PRO:HD2	1:A:183:GLU:OE1	2.16	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:B:1313:VAL:CG1	1:B:1538:VAL:HG22	2.44	0.45
1:B:1558:HIS:HD2	1:B:1561:VAL:CG2	2.28	0.45
1:B:1546:ARG:O	1:B:1615:HIS:HA	2.16	0.45
1:B:1581:ILE:HA	1:B:1711:LEU:O	2.16	0.45
1:B:1126:LEU:O	1:B:1127:LEU:HD23	2.15	0.45
1:A:718:GLU:OE1	1:A:723:VAL:HG11	2.16	0.45
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: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:B:1184:LEU:HB3	1:B:1190:PHE:CE2	2.52	0.45
1:A:558:HIS:CE1	1:A:598:LEU:HD11	2.50	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:B:1711:LEU:HD22	1:B:1730:PRO:HA	1.98	0.45
1:B:1120:THR:HA	1:B:1150:VAL:CG1	2.47	0.45
1:A:278:GLU:OE1	1:A:536:VAL:HG22	2.16	0.45
1:B:1522:ARG:NH1	1:B:1522:ARG:HG2	2.28	0.45
1:B:1380:GLU:HA	1:B:1383:GLU:OE1	2.17	0.45
1:B:1623:TYR:CD1	1:B:1623:TYR:N	2.84	0.45
1:A:260:LEU:N	1:A:260:LEU:HD12	2.32	0.45
1:A:544:ARG:HB2	1:A:608:PHE:CZ	2.51	0.45
1:B:1318:LEU:HD11	1:B:1366:LEU:HD23	1.99	0.45
1:A:692:LEU:HA	1:A:692:LEU:HD23	1.79	0.45
1:A:534:ALA:O	1:A:538:VAL:HG23	2.16	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:556:GLY:C	1:A:557:ARG:HG3	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:B:1298:ASP:C	1:B:1301:PRO:HD2	2.37	0.45
1:A:280:ARG:NH1	1:A:280:ARG:HG3	2.30	0.45
1:A:578:LEU:C	1:A:578:LEU:CD2	2.85	0.45
1:A:170:LEU:HD13	1:A:170:LEU:C	2.36	0.45
1:B:1537:ALA:HA	1:B:1542:TYR:HB2	1.98	0.45
1:B:1281:THR:HB	1:B:1283:PRO:HD2	1.99	0.45
1:A:581:ILE:HB	1:A:694:ALA:HA	1.98	0.45
1:B:1250:MSE:CE	1:B:1604:GLN:OE1	2.63	0.45
1:B:1161:LYS:HE2	1:B:1161:LYS:N	2.19	0.45
1:B:1563:ARG:HA	1:B:1563:ARG:NE	2.23	0.45
1:B:1555:ALA:HA	1:B:1570:ASN:O	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:B:1301:PRO:O	1:B:1304:ALA:HB3	2.17	0.45
1:A:296:LEU:HB2	1:A:302:LEU:HD11	1.98	0.45
1:A:250:MSE:HE1	1:A:622:ILE:HD11	2.00	0.45
1:B:1708:LEU:HG	1:B:1709:LYS:N	2.26	0.45
1:A:518:ARG:HD2	1:A:522:ARG:HH21	1.82	0.45
1:A:232:GLN:HG3	1:A:236:LEU:CD2	2.46	0.45
1:B:1678:THR:O	1:B:1682:GLU:HG3	2.17	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:1263:PHE:HE1	1:B:1293:ARG:HG2	1.82	0.44
1:A:590:SER:HA	1:A:593:LEU:CD1	2.38	0.44
1:B:1722:LEU:O	1:B:1723:VAL:HG23	2.17	0.44
1:A:138:ALA:HB3	1:A:216:ALA:O	2.16	0.44
1:B:1180:LEU:HD11	1:B:1194:PHE:CD2	2.52	0.44
1:A:654:THR:H	1:A:657:SER:CB	2.31	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:B:1291:TRP:HH2	1:B:1530:TYR:CE2	2.35	0.44
1:A:247:GLY:HA2	1:A:251:ARG:NH2	2.31	0.44
1:B:1557:ARG:HB2	1:B:1610:PRO:HB2	1.99	0.44
1:A:746:GLY:O	1:B:1651:LYS:NZ	2.44	0.44
1:A:553:ILE:HD13	1:A:599:ILE:HD12	1.98	0.44
1:B:1639:PHE:CE1	1:B:1643:MSE:HE3	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1540:TYR:CD1	1:B:1563:ARG:NH1	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:623:TYR:N	1:A:623:TYR:CD1	2.85	0.44
1:B:1536:VAL:CG1	1:B:1537:ALA:N	2.80	0.44
1:B:1120:THR:HA	1:B:1150:VAL:HG13	2.00	0.44
1:A:693:PHE:CD2	1:A:693:PHE:C	2.91	0.44
1:B:1373:PRO:CG	1:B:1519:GLU:HG2	2.45	0.44
1:B:1179:LEU:HD22	1:B:1203:SER:O	2.18	0.44
1:B:1581:ILE:HB	1:B:1694:ALA:HA	1.98	0.44
1:B:1117:THR:C	1:B:1119:GLY:N	2.71	0.44
1:A:251:ARG:NH1	1:A:251:ARG:HG2	2.33	0.44
1:B:1535:GLU:O	1:B:1536:VAL:C	2.55	0.44
1:B:1143:TRP:HH2	1:B:1163:LYS:HD3	1.80	0.44
1:B:1742:ALA:O	1:B:1747:LEU:HD12	2.16	0.44
1:A:739:VAL:HA	1:B:1676:ILE:HD11	2.00	0.44
1:B:1682:GLU:HA	1:B:1685:HIS:HB3	1.98	0.44
1:B:1363:ARG:NH2	1:B:1368:GLU:HG3	2.33	0.44
1:B:1220:ALA:O	1:B:1223:ALA:HB3	2.18	0.44
1:A:191:LEU:HD21	1:A:195:ARG:NH2	2.33	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: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:A:171:PHE:CZ	1:A:254:GLU:HG3	2.52	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: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:581:ILE:HA	1:A:711:LEU:O	2.18	0.43
1:A:559:PRO:HB3	1:A:610:PRO:HG3	2.00	0.43
1:B:1659:VAL:C	1:B:1660:LEU:HD23	2.39	0.43
1:A:724:PHE:HD1	1:A:724:PHE:H	1.64	0.43
1:B:1359:LEU:CB	1:B:1360:PRO:HD3	2.48	0.43
1:A:143:TRP:HH2	1:A:163:LYS:HD3	1.82	0.43
1:B:1685:HIS:HE1	1:B:1707:ARG:H	1.66	0.43
1:B:1181:ALA:HB1	1:B:1219:ARG:NH2	2.33	0.43
1:A:230:ARG:HD2	1:A:230:ARG:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1252:LEU:HA	1:B:1252:LEU:HD23	1.80	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:1718:GLU:CG	1:B:1723:VAL:HG21	2.48	0.43
1:A:540:TYR:CD2	1:A:563:ARG:HD3	2.53	0.43
1:B:1663:GLU:CB	1:B:1666:ARG:HD3	2.47	0.43
1:A:553:ILE:O	1:A:571:ASP:HA	2.18	0.43
1:B:1579:VAL:HG13	1:B:1709:LYS:HG2	2.00	0.43
1:A:563:ARG:HA	1:A:563:ARG:NE	2.26	0.43
1:B:1753:ALA:C	1:B:1755:ALA:H	2.21	0.43
1:B:1673:GLY:HA3	1:B:1697:TYR:OH	2.18	0.43
1:B:1125:SER:O	1:B:1126:LEU:HD23	2.19	0.43
1:A:581:ILE:HG22	1:A:589:LYS:CG	2.47	0.43
1:B:1717:GLU:HA	1:B:1721:GLY:O	2.18	0.43
1:A:757:ALA:O	1:A:759:LEU:N	2.52	0.43
1:B:1138:ALA:O	1:B:1216:ALA:HB1	2.18	0.43
1:B:1743:ALA:HB2	1:B:1752:VAL:HG13	1.99	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: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:1592:PHE:CD1	1:B:1728:VAL:HG21	2.53	0.43
1:B:1331:ASP:O	1:B:1333:GLU:N	2.52	0.43
1:B:1252:LEU:HD21	1:B:1256:THR:CG2	2.48	0.43
1:A:699:GLU:CD	1:A:699:GLU:H	2.20	0.43
1:B:1714:ALA:O	1:B:1724:PHE:HA	2.19	0.43
1:B:1152:THR:O	1:B:1239:GLN:OE1	2.37	0.43
1:A:760:GLN:O	1:A:761:ALA:C	2.56	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:1150:VAL:CG2	1:B:1151:SER:N	2.82	0.43
1:B:1130:GLU:HG2	1:B:1289:GLN:NE2	2.33	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:1557:ARG:CZ	1:B:1562:GLU:OE2	2.66	0.43
1:B:1717:GLU:H	1:B:1717:GLU:HG3	1.63	0.43
1:B:1654:THR:H	1:B:1657:SER:HB2	1.83	0.43
1:B:1183:GLU:OE2	1:B:1219:ARG:NH1	2.51	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:B:1127:LEU:HD13	1:B:1151:SER:CB	2.49	0.42
1:B:1568:VAL:CG1	1:B:1727:GLN:NE2	2.79	0.42
1:A:743:ALA:HB2	1:A:752:VAL:HG13	2.01	0.42
1:A:180:LEU:HD22	1:A:184:LEU:CD1	2.48	0.42
1:A:138:ALA:HB2	1:A:207:PHE:CD2	2.54	0.42
1:B:1518:ARG:HG2	1:B:1518:ARG:HH11	1.84	0.42
1:A:669:SER:HB3	1:B:1696:HIS:O	2.18	0.42
1:A:586:MSE:HE1	1:B:1640:MSE:HE1	2.00	0.42
1:B:1748:PRO:O	1:B:1752:VAL:HG23	2.19	0.42
1:A:256:THR:HA	1:A:624:THR:OG1	2.18	0.42
1:A:289:GLN:O	1:A:293:ARG:NH1	2.52	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: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:A:278:GLU:HB2	1:A:536:VAL:CG2	2.49	0.42
1:A:236:LEU:HB3	1:A:238:LEU:HD21	2.02	0.42
1:B:1367:GLY:O	1:B:1369:GLU:N	2.51	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:B:1296:LEU:CD1	1:B:1301:PRO:HB2	2.42	0.42
1:A:143:TRP:CZ3	1:A:166:LEU:HD22	2.53	0.42
1:B:1750:GLU:O	1:B:1753:ALA:HB3	2.19	0.42
1:A:237:SER:C	1:A:238:LEU:HD23	2.40	0.42
1:A:150:VAL:CG2	1:A:151:SER:N	2.83	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: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:B:1117:THR:HG22	1:B:1119:GLY:CA	2.49	0.42
1:A:676:ILE:O	1:A:680:VAL:HG23	2.20	0.42
1:B:1222:GLY:HA2	1:B:1225:LEU:CD1	2.44	0.42
1:B:1135:ALA:O	1:B:1178:VAL:HA	2.20	0.42
1:B:1603:ALA:CB	1:B:1616:LEU:HD12	2.50	0.42
1:A:710:ASN:HB2	1:A:732:PRO:HD3	2.02	0.42
1:B:1742:ALA:HB1	1:B:1747:LEU:HD12	1.99	0.42
1:A:345:SER:HB2	1:A:346:PRO:CD	2.39	0.42
1:B:1533:LEU:O	1:B:1534:ALA:C	2.58	0.42
1:B:1250:MSE:CA	1:B:1297:LEU:HD21	2.49	0.42
1:B:1354:ARG:HA	1:B:1357:GLN:OE1	2.19	0.42
1:B:1261:GLU:HG2	1:B:1266:LEU:HG	1.98	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:236:LEU:CB	1:A:238:LEU:HD21	2.50	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:A:135:ALA:HB2	1:A:147:PHE:CE2	2.55	0.42
1:B:1515:GLU:C	1:B:1517:LEU:N	2.73	0.42
1:A:563:ARG:CA	1:A:563:ARG:NE	2.79	0.41
1:A:133:TYR:CD2	1:A:147:PHE:HB3	2.55	0.41
1:A:243:PHE:C	1:A:243:PHE:CD2	2.93	0.41
1:B:1699:GLU:CD	1:B:1699:GLU:H	2.22	0.41
1:B:1710:ASN:HB2	1:B:1732:PRO:HD3	2.02	0.41
1:B:1312:PHE:HB3	1:B:1319:ARG:HB2	2.02	0.41
1:B:1117:THR:C	1:B:1119:GLY:H	2.22	0.41
1:A:637:SER:O	1:A:638:THR:C	2.57	0.41
1:A:190:PHE:C	1:A:190:PHE:CD2	2.93	0.41
1:B:1581:ILE:HG22	1:B:1589:LYS:HD3	2.02	0.41
1:B:1659:VAL:O	1:B:1691:THR:HA	2.19	0.41
1:B:1293:ARG:NH1	1:B:1293:ARG:HB2	2.35	0.41
1:B:1637:SER:O	1:B:1638:THR:C	2.58	0.41
1:A:757:ALA:O	1:A:758:LEU:C	2.57	0.41
1:A:555:ALA:HA	1:A:570:ASN:O	2.20	0.41
1:A:262:VAL:HG12	1:A:263:PHE:N	2.35	0.41
1:B:1537:ALA:CB	1:B:1542:TYR:HB2	2.50	0.41
1:B:1578:LEU:HD21	1:B:1580:LEU:CD2	2.51	0.41
1:B:1658:LEU:HD12	1:B:1659:VAL:H	1.83	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:A:279:THR:HG21	1:A:285:ARG:CA	2.50	0.41
1:B:1345:SER:HB2	1:B:1346:PRO:HD2	2.03	0.41
1:B:1620:ASP:OD1	1:B:1657:SER:CA	2.68	0.41
1:B:1291:TRP:CH2	1:B:1530:TYR:CE2	3.09	0.41
1:A:685:HIS:CE1	1:A:707:ARG:H	2.39	0.41
1:A:265:PRO:HB3	1:A:270:ASP:O	2.21	0.41
1:B:1124:GLU:HB2	1:B:1338:ARG:NH1	2.35	0.41
1:B:1554:ARG:HB3	1:B:1613:GLU:HB3	2.01	0.41
1:B:1740:GLU:O	1:B:1741:VAL:C	2.58	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:557:ARG:HB2	1:A:610:PRO:HB2	2.03	0.41
1:B:1129:ARG:HA	1:B:1282:ALA:HB1	2.02	0.41
1:A:711:LEU:HD22	1:A:730:PRO:HA	2.02	0.41
1:B:1618:LEU:HA	1:B:1618:LEU:HD23	1.83	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:A:161:LYS:HD2	1:A:162:SER:N	2.32	0.41
1:A:575:ALA:O	1:A:576:HIS:HB2	2.19	0.41
1:A:603:ALA:CB	1:A:616:LEU:HD12	2.50	0.41
1:B:1160:LEU:HD22	1:B:1166:LEU:N	2.35	0.41
1:B:1287:LEU:O	1:B:1290:SER:HB3	2.20	0.41
1:A:693:PHE:HD2	1:A:694:ALA:N	2.19	0.41
1:A:589:LYS:NZ	1:A:696:HIS:HD1	2.19	0.41
1:A:718:GLU:O	1:A:719:ALA:C	2.60	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:A:222:GLY:HA2	1:A:225:LEU:HD12	2.03	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:1261:GLU:HG2	1:B:1266:LEU:H	1.86	0.41
1:B:1387:VAL:HG12	1:B:1389:ASP:H	1.86	0.41
1:B:1693:PHE:HD2	1:B:1694:ALA:N	2.19	0.41
1:B:1594:ARG:O	1:B:1596:THR:N	2.54	0.41
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:A:326:LEU:CD1	1:A:528:ASP:HA	2.50	0.40
1:B:1232:GLN:HE22	1:B:1343:ARG:CZ	2.34	0.40
1:A:518:ARG:CD	1:A:522:ARG:HH21	2.35	0.40
1:B:1685:HIS:CE1	1:B:1707:ARG:NH2	2.90	0.40
1:A:320:GLU:O	1:A:324:ARG:HG3	2.20	0.40
1:A:135:ALA:O	1:A:178:VAL:HA	2.22	0.40
1:B:1145:LEU:HD22	1:B:1147:PHE:CE1	2.56	0.40
1:B:1547:PHE:HA	1:B:1616:LEU:O	2.21	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:A:554:ARG:HB3	1:A:613:GLU:HB3	2.02	0.40
1:A:301:PRO:O	1:A:304:ALA:HB3	2.21	0.40
1:A:589:LYS:HZ2	1:A:696:HIS:HD1	1.70	0.40
1:A:225:LEU:O	1:A:227:TYR:N	2.55	0.40
1:B:1232:GLN:C	1:B:1234:GLY:H	2.25	0.40
1:A:312:PHE:HB3	1:A:319:ARG:HG3	2.03	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:152:THR:O	1:A:239:GLN:OE1	2.39	0.40
1:B:1575:ALA:O	1:B:1576:HIS:HB2	2.20	0.40
1:B:1556:GLY:O	1:B:1557:ARG:HG3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1339:LEU:HD22	1:B:1511:LYS:HB2	2.03	0.40
1:B:1247:GLY:HA2	1:B:1251:ARG:NH2	2.37	0.40
1:B:1246:PRO:O	1:B:1251:ARG:CZ	2.70	0.40
1:B:1382:LEU:HD23	1:B:1506:VAL:CG1	2.52	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 18
1	B	521/649 (80%)	406 (78%)	87 (17%)	28 (5%)	2 19
All	All	958/1298 (74%)	750 (78%)	156 (16%)	52 (5%)	2 19

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%)	13	45
1	B	419/515 (81%)	385 (92%)	34 (8%)	15	51
All	All	765/1030 (74%)	701 (92%)	64 (8%)	14	48

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

Some 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 carbohydrates 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

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%)	1.89	168 (38%)	0	0	34, 104, 154, 181	0
1	B	522/649 (80%)	1.74	163 (31%)	1	0	14, 98, 158, 188	0
All	All	962/1298 (74%)	1.81	331 (34%)	0	0	14, 102, 156, 188	0

All (331) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1142	GLY	13.7
1	A	530	TYR	8.8
1	A	216	ALA	8.3
1	B	1726	HIS	8.2
1	B	1719	ALA	8.2
1	A	279	THR	8.0
1	A	725	TYR	7.6
1	A	726	HIS	7.5
1	A	549	ASP	7.3
1	A	236	LEU	7.2
1	A	533	LEU	7.1
1	B	1267	ARG	7.1
1	A	550	ARG	6.9
1	B	1235	ALA	6.7
1	A	280	ARG	6.6
1	B	1362	LEU	6.4
1	A	720	GLY	6.3
1	B	1140	GLY	6.3
1	B	1223	ALA	6.3
1	B	1143	TRP	6.2
1	B	1344	ALA	6.1
1	B	1231	THR	6.1
1	A	525	ALA	6.1
1	B	1718	GLU	6.0

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Mol	Chain	Res	Type	RSRZ
1	B	1337	THR	6.0
1	B	1720	GLY	5.9
1	A	192	ASP	5.9
1	B	1241	PHE	5.8
1	B	1220	ALA	5.8
1	B	1149	ASP	5.8
1	A	188	GLY	5.7
1	B	1378	LEU	5.7
1	B	1737	TYR	5.7
1	A	719	ALA	5.5
1	A	210	GLU	5.4
1	A	302	LEU	5.4
1	A	544	ARG	5.2
1	B	1148	LEU	5.1
1	A	690	TYR	5.0
1	A	240	PRO	5.0
1	B	1345	SER	4.9
1	B	1244	TYR	4.9
1	B	1725	TYR	4.9
1	B	1191	LEU	4.9
1	B	1188	GLY	4.8
1	A	179	LEU	4.8
1	B	1178	VAL	4.7
1	A	283	PRO	4.7
1	A	159	VAL	4.7
1	B	1180	LEU	4.7
1	A	571	ASP	4.7
1	B	1192	ASP	4.7
1	B	1152	THR	4.7
1	B	1224	LEU	4.6
1	B	1269	GLN	4.6
1	A	284	GLY	4.6
1	B	1373	PRO	4.6
1	B	1363	ARG	4.5
1	B	1635	GLY	4.5
1	A	223	ALA	4.5
1	A	133	TYR	4.5
1	B	1173	HIS	4.5
1	B	1330	ALA	4.5
1	B	1587	ALA	4.5
1	B	1379	LYS	4.4
1	B	1277	ASP	4.4

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Mol	Chain	Res	Type	RSRZ
1	B	1202	LEU	4.4
1	A	716	ARG	4.3
1	B	1134	LEU	4.3
1	A	345	SER	4.2
1	B	1203	SER	4.2
1	A	310	GLU	4.2
1	A	265	PRO	4.2
1	A	149	ASP	4.2
1	A	584	PRO	4.1
1	A	178	VAL	4.1
1	B	1139	THR	4.1
1	B	1146	ALA	4.1
1	A	570	ASN	4.0
1	A	290	SER	4.0
1	A	721	GLY	4.0
1	A	524	LEU	4.0
1	A	206	PRO	3.9
1	A	617	PRO	3.9
1	B	1215	LEU	3.9
1	A	160	LEU	3.9
1	A	295	PRO	3.9
1	A	715	ALA	3.9
1	B	1189	ALA	3.9
1	A	722	LEU	3.9
1	A	177	GLU	3.9
1	B	1243	PHE	3.9
1	A	241	PHE	3.8
1	A	244	TYR	3.8
1	B	1505	GLU	3.8
1	B	1185	LEU	3.8
1	B	1375	LEU	3.8
1	A	614	ALA	3.8
1	A	143	TRP	3.8
1	B	1721	GLY	3.8
1	B	1525	ALA	3.7
1	B	1368	GLU	3.7
1	B	1153	GLY	3.7
1	B	1553	ILE	3.7
1	B	1504	LEU	3.7
1	A	275	VAL	3.6
1	A	323	ARG	3.6
1	B	1662	ASP	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	1279	THR	3.6
1	A	545	PRO	3.6
1	A	217	LEU	3.6
1	A	727	GLN	3.6
1	B	1327	TYR	3.6
1	B	1186	GLU	3.5
1	B	1221	ARG	3.5
1	A	605	VAL	3.5
1	A	534	ALA	3.5
1	B	1172	ARG	3.5
1	A	237	SER	3.5
1	B	1150	VAL	3.5
1	A	175	PRO	3.4
1	A	677	ALA	3.4
1	A	737	TYR	3.4
1	A	186	GLU	3.3
1	A	207	PHE	3.3
1	A	745	ALA	3.3
1	A	203	SER	3.3
1	A	344	ALA	3.2
1	B	1580	LEU	3.2
1	B	1144	GLY	3.2
1	A	292	LEU	3.2
1	A	138	ALA	3.2
1	A	547	PHE	3.2
1	A	155	PHE	3.2
1	A	536	VAL	3.2
1	A	765	ARG	3.2
1	A	142	GLY	3.2
1	A	618	LEU	3.2
1	A	611	ALA	3.1
1	B	1736	SER	3.1
1	A	184	LEU	3.1
1	B	1390	PRO	3.1
1	A	529	VAL	3.1
1	B	1160	LEU	3.1
1	A	582	THR	3.1
1	A	312	PHE	3.1
1	B	1151	SER	3.1
1	B	1677	ALA	3.0
1	B	1506	VAL	3.0
1	A	606	GLY	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	1289	GLN	3.0
1	A	341	LEU	3.0
1	B	1207	PHE	3.0
1	B	1690	TYR	3.0
1	B	1372	LEU	3.0
1	B	1752	VAL	3.0
1	A	596	THR	3.0
1	A	156	LYS	3.0
1	A	616	LEU	3.0
1	B	1210	GLU	3.0
1	A	555	ALA	3.0
1	A	718	GLU	3.0
1	A	561	VAL	2.9
1	A	577	GLU	2.9
1	B	1622	ILE	2.9
1	A	286	ARG	2.9
1	A	251	ARG	2.9
1	B	1123	GLN	2.9
1	B	1127	LEU	2.9
1	B	1727	GLN	2.9
1	A	608	PHE	2.9
1	A	193	GLU	2.9
1	A	131	ALA	2.9
1	A	624	THR	2.9
1	B	1182	PRO	2.9
1	A	209	PRO	2.9
1	B	1147	PHE	2.8
1	A	327	TYR	2.8
1	A	293	ARG	2.8
1	B	1558	HIS	2.8
1	A	560	VAL	2.8
1	A	669	SER	2.8
1	B	1237	SER	2.8
1	A	587	ALA	2.8
1	B	1219	ARG	2.8
1	A	180	LEU	2.8
1	A	196	LYS	2.8
1	A	134	LEU	2.8
1	B	1167	TYR	2.8
1	A	628	ALA	2.8
1	A	554	ARG	2.7
1	B	1669	SER	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	543	VAL	2.7
1	A	145	LEU	2.7
1	B	1272	LEU	2.7
1	B	1242	ARG	2.7
1	B	1168	ASP	2.7
1	B	1530	TYR	2.7
1	A	601	LEU	2.7
1	B	1179	LEU	2.7
1	A	518	ARG	2.7
1	B	1213	GLY	2.7
1	A	172	ARG	2.7
1	A	573	GLU	2.7
1	A	585	ASN	2.7
1	B	1306	LEU	2.7
1	B	1226	ALA	2.6
1	A	711	LEU	2.6
1	B	1607	SER	2.6
1	B	1581	ILE	2.6
1	B	1512	ARG	2.6
1	A	559	PRO	2.6
1	A	622	ILE	2.6
1	B	1564	ARG	2.6
1	A	144	GLY	2.6
1	B	1689	ALA	2.6
1	B	1131	ALA	2.6
1	B	1724	PHE	2.6
1	A	657	SER	2.6
1	B	1668	THR	2.6
1	B	1686	GLU	2.5
1	B	1702	ALA	2.5
1	A	137	ILE	2.5
1	A	222	GLY	2.5
1	A	285	ARG	2.5
1	B	1353	ARG	2.5
1	B	1287	LEU	2.5
1	B	1130	GLU	2.5
1	B	1268	GLY	2.5
1	A	150	VAL	2.5
1	B	1546	ARG	2.5
1	A	182	PRO	2.4
1	B	1387	VAL	2.4
1	B	1209	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	269	GLN	2.4
1	A	539	ARG	2.4
1	B	1308	ARG	2.4
1	A	197	ARG	2.4
1	B	1584	PRO	2.4
1	A	245	ASP	2.4
1	B	1305	ARG	2.4
1	A	346	PRO	2.4
1	B	1240	PRO	2.4
1	B	1624	THR	2.4
1	B	1547	PHE	2.4
1	B	1293	ARG	2.4
1	B	1137	ILE	2.4
1	B	1163	LYS	2.4
1	B	1551	LEU	2.4
1	A	609	VAL	2.3
1	A	658	LEU	2.3
1	A	659	VAL	2.3
1	B	1266	LEU	2.3
1	B	1322	VAL	2.3
1	A	161	LYS	2.3
1	B	1285	ARG	2.3
1	A	132	ASN	2.3
1	B	1623	TYR	2.3
1	B	1613	GLU	2.3
1	A	597	ALA	2.3
1	B	1194	PHE	2.3
1	B	1616	LEU	2.3
1	A	257	LEU	2.3
1	B	1593	LEU	2.3
1	A	732	PRO	2.3
1	B	1333	GLU	2.3
1	A	270	ASP	2.3
1	A	318	LEU	2.3
1	B	1733	ALA	2.3
1	B	1758	LEU	2.3
1	B	1298	ASP	2.3
1	A	319	ARG	2.2
1	B	1391	PRO	2.2
1	B	1665	GLY	2.2
1	B	1340	GLU	2.2
1	A	306	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	1248	ALA	2.2
1	B	1329	LEU	2.2
1	A	553	ILE	2.2
1	A	691	THR	2.2
1	B	1312	PHE	2.2
1	B	1154	GLU	2.2
1	A	263	PHE	2.2
1	B	1304	ALA	2.2
1	B	1559	PRO	2.2
1	A	147	PHE	2.2
1	A	674	VAL	2.2
1	A	226	ALA	2.2
1	A	537	ALA	2.2
1	B	1246	PRO	2.2
1	B	1706	PRO	2.2
1	A	595	GLN	2.1
1	B	1567	PHE	2.1
1	A	148	LEU	2.1
1	B	1222	GLY	2.1
1	B	1284	GLY	2.1
1	A	578	LEU	2.1
1	B	1355	SER	2.1
1	A	305	ARG	2.1
1	B	1302	LEU	2.1
1	A	694	ALA	2.1
1	B	1694	ALA	2.1
1	A	644	GLU	2.1
1	A	590	SER	2.1
1	A	219	ARG	2.1
1	B	1693	PHE	2.1
1	A	171	PHE	2.1
1	B	1710	ASN	2.1
1	A	195	ARG	2.1
1	A	531	ALA	2.1
1	B	1654	THR	2.1
1	A	266	LEU	2.1
1	B	1621	GLY	2.1
1	A	220	ALA	2.1
1	A	686	GLU	2.1
1	B	1748	PRO	2.1
1	A	589	LYS	2.1
1	A	692	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	316	GLY	2.0
1	B	1526	GLU	2.0
1	A	743	ALA	2.0
1	B	1661	LEU	2.0
1	B	1228	ALA	2.0
1	B	1529	VAL	2.0
1	A	170	LEU	2.0
1	B	1695	THR	2.0
1	A	567	PHE	2.0
1	A	593	LEU	2.0
1	A	599	ILE	2.0
1	B	1136	ALA	2.0
1	A	243	PHE	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.