



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:23 AM GMT

PDB ID : 2GW1
Title : Crystal Structure of the Yeast Tom70
Authors : Wu, Y.; Sha, B.
Deposited on : 2006-05-03
Resolution : 3.00 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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) 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

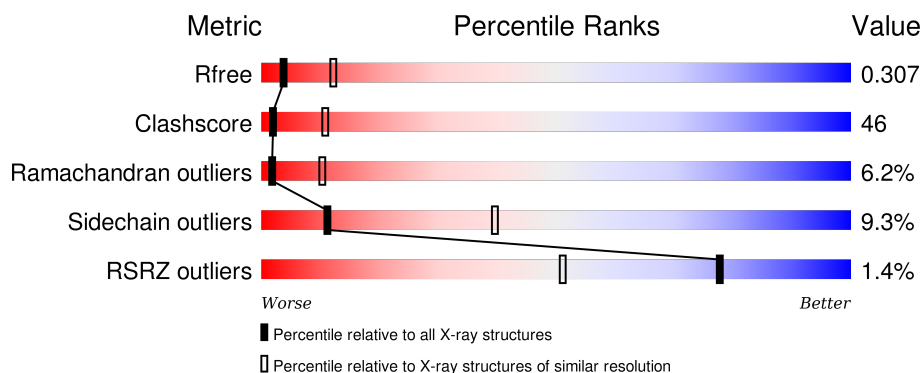
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	514	
1	B	514	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7984 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 Mitochondrial precursor proteins import receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	487	Total	C	N	O	S	0	0	0
			3929	2500	642	773	14			
1	B	487	Total	C	N	O	S	0	0	0
			3929	2500	642	773	14			

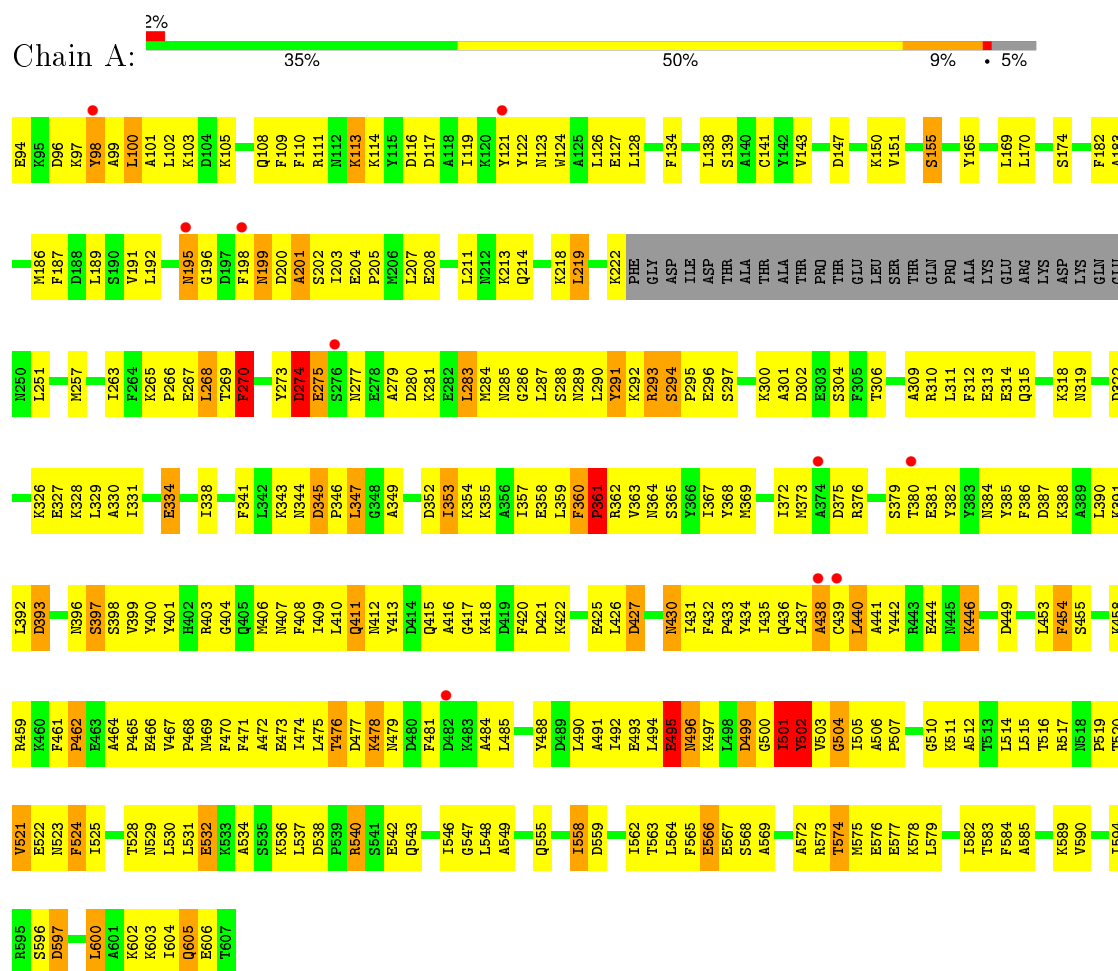
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	65	Total	O	0	0
			65	65		
2	B	61	Total	O	0	0
			61	61		

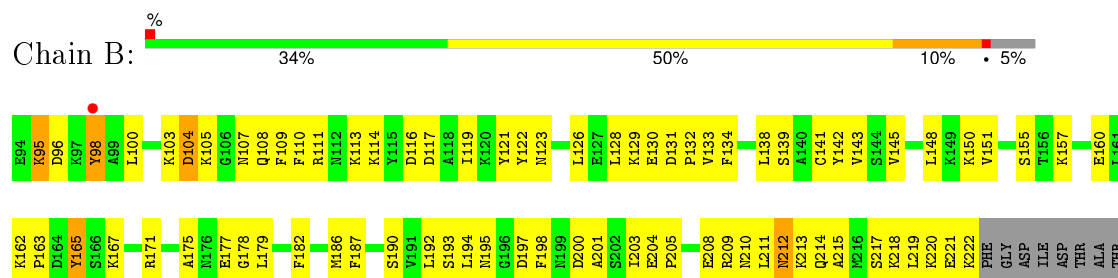
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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: Mitochondrial precursor proteins import receptor



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4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	44.88 Å 168.60 Å 82.99 Å 90.00° 102.59° 90.00°	Depositor
Resolution (Å)	46.17 – 3.00 46.17 – 2.90	Depositor EDS
% Data completeness (in resolution range)	97.0 (46.17-3.00) 94.7 (46.17-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.13 (at 2.91 Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.259 , 0.316 0.254 , 0.307	Depositor DCC
R_{free} test set	1128 reflections (4.83%)	DCC
Wilson B-factor (Å ²)	83.2	Xtriage
Anisotropy	0.200	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 58.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	2 of 25246 reflections (0.008%)	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	7984	wwPDB-VP
Average B, all atoms (Å ²)	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.25% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.29	0/3999	0.53	1/5379 (0.0%)
1	B	0.29	0/3999	0.51	0/5379
All	All	0.29	0/7998	0.52	1/10758 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	275	GLU	N-CA-C	-5.31	96.66	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	3929	0	3885	383	0
1	B	3929	0	3885	357	0
2	A	65	0	0	22	0
2	B	61	0	0	25	0
All	All	7984	0	7770	726	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 46.

All (726) 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:B:439:CYS:SG	1:B:442:TYR:HB2	2.02	0.99
1:A:478:LYS:HE3	1:A:478:LYS:HA	1.45	0.98
1:B:148:LEU:HB3	1:B:179:LEU:HD11	1.46	0.96
1:B:255:THR:HG22	2:B:660:HOH:O	1.66	0.93
1:B:344:ASN:O	1:B:345:ASP:HB3	1.66	0.93
1:B:431:ILE:HD11	1:B:467:VAL:HG23	1.50	0.92
1:B:558:ILE:HG12	1:B:559:ASP:H	1.35	0.91
1:A:469:ASN:HD22	1:A:507:PRO:HG3	1.35	0.91
1:A:283:LEU:HD11	1:A:331:ILE:HD11	1.52	0.91
1:A:506:ALA:HB3	1:A:507:PRO:HD3	1.54	0.90
1:A:369:MET:SD	1:A:372:ILE:HD11	2.12	0.90
1:A:455:SER:HA	1:A:458:LYS:HB2	1.53	0.89
1:A:606:GLU:HG2	2:A:636:HOH:O	1.71	0.89
1:B:376:ARG:HH21	1:B:377:ASN:HB3	1.39	0.88
1:A:269:THR:HG23	1:A:270:PHE:H	1.38	0.88
1:A:439:CYS:SG	1:A:442:TYR:HB2	2.16	0.86
1:B:478:LYS:HE3	1:B:478:LYS:HA	1.56	0.86
1:B:376:ARG:HE	1:B:377:ASN:H	1.23	0.85
1:A:274:ASP:HA	1:A:280:ASP:HB3	1.59	0.84
1:B:468:PRO:HB2	1:B:491:ALA:HB2	1.58	0.84
1:A:293:ARG:HD2	1:A:501:ILE:HG22	1.60	0.82
1:A:341:PHE:HD2	1:A:372:ILE:HG22	1.43	0.82
1:A:435:ILE:HG21	1:A:470:PHE:HD2	1.45	0.82
1:A:331:ILE:HG22	1:A:362:ARG:HE	1.44	0.82
1:B:435:ILE:HG21	1:B:470:PHE:HD2	1.45	0.82
1:A:499:ASP:HA	2:A:611:HOH:O	1.79	0.81
1:B:488:TYR:O	1:B:492:ILE:HG13	1.79	0.81
1:B:105:LYS:HA	1:B:108:GLN:HE21	1.41	0.81
1:A:522:GLU:O	1:A:525:ILE:HG22	1.80	0.81
1:A:291:TYR:O	1:A:292:LYS:HG2	1.81	0.80
1:A:349:ALA:O	1:A:353:ILE:HG23	1.81	0.80
1:A:390:LEU:HD21	1:A:399:VAL:HG21	1.64	0.80
1:B:458:LYS:HE2	1:B:468:PRO:HG3	1.64	0.79
1:A:331:ILE:HG22	1:A:362:ARG:NE	1.99	0.78
1:A:521:VAL:HG23	1:A:522:GLU:HG3	1.66	0.77
1:A:344:ASN:CG	1:A:345:ASP:H	1.88	0.77
1:B:587:ALA:O	1:B:590:VAL:HG12	1.85	0.77
1:A:98:TYR:O	1:A:102:LEU:HG	1.85	0.76
1:B:558:ILE:HG12	1:B:559:ASP:N	1.99	0.76
1:A:222:LYS:HB2	2:A:651:HOH:O	1.84	0.76
1:B:551:MET:HE3	2:B:662:HOH:O	1.85	0.76
1:A:341:PHE:CD2	1:A:372:ILE:HG22	2.21	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:273:TYR:CE2	1:A:274:ASP:HB3	2.21	0.75
1:B:367:ILE:HD11	1:B:399:VAL:HG12	1.67	0.75
1:B:467:VAL:HB	1:B:468:PRO:HD3	1.68	0.74
1:A:473:GLU:O	1:A:476:THR:HG22	1.87	0.74
1:B:329:LEU:HD22	1:B:333:LEU:HG	1.68	0.74
1:B:506:ALA:HB3	1:B:507:PRO:HD3	1.68	0.74
1:B:293:ARG:HH21	1:B:502:TYR:HA	1.53	0.73
1:A:427:ASP:OD2	1:A:430:ASN:HB2	1.87	0.73
1:A:139:SER:O	1:A:143:VAL:HG23	1.89	0.73
1:B:253:SER:HB2	2:B:660:HOH:O	1.87	0.73
1:A:420:PHE:CZ	1:A:436:GLN:HG2	2.24	0.73
1:B:437:LEU:HD23	1:B:440:LEU:HD23	1.69	0.73
1:B:251:LEU:HD12	2:B:628:HOH:O	1.89	0.73
1:A:396:ASN:O	1:A:399:VAL:HG22	1.89	0.72
1:B:439:CYS:SG	1:B:474:ILE:HD13	2.30	0.72
1:A:390:LEU:CD2	1:A:399:VAL:HG21	2.19	0.71
1:A:274:ASP:HA	1:A:280:ASP:CB	2.20	0.71
1:B:331:ILE:HG22	1:B:362:ARG:HE	1.54	0.71
1:B:278:GLU:HG3	1:B:311:LEU:HD13	1.71	0.71
1:A:594:ILE:HG22	1:A:604:ILE:HD11	1.72	0.71
1:A:119:ILE:HG22	1:A:123:ASN:ND2	2.06	0.71
1:B:217:SER:O	1:B:220:LYS:HG2	1.90	0.71
1:A:360:PHE:HD2	1:A:361:PRO:HD2	1.56	0.70
1:A:269:THR:HA	2:A:630:HOH:O	1.91	0.70
1:A:312:PHE:HB3	1:A:329:LEU:HB2	1.74	0.70
1:A:505:ILE:HG23	1:A:534:ALA:HB1	1.72	0.70
1:A:503:VAL:HG12	1:A:507:PRO:HD3	1.74	0.70
1:A:505:ILE:HG12	1:A:538:ASP:HB2	1.72	0.70
1:B:399:VAL:HG23	1:B:400:TYR:H	1.57	0.70
1:A:98:TYR:HA	1:A:101:ALA:HB3	1.74	0.70
1:B:463:GLU:HA	1:B:494:LEU:HD22	1.73	0.70
1:A:214:GLN:HG3	1:B:586:GLU:HG2	1.72	0.70
1:A:379:SER:C	1:A:381:GLU:H	1.96	0.69
1:A:273:TYR:CE2	1:A:284:MET:HG3	2.27	0.69
1:A:363:VAL:HG11	1:A:396:ASN:ND2	2.06	0.69
1:B:418:LYS:HE2	2:B:610:HOH:O	1.91	0.69
1:A:467:VAL:HB	1:A:468:PRO:HD3	1.75	0.69
1:B:520:THR:HG22	1:B:522:GLU:H	1.57	0.69
1:A:207:LEU:HD13	1:B:204:GLU:CD	2.14	0.68
1:A:169:LEU:HD23	1:A:192:LEU:HD13	1.73	0.68
1:B:598:PRO:HA	1:B:601:ALA:HB3	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:522:GLU:O	1:B:525:ILE:HG22	1.92	0.68
1:B:409:ILE:HD12	1:B:410:LEU:N	2.08	0.68
1:A:361:PRO:O	1:A:362:ARG:HB3	1.91	0.68
1:B:431:ILE:HG12	1:B:435:ILE:HD11	1.75	0.68
1:B:331:ILE:HG22	1:B:362:ARG:NE	2.08	0.67
1:B:353:ILE:O	1:B:357:ILE:HG13	1.95	0.67
1:B:349:ALA:O	1:B:353:ILE:HG23	1.94	0.67
1:B:525:ILE:HD12	1:B:528:THR:HG21	1.76	0.67
1:A:455:SER:HA	1:A:458:LYS:CB	2.25	0.67
1:B:302:ASP:HB2	1:B:339:PHE:CE2	2.29	0.67
1:A:322:ASP:O	1:A:326:LYS:HG3	1.94	0.67
1:B:427:ASP:OD2	1:B:430:ASN:HB2	1.95	0.67
1:A:488:TYR:O	1:A:492:ILE:HG13	1.95	0.67
1:B:151:VAL:O	1:B:155:SER:HB2	1.94	0.67
1:A:449:ASP:O	1:A:453:LEU:HB2	1.94	0.66
1:B:420:PHE:CZ	1:B:436:GLN:HG2	2.29	0.66
1:A:105:LYS:HD3	1:A:121:TYR:HE2	1.60	0.66
1:A:579:LEU:O	1:A:583:THR:HG23	1.95	0.66
1:A:285:ASN:HD21	1:A:300:LYS:NZ	1.94	0.66
1:A:558:ILE:HD13	1:A:559:ASP:H	1.61	0.66
1:B:503:VAL:HG12	1:B:507:PRO:HD3	1.77	0.66
1:A:151:VAL:O	1:A:155:SER:HB2	1.96	0.66
1:B:431:ILE:HD13	1:B:466:GLU:HB2	1.77	0.66
1:A:275:GLU:C	1:A:277:ASN:H	1.99	0.66
1:B:376:ARG:HE	1:B:377:ASN:N	1.93	0.66
1:A:386:PHE:HB2	2:A:631:HOH:O	1.94	0.66
1:B:182:PHE:CE2	1:B:213:LYS:HD3	2.31	0.66
1:A:441:ALA:HA	2:A:656:HOH:O	1.95	0.65
1:B:511:LYS:O	1:B:515:LEU:HB2	1.95	0.65
1:B:119:ILE:HG23	1:B:138:LEU:HD21	1.78	0.65
1:B:293:ARG:HB3	1:B:501:ILE:HG22	1.78	0.65
1:A:293:ARG:CD	1:A:501:ILE:HG22	2.25	0.65
1:A:522:GLU:HB2	2:A:635:HOH:O	1.95	0.65
1:A:399:VAL:HG23	1:A:400:TYR:N	2.12	0.65
1:A:219:LEU:HD12	1:B:579:LEU:HD23	1.79	0.65
1:A:318:LYS:HD3	1:A:318:LYS:O	1.96	0.65
1:B:263:ILE:HD12	1:B:263:ILE:N	2.11	0.65
1:B:596:SER:O	1:B:597:ASP:C	2.35	0.65
1:B:353:ILE:O	1:B:353:ILE:HD12	1.97	0.64
1:A:397:SER:HB2	1:A:426:LEU:CB	2.28	0.64
1:B:558:ILE:HD13	1:B:558:ILE:H	1.62	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:276:SER:O	1:B:281:LYS:HE2	1.97	0.64
1:B:505:ILE:CD1	1:B:538:ASP:HB2	2.27	0.64
1:A:119:ILE:HG22	1:A:123:ASN:HD21	1.61	0.64
1:B:329:LEU:CD2	1:B:333:LEU:HG	2.27	0.64
1:B:369:MET:O	1:B:372:ILE:HG13	1.97	0.64
1:B:532:GLU:HG3	2:B:646:HOH:O	1.98	0.64
1:B:114:LYS:HB3	1:B:117:ASP:HB2	1.79	0.64
1:B:558:ILE:CG1	1:B:559:ASP:H	2.09	0.64
1:B:316:LEU:HD12	1:B:329:LEU:HD12	1.80	0.64
1:B:142:TYR:CD1	1:B:150:LYS:HB3	2.33	0.64
1:B:556:GLU:HA	2:B:637:HOH:O	1.98	0.64
1:A:431:ILE:HD13	1:A:466:GLU:HB2	1.80	0.64
1:A:459:ARG:O	1:A:462:PRO:HD3	1.98	0.63
1:A:182:PHE:CE1	1:A:213:LYS:HB3	2.32	0.63
1:A:353:ILE:HD11	1:A:369:MET:HB2	1.80	0.63
1:B:372:ILE:HD12	1:B:373:MET:N	2.14	0.63
1:B:341:PHE:CD2	1:B:372:ILE:HG22	2.33	0.63
1:A:251:LEU:HD23	1:A:257:MET:HE3	1.80	0.63
1:A:520:THR:HB	1:A:523:ASN:CB	2.28	0.63
1:B:178:GLY:O	1:B:517:ARG:HD2	1.99	0.63
1:B:289:ASN:HB3	1:B:297:SER:O	1.99	0.63
1:B:327:GLU:O	1:B:331:ILE:HG23	1.98	0.63
1:A:520:THR:HB	1:A:523:ASN:HB3	1.81	0.63
1:B:192:LEU:HD11	1:B:198:PHE:CD1	2.34	0.63
1:A:576:GLU:HG2	1:A:577:GLU:OE2	1.99	0.62
1:B:473:GLU:O	1:B:476:THR:HG22	1.98	0.62
1:A:251:LEU:HD23	1:A:257:MET:CE	2.29	0.62
1:B:160:GLU:HA	2:B:613:HOH:O	1.98	0.62
1:A:397:SER:HB2	1:A:426:LEU:HB2	1.81	0.62
1:B:192:LEU:HD11	1:B:198:PHE:HD1	1.64	0.62
1:B:505:ILE:HG22	1:B:509:VAL:HG23	1.81	0.62
1:B:277:ASN:HD21	1:B:279:ALA:HB3	1.65	0.62
1:A:458:LYS:HA	1:A:467:VAL:HG11	1.80	0.62
1:B:411:GLN:HB2	2:B:632:HOH:O	2.00	0.62
1:A:103:LYS:HB2	1:A:134:PHE:HE1	1.65	0.62
1:A:505:ILE:HD12	1:A:505:ILE:N	2.15	0.61
1:B:406:MET:O	1:B:409:ILE:HG13	1.99	0.61
1:B:505:ILE:HD12	1:B:505:ILE:N	2.15	0.61
1:B:387:ASP:HA	1:B:390:LEU:HD12	1.83	0.61
1:A:147:ASP:O	1:A:151:VAL:HG23	2.00	0.61
1:B:204:GLU:HG2	1:B:208:GLU:OE2	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:204:GLU:N	1:A:205:PRO:HD2	2.16	0.61
1:B:105:LYS:HD3	1:B:121:TYR:CE2	2.36	0.61
1:A:287:LEU:O	1:A:287:LEU:HD23	1.99	0.61
1:A:502:TYR:CD1	1:A:502:TYR:N	2.67	0.61
1:B:555:GLN:CA	1:B:555:GLN:HE21	2.14	0.61
1:A:431:ILE:HG12	1:A:435:ILE:HD11	1.83	0.61
1:B:105:LYS:HA	1:B:108:GLN:NE2	2.14	0.60
1:A:525:ILE:HA	1:A:528:THR:HG22	1.83	0.60
1:B:489:ASP:HA	1:B:492:ILE:HD12	1.83	0.60
1:A:446:LYS:HA	1:A:446:LYS:HE2	1.82	0.60
1:B:182:PHE:HE2	1:B:213:LYS:HD3	1.67	0.60
1:B:119:ILE:HG22	1:B:123:ASN:HD22	1.67	0.60
1:B:449:ASP:O	1:B:453:LEU:HB2	2.00	0.60
1:B:558:ILE:N	1:B:558:ILE:HD13	2.17	0.60
1:B:454:PHE:O	1:B:458:LYS:HB2	2.01	0.60
1:B:268:LEU:HD12	1:B:268:LEU:N	2.16	0.60
1:B:212:ASN:HD22	1:B:212:ASN:C	2.04	0.60
1:A:468:PRO:HG2	1:A:494:LEU:HD12	1.84	0.59
1:A:422:LYS:O	1:A:426:LEU:HD13	2.02	0.59
1:B:386:PHE:O	1:B:390:LEU:HG	2.03	0.59
1:B:197:ASP:HA	2:B:615:HOH:O	2.01	0.59
1:B:221:GLU:HG3	1:B:222:LYS:HD2	1.84	0.59
1:A:353:ILE:HD12	1:A:353:ILE:O	2.03	0.59
1:A:426:LEU:O	1:A:427:ASP:HB2	2.01	0.59
1:A:334:GLU:O	1:A:338:ILE:HG12	2.01	0.59
1:A:594:ILE:CG2	1:A:604:ILE:HD11	2.33	0.59
1:B:260:PHE:HE1	1:B:338:ILE:CD1	2.16	0.59
1:B:336:THR:O	1:B:340:LYS:HG2	2.02	0.59
1:A:396:ASN:O	1:A:398:SER:N	2.36	0.59
1:A:500:GLY:HA3	1:A:502:TYR:HE1	1.68	0.58
1:A:334:GLU:HG3	1:A:365:SER:OG	2.02	0.58
1:A:431:ILE:CD1	1:A:466:GLU:HB2	2.32	0.58
1:B:324:LYS:O	1:B:328:LYS:HD3	2.03	0.58
1:A:454:PHE:CD2	1:A:471:PHE:HB2	2.38	0.58
1:B:374:ALA:HB1	1:B:406:MET:HE1	1.85	0.58
1:A:488:TYR:CE2	1:A:510:GLY:HA3	2.38	0.58
1:B:422:LYS:O	1:B:426:LEU:HD13	2.03	0.58
1:A:505:ILE:CD1	1:A:538:ASP:HB2	2.34	0.58
1:A:379:SER:O	1:A:381:GLU:N	2.36	0.58
1:A:440:LEU:HD23	2:A:656:HOH:O	2.04	0.58
1:B:367:ILE:HD11	1:B:399:VAL:CG1	2.34	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:558:ILE:H	1:B:558:ILE:CD1	2.16	0.58
1:A:439:CYS:HB2	1:A:454:PHE:CE1	2.38	0.58
1:A:293:ARG:HB3	1:A:501:ILE:HB	1.85	0.58
1:B:130:GLU:HB3	2:B:630:HOH:O	2.03	0.57
1:A:511:LYS:HD3	1:A:530:LEU:HD11	1.86	0.57
1:A:435:ILE:HG21	1:A:470:PHE:CD2	2.33	0.57
1:A:455:SER:CA	1:A:458:LYS:HB2	2.29	0.57
1:A:263:ILE:N	1:A:263:ILE:HD12	2.19	0.57
1:B:263:ILE:HG13	1:B:432:PHE:CD1	2.39	0.57
1:B:435:ILE:HG21	1:B:470:PHE:CD2	2.35	0.57
1:B:552:LYS:NZ	1:B:560:GLU:HB3	2.20	0.57
1:A:542:GLU:OE2	1:A:572:ALA:HB2	2.04	0.57
1:A:468:PRO:HB2	1:A:491:ALA:HB2	1.85	0.57
1:B:145:VAL:O	1:B:145:VAL:HG12	2.03	0.57
1:B:575:MET:HA	1:B:578:LYS:HG3	1.86	0.57
1:A:470:PHE:O	1:A:473:GLU:HG2	2.05	0.57
1:B:107:ASN:O	1:B:111:ARG:HG3	2.05	0.57
1:A:505:ILE:H	1:A:505:ILE:HD12	1.70	0.57
1:B:119:ILE:HG22	1:B:123:ASN:ND2	2.20	0.57
1:A:435:ILE:O	1:A:438:ALA:HB3	2.05	0.56
1:B:252:PRO:HG2	1:B:257:MET:HG3	1.88	0.56
1:A:491:ALA:O	1:A:495:GLU:HB2	2.05	0.56
1:A:334:GLU:OE2	1:A:364:ASN:HB2	2.06	0.56
1:B:331:ILE:CG2	1:B:362:ARG:HE	2.18	0.56
1:B:601:ALA:HA	1:B:604:ILE:HD12	1.88	0.56
1:B:422:LYS:HD3	1:B:422:LYS:O	2.05	0.56
1:B:273:TYR:CE2	1:B:274:ASP:HB2	2.39	0.56
1:A:367:ILE:HD11	1:A:399:VAL:HG12	1.87	0.56
1:A:211:LEU:HD22	1:B:208:GLU:OE1	2.06	0.56
1:A:344:ASN:CG	1:A:345:ASP:N	2.57	0.56
1:A:525:ILE:HA	1:A:528:THR:CG2	2.36	0.56
1:B:525:ILE:O	1:B:528:THR:HG22	2.06	0.56
1:A:354:LYS:O	1:A:358:GLU:HG3	2.06	0.56
1:A:295:PRO:C	1:A:297:SER:H	2.09	0.56
1:A:524:PHE:O	1:A:528:THR:HG22	2.05	0.56
1:A:310:ARG:O	1:A:314:GLU:HG3	2.05	0.56
1:B:148:LEU:HB3	1:B:179:LEU:CD1	2.29	0.56
1:A:540:ARG:HB3	1:A:540:ARG:HH11	1.70	0.56
1:B:600:LEU:O	1:B:604:ILE:HG13	2.06	0.56
1:B:295:PRO:C	1:B:297:SER:H	2.09	0.56
1:A:505:ILE:CG1	1:A:538:ASP:HB2	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:221:GLU:C	1:B:222:LYS:HD2	2.26	0.55
1:B:95:LYS:HD3	1:B:128:LEU:HD22	1.88	0.55
1:A:575:MET:HB3	1:B:576:GLU:HG2	1.86	0.55
1:B:260:PHE:CE1	1:B:338:ILE:HD11	2.42	0.55
1:A:563:THR:O	1:A:567:GLU:HG3	2.06	0.55
1:B:435:ILE:O	1:B:438:ALA:HB3	2.06	0.55
1:A:363:VAL:HG21	1:A:393:ASP:HB2	1.87	0.55
1:B:545:LYS:HG3	1:B:571:LEU:HD12	1.88	0.55
1:B:461:PHE:N	1:B:462:PRO:CD	2.70	0.55
1:A:393:ASP:CB	1:A:396:ASN:HB2	2.37	0.55
1:B:410:LEU:C	1:B:412:ASN:H	2.10	0.55
1:A:481:PHE:HE2	1:A:517:ARG:HG2	1.71	0.55
1:A:265:LYS:HG3	1:A:265:LYS:O	2.06	0.55
1:A:382:TYR:HA	1:A:385:TYR:CD1	2.42	0.55
1:B:418:LYS:HD3	1:B:418:LYS:O	2.06	0.55
1:A:286:GLY:HA2	1:A:301:ALA:HA	1.88	0.55
1:B:520:THR:HB	1:B:523:ASN:HB2	1.89	0.55
1:B:119:ILE:HD13	1:B:142:TYR:CE2	2.42	0.55
1:A:200:ASP:C	1:A:202:SER:H	2.11	0.55
1:B:439:CYS:C	1:B:441:ALA:H	2.11	0.54
1:B:342:LEU:C	1:B:344:ASN:N	2.58	0.54
1:B:431:ILE:CD1	1:B:466:GLU:HB2	2.37	0.54
1:B:203:ILE:HD12	1:B:204:GLU:N	2.21	0.54
1:A:279:ALA:HA	1:A:311:LEU:HD12	1.89	0.54
1:A:360:PHE:CD2	1:A:361:PRO:HD2	2.40	0.54
1:B:342:LEU:C	1:B:344:ASN:H	2.11	0.54
1:B:468:PRO:HA	1:B:487:GLN:OE1	2.08	0.54
1:A:288:SER:O	1:A:292:LYS:HD2	2.07	0.54
1:A:334:GLU:OE2	1:A:362:ARG:HD3	2.07	0.54
1:B:373:MET:O	1:B:376:ARG:HG3	2.07	0.54
1:A:277:ASN:O	1:A:281:LYS:HG3	2.07	0.54
1:A:469:ASN:O	1:A:472:ALA:HB3	2.07	0.54
1:A:109:PHE:HB3	1:A:117:ASP:HB2	1.90	0.54
1:B:338:ILE:HD13	1:B:338:ILE:O	2.08	0.54
1:A:410:LEU:C	1:A:412:ASN:H	2.10	0.54
1:A:309:ALA:O	1:A:313:GLU:HB2	2.07	0.54
1:B:268:LEU:HD12	1:B:268:LEU:H	1.73	0.54
1:A:546:ILE:HG23	1:A:568:SER:HB3	1.90	0.54
1:A:347:LEU:HG	1:B:376:ARG:HB3	1.90	0.53
1:A:393:ASP:HB3	1:A:396:ASN:HB2	1.89	0.53
1:B:563:THR:O	1:B:567:GLU:HG3	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:134:PHE:O	1:A:138:LEU:HG	2.07	0.53
1:A:204:GLU:O	1:A:208:GLU:HG3	2.07	0.53
1:A:578:LYS:O	1:A:582:ILE:HG13	2.08	0.53
1:B:514:LEU:HD23	1:B:515:LEU:N	2.24	0.53
1:A:496:ASN:HA	2:A:669:HOH:O	2.09	0.53
1:B:446:LYS:HD2	1:B:449:ASP:OD1	2.08	0.53
1:B:110:PHE:HD2	1:B:141:CYS:HG	1.55	0.53
1:A:382:TYR:C	1:A:384:ASN:H	2.12	0.53
1:A:94:GLU:O	1:A:97:LYS:HB3	2.08	0.53
1:B:334:GLU:OE1	1:B:364:ASN:HB3	2.09	0.53
1:A:431:ILE:O	1:A:435:ILE:HG13	2.09	0.53
1:A:100:LEU:HD13	1:A:100:LEU:C	2.29	0.53
1:A:530:LEU:HG	2:A:654:HOH:O	2.09	0.53
1:B:525:ILE:C	1:B:528:THR:HG22	2.30	0.52
1:A:200:ASP:O	1:A:202:SER:N	2.42	0.52
1:A:399:VAL:HG23	1:A:400:TYR:H	1.73	0.52
1:B:363:VAL:HG23	1:B:392:LEU:HB2	1.89	0.52
1:A:345:ASP:OD1	1:B:376:ARG:HB2	2.10	0.52
1:B:431:ILE:CD1	1:B:467:VAL:HG23	2.31	0.52
1:B:575:MET:HA	1:B:578:LYS:CG	2.40	0.52
1:B:439:CYS:C	1:B:441:ALA:N	2.63	0.52
1:A:499:ASP:HB3	2:A:618:HOH:O	2.10	0.52
1:B:291:TYR:O	1:B:292:LYS:HB3	2.09	0.52
1:B:361:PRO:O	1:B:362:ARG:CB	2.57	0.52
1:B:277:ASN:ND2	1:B:279:ALA:HB3	2.24	0.52
1:A:386:PHE:CE1	1:A:403:ARG:HA	2.45	0.52
1:A:381:GLU:O	1:A:384:ASN:HB3	2.09	0.52
1:B:270:PHE:CE2	1:B:328:LYS:HE2	2.45	0.52
1:B:219:LEU:O	1:B:219:LEU:HD13	2.09	0.51
1:A:537:LEU:HD12	1:A:537:LEU:N	2.25	0.51
1:A:319:ASN:HB3	1:A:322:ASP:HB2	1.93	0.51
1:A:147:ASP:OD1	1:A:150:LYS:HB2	2.09	0.51
1:A:96:ASP:HA	1:A:99:ALA:HB3	1.91	0.51
1:B:107:ASN:HA	1:B:122:TYR:OH	2.10	0.51
1:B:421:ASP:O	1:B:425:GLU:HG3	2.10	0.51
1:B:148:LEU:HD21	1:B:518:ASN:HD22	1.75	0.51
1:B:556:GLU:HG2	2:B:637:HOH:O	2.10	0.51
1:A:546:ILE:HG13	1:A:547:GLY:N	2.25	0.51
1:B:439:CYS:SG	1:B:442:TYR:CB	2.89	0.51
1:B:458:LYS:NZ	1:B:490:LEU:HD11	2.25	0.51
1:A:285:ASN:HD22	1:A:304:SER:HB3	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:469:ASN:ND2	1:B:507:PRO:HG3	2.25	0.51
1:B:579:LEU:HD13	1:B:579:LEU:O	2.10	0.51
1:B:552:LYS:HZ2	1:B:560:GLU:HB3	1.76	0.51
1:A:195:ASN:OD1	1:A:196:GLY:N	2.42	0.51
1:B:219:LEU:C	1:B:219:LEU:HD13	2.31	0.51
1:A:379:SER:C	1:A:381:GLU:N	2.64	0.51
1:A:326:LYS:HD2	1:A:359:LEU:HD23	1.92	0.51
1:B:431:ILE:HG23	1:B:432:PHE:N	2.26	0.51
1:B:554:GLN:C	1:B:556:GLU:H	2.13	0.51
1:B:546:ILE:HG23	1:B:568:SER:HB3	1.93	0.51
1:A:472:ALA:HB1	1:A:488:TYR:CD1	2.46	0.51
1:B:409:ILE:C	1:B:411:GLN:H	2.15	0.51
1:A:446:LYS:HD3	1:A:449:ASP:OD2	2.10	0.51
1:A:574:THR:HB	1:A:577:GLU:OE2	2.11	0.51
1:B:322:ASP:OD1	1:B:324:LYS:HB2	2.11	0.51
1:B:167:LYS:HE2	1:B:171:ARG:NH2	2.26	0.51
1:B:255:THR:N	2:B:660:HOH:O	2.33	0.50
1:A:514:LEU:HD12	1:A:515:LEU:N	2.26	0.50
1:B:501:ILE:O	1:B:501:ILE:HD13	2.11	0.50
1:B:270:PHE:HE2	1:B:328:LYS:HE2	1.76	0.50
1:B:408:PHE:CD1	1:B:440:LEU:HD13	2.45	0.50
1:B:597:ASP:O	1:B:599:VAL:N	2.44	0.50
1:A:575:MET:CB	1:B:576:GLU:HG2	2.41	0.50
1:A:605:GLN:HE21	1:A:605:GLN:CA	2.23	0.50
1:B:363:VAL:CG2	1:B:392:LEU:HB2	2.41	0.50
1:A:355:LYS:NZ	1:A:355:LYS:HB2	2.27	0.50
1:B:344:ASN:O	1:B:345:ASP:CB	2.49	0.50
1:A:295:PRO:O	1:A:297:SER:N	2.44	0.50
1:A:602:LYS:O	2:A:636:HOH:O	2.19	0.50
1:B:260:PHE:HE1	1:B:338:ILE:HD11	1.77	0.50
1:B:546:ILE:HG23	1:B:568:SER:CB	2.42	0.50
1:B:594:ILE:C	1:B:596:SER:H	2.15	0.50
1:A:493:GLU:O	1:A:496:ASN:ND2	2.45	0.50
1:B:263:ILE:HD13	2:B:616:HOH:O	2.12	0.50
1:A:302:ASP:O	1:A:306:THR:HG23	2.11	0.50
1:A:275:GLU:C	1:A:277:ASN:N	2.65	0.50
1:B:572:ALA:O	1:B:578:LYS:HE2	2.11	0.50
1:A:283:LEU:CD1	1:A:331:ILE:HD11	2.32	0.50
1:B:372:ILE:C	1:B:372:ILE:HD12	2.31	0.50
1:B:505:ILE:HD13	1:B:538:ASP:HB2	1.94	0.50
1:A:431:ILE:HD12	1:A:464:ALA:HB1	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:506:ALA:HB3	1:A:507:PRO:CD	2.36	0.50
1:B:501:ILE:HG23	1:B:502:TYR:N	2.26	0.50
1:A:415:GLN:HA	1:A:415:GLN:HE21	1.75	0.50
1:B:108:GLN:HG2	1:B:111:ARG:NH2	2.27	0.49
1:A:515:LEU:HB3	1:A:523:ASN:OD1	2.12	0.49
1:B:126:LEU:HD21	1:B:134:PHE:HB2	1.94	0.49
1:B:221:GLU:HG3	1:B:222:LYS:CD	2.42	0.49
1:B:167:LYS:HE2	1:B:171:ARG:HH22	1.77	0.49
1:A:532:GLU:HA	1:A:548:LEU:HD11	1.93	0.49
1:A:270:PHE:HE1	1:A:284:MET:HG2	1.77	0.49
1:B:532:GLU:O	1:B:536:LYS:HG2	2.12	0.49
1:B:131:ASP:HB3	1:B:134:PHE:CD2	2.46	0.49
1:B:266:PRO:HA	1:B:291:TYR:CE1	2.47	0.49
1:A:274:ASP:CA	1:A:280:ASP:HB3	2.38	0.49
1:A:504:GLY:O	1:A:507:PRO:HD2	2.12	0.49
1:A:345:ASP:CG	1:A:347:LEU:HB2	2.32	0.49
1:A:440:LEU:HA	2:A:670:HOH:O	2.12	0.49
1:B:163:PRO:HG3	2:B:613:HOH:O	2.13	0.49
1:A:267:GLU:C	1:A:287:LEU:HD21	2.33	0.49
1:B:444:GLU:O	1:B:446:LYS:N	2.35	0.49
1:A:566:GLU:O	1:A:569:ALA:HB3	2.13	0.49
1:B:424:LYS:HD2	1:B:434:TYR:CZ	2.48	0.49
1:A:396:ASN:HD22	1:A:399:VAL:HG13	1.77	0.49
1:A:415:GLN:NE2	1:A:415:GLN:HA	2.28	0.49
1:A:505:ILE:H	1:A:505:ILE:CD1	2.24	0.49
1:A:369:MET:O	1:A:372:ILE:HG12	2.13	0.48
1:A:347:LEU:HG	1:B:376:ARG:CB	2.43	0.48
1:A:446:LYS:HA	1:A:446:LYS:CE	2.43	0.48
1:A:585:ALA:O	1:A:589:LYS:HG3	2.12	0.48
1:A:189:LEU:HD22	1:A:203:ILE:HG13	1.94	0.48
1:A:594:ILE:HD13	1:B:187:PHE:CE2	2.47	0.48
1:A:269:THR:CG2	1:A:270:PHE:H	2.17	0.48
1:A:397:SER:HB2	1:A:426:LEU:HB3	1.95	0.48
1:A:385:TYR:HD2	1:A:388:LYS:HD2	1.77	0.48
1:B:548:LEU:HB3	1:B:564:LEU:HD13	1.95	0.48
1:B:516:THR:C	1:B:518:ASN:H	2.17	0.48
1:A:338:ILE:HD13	1:A:338:ILE:N	2.27	0.48
1:B:499:ASP:OD2	1:B:500:GLY:N	2.47	0.48
1:B:469:ASN:HD21	1:B:507:PRO:HA	1.78	0.48
1:B:598:PRO:C	1:B:600:LEU:N	2.65	0.48
1:A:454:PHE:O	1:A:458:LYS:N	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:251:LEU:CD2	1:B:252:PRO:HD2	2.44	0.48
1:B:598:PRO:C	1:B:600:LEU:H	2.14	0.48
1:B:505:ILE:CD1	1:B:505:ILE:N	2.77	0.48
1:A:114:LYS:HB3	1:A:114:LYS:NZ	2.28	0.48
1:B:251:LEU:HD21	1:B:339:PHE:CD2	2.48	0.48
1:B:411:GLN:O	1:B:413:TYR:N	2.39	0.48
1:A:442:TYR:C	1:A:444:GLU:H	2.17	0.48
1:B:501:ILE:CG2	1:B:502:TYR:N	2.77	0.48
1:A:251:LEU:HB3	1:A:257:MET:HE1	1.96	0.48
1:B:214:GLN:HE21	1:B:218:LYS:HG2	1.78	0.48
1:B:293:ARG:NH2	1:B:502:TYR:HA	2.24	0.48
1:B:430:ASN:O	1:B:433:PRO:HD2	2.14	0.48
1:A:289:ASN:ND2	1:A:300:LYS:HD2	2.29	0.47
1:A:417:GLY:HA2	1:A:420:PHE:CD1	2.49	0.47
1:B:204:GLU:N	1:B:205:PRO:HD2	2.29	0.47
1:B:114:LYS:HB3	1:B:117:ASP:CB	2.44	0.47
1:B:212:ASN:ND2	1:B:212:ASN:C	2.67	0.47
1:B:332:SER:O	1:B:336:THR:HG23	2.14	0.47
1:B:485:LEU:HD23	1:B:485:LEU:O	2.13	0.47
1:B:399:VAL:HG23	1:B:400:TYR:HD1	1.79	0.47
1:B:203:ILE:C	1:B:203:ILE:HD12	2.34	0.47
1:A:263:ILE:HG21	1:A:401:TYR:CD1	2.49	0.47
1:A:174:SER:HA	2:A:644:HOH:O	2.14	0.47
1:B:490:LEU:O	1:B:493:GLU:HB3	2.14	0.47
1:A:431:ILE:HD12	1:A:464:ALA:CB	2.44	0.47
1:A:475:LEU:HB2	1:A:484:ALA:HB2	1.96	0.47
1:A:382:TYR:C	1:A:384:ASN:N	2.66	0.47
1:B:475:LEU:HB2	1:B:484:ALA:HB2	1.96	0.47
1:B:465:PRO:C	1:B:468:PRO:HD2	2.34	0.47
1:A:417:GLY:HA2	1:A:420:PHE:HD1	1.80	0.47
1:A:505:ILE:CG2	1:A:534:ALA:HB1	2.43	0.47
1:A:384:ASN:O	1:A:387:ASP:HB3	2.13	0.47
1:B:409:ILE:CD1	1:B:410:LEU:HG	2.44	0.47
1:A:124:TRP:HA	1:A:127:GLU:HG2	1.96	0.47
1:A:549:ALA:HB2	1:A:564:LEU:CB	2.45	0.47
1:A:506:ALA:CB	1:A:507:PRO:HD3	2.36	0.47
1:A:263:ILE:HG22	1:A:263:ILE:O	2.15	0.47
1:A:512:ALA:O	1:A:516:THR:HG23	2.14	0.47
1:B:511:LYS:HA	1:B:514:LEU:HD22	1.96	0.47
1:B:190:SER:O	1:B:193:SER:HB3	2.15	0.47
1:A:289:ASN:HB3	1:A:297:SER:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:468:PRO:O	1:A:472:ALA:HB2	2.14	0.47
1:B:525:ILE:HA	1:B:528:THR:CG2	2.45	0.47
1:A:496:ASN:ND2	1:A:496:ASN:N	2.62	0.47
1:A:477:ASP:C	1:A:479:ASN:H	2.17	0.47
1:A:294:SER:OG	1:A:297:SER:HB2	2.15	0.47
1:A:393:ASP:HB3	2:A:622:HOH:O	2.15	0.47
1:A:387:ASP:O	1:A:391:LYS:HG3	2.15	0.47
1:A:195:ASN:CG	1:A:196:GLY:H	2.17	0.47
1:A:549:ALA:HA	1:A:564:LEU:HD12	1.96	0.47
1:A:416:ALA:C	1:A:418:LYS:H	2.18	0.47
1:B:468:PRO:CB	1:B:491:ALA:HB2	2.39	0.47
1:A:266:PRO:HA	1:A:291:TYR:CE1	2.50	0.47
1:A:292:LYS:HG3	1:A:292:LYS:O	2.15	0.47
1:B:209:ARG:HD2	1:B:213:LYS:HZ3	1.80	0.47
1:A:549:ALA:HB2	1:A:564:LEU:HB3	1.96	0.47
1:A:207:LEU:HD13	1:B:204:GLU:OE1	2.15	0.47
1:B:555:GLN:O	1:B:556:GLU:HB2	2.15	0.47
1:A:201:ALA:HA	1:A:204:GLU:CG	2.45	0.46
1:A:285:ASN:HD21	1:A:300:LYS:HZ3	1.61	0.46
1:B:525:ILE:HA	1:B:528:THR:HG22	1.97	0.46
1:A:187:PHE:O	1:A:191:VAL:HG23	2.15	0.46
1:A:292:LYS:O	1:A:293:ARG:C	2.53	0.46
1:A:289:ASN:HA	1:A:292:LYS:HD3	1.98	0.46
1:B:369:MET:SD	1:B:372:ILE:HD11	2.56	0.46
1:B:511:LYS:CE	1:B:530:LEU:HD11	2.46	0.46
1:A:266:PRO:HB3	1:A:291:TYR:CG	2.50	0.46
1:A:367:ILE:HD11	1:A:399:VAL:CG1	2.46	0.46
1:A:496:ASN:HD22	1:A:496:ASN:N	2.12	0.46
1:A:399:VAL:HG23	1:A:400:TYR:CD1	2.51	0.46
1:B:103:LYS:HB2	1:B:134:PHE:HE1	1.80	0.46
1:A:410:LEU:C	1:A:412:ASN:N	2.69	0.46
1:A:183:ALA:HB3	2:A:632:HOH:O	2.14	0.46
1:B:525:ILE:O	1:B:529:ASN:ND2	2.49	0.46
1:A:458:LYS:HG2	1:A:467:VAL:CG1	2.45	0.46
1:A:327:GLU:O	1:A:331:ILE:HG23	2.15	0.46
1:A:360:PHE:HD2	1:A:361:PRO:CD	2.26	0.46
1:A:540:ARG:CB	1:A:540:ARG:HH11	2.28	0.46
1:B:186:MET:SD	1:B:211:LEU:HA	2.55	0.46
1:A:214:GLN:HE21	1:A:218:LYS:HG2	1.80	0.46
1:B:529:ASN:HA	2:B:646:HOH:O	2.15	0.46
1:A:469:ASN:CB	1:A:503:VAL:HG11	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:338:ILE:HD12	1:A:368:TYR:CG	2.51	0.46
1:A:273:TYR:O	1:A:274:ASP:O	2.33	0.46
1:A:439:CYS:HB2	1:A:454:PHE:HE1	1.80	0.45
1:A:503:VAL:O	1:A:503:VAL:HG12	2.16	0.45
1:A:430:ASN:O	1:A:433:PRO:HD2	2.16	0.45
1:B:186:MET:CE	1:B:211:LEU:HA	2.46	0.45
1:A:373:MET:C	1:A:375:ASP:N	2.68	0.45
1:B:175:ALA:O	1:B:179:LEU:HD12	2.16	0.45
1:B:447:PHE:O	1:B:450:CYS:N	2.48	0.45
1:A:432:PHE:HA	1:A:435:ILE:HG13	1.98	0.45
1:A:520:THR:HB	1:A:523:ASN:HB2	1.99	0.45
1:A:558:ILE:O	1:A:562:ILE:HG13	2.16	0.45
1:B:212:ASN:HD21	1:B:580:GLN:HG3	1.81	0.45
1:B:98:TYR:HB3	1:B:128:LEU:CD1	2.47	0.45
1:B:402:HIS:O	1:B:405:GLN:HB2	2.15	0.45
1:A:485:LEU:O	1:A:485:LEU:HD23	2.16	0.45
1:B:157:LYS:HE3	2:B:626:HOH:O	2.16	0.45
1:B:597:ASP:OD1	1:B:597:ASP:O	2.34	0.45
1:A:605:GLN:HE21	1:A:605:GLN:HA	1.81	0.45
1:B:491:ALA:O	1:B:495:GLU:HB2	2.17	0.45
1:A:399:VAL:CG2	1:A:400:TYR:N	2.79	0.45
1:A:108:GLN:C	1:A:110:PHE:N	2.70	0.45
1:A:289:ASN:HA	1:A:292:LYS:CD	2.47	0.45
1:A:495:GLU:OE2	1:A:502:TYR:O	2.35	0.45
1:A:520:THR:HG22	1:A:522:GLU:H	1.81	0.45
1:B:594:ILE:HG22	1:B:604:ILE:HD11	1.99	0.45
1:A:558:ILE:HG12	1:A:559:ASP:N	2.30	0.45
1:B:131:ASP:OD1	1:B:133:VAL:N	2.50	0.45
1:A:469:ASN:HB2	1:A:503:VAL:HG11	1.99	0.45
1:A:461:PHE:C	2:A:671:HOH:O	2.55	0.45
1:B:393:ASP:O	1:B:396:ASN:N	2.50	0.45
1:A:596:SER:O	1:A:597:ASP:O	2.35	0.45
1:A:273:TYR:CD2	1:A:274:ASP:N	2.85	0.45
1:B:119:ILE:HG23	1:B:138:LEU:CD2	2.45	0.45
1:B:575:MET:HA	1:B:578:LYS:HB2	1.99	0.45
1:B:263:ILE:O	1:B:263:ILE:HG22	2.17	0.44
1:A:454:PHE:CE2	1:A:471:PHE:HB2	2.51	0.44
1:A:277:ASN:HD21	1:A:279:ALA:HB3	1.82	0.44
1:A:406:MET:O	1:A:410:LEU:HG	2.17	0.44
1:B:432:PHE:CD2	1:B:435:ILE:HD12	2.52	0.44
1:B:528:THR:N	2:B:657:HOH:O	2.49	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:96:ASP:OD2	1:B:129:LYS:HD2	2.17	0.44
1:B:438:ALA:O	1:B:450:CYS:HA	2.18	0.44
1:A:119:ILE:HG12	1:A:141:CYS:SG	2.57	0.44
1:B:533:LYS:O	1:B:536:LYS:HB2	2.18	0.44
1:A:481:PHE:HD1	1:A:481:PHE:H	1.64	0.44
1:A:465:PRO:C	1:A:468:PRO:HD2	2.37	0.44
1:B:440:LEU:O	1:B:440:LEU:HD12	2.16	0.44
1:B:443:ARG:NH2	2:B:635:HOH:O	2.49	0.44
1:A:361:PRO:CB	1:A:392:LEU:HD11	2.47	0.44
1:B:382:TYR:HA	1:B:385:TYR:CD1	2.53	0.44
1:A:500:GLY:HA3	1:A:502:TYR:CE1	2.50	0.44
1:A:520:THR:O	1:A:521:VAL:C	2.56	0.44
1:B:399:VAL:HG23	1:B:400:TYR:CD1	2.53	0.44
1:B:331:ILE:CG2	1:B:362:ARG:NE	2.80	0.44
1:A:590:VAL:O	1:A:594:ILE:HG12	2.18	0.44
1:A:263:ILE:HD12	1:A:263:ILE:H	1.83	0.44
1:A:407:ASN:O	1:A:412:ASN:HB3	2.18	0.44
1:A:582:ILE:HD12	1:B:219:LEU:HB2	1.99	0.44
1:B:378:ASP:HB2	2:B:667:HOH:O	2.17	0.44
1:B:379:SER:C	1:B:381:GLU:H	2.20	0.44
1:A:475:LEU:CB	1:A:484:ALA:HB2	2.48	0.44
1:A:283:LEU:HD11	1:A:331:ILE:CD1	2.35	0.44
1:B:353:ILE:HD11	1:B:369:MET:HB2	1.99	0.44
1:A:521:VAL:HG23	1:A:522:GLU:N	2.33	0.44
1:B:293:ARG:O	1:B:294:SER:O	2.35	0.44
1:A:119:ILE:CG2	1:A:123:ASN:HD21	2.30	0.44
1:A:99:ALA:HA	1:A:128:LEU:HD12	2.00	0.44
1:B:177:GLU:HB2	1:B:210:ASN:OD1	2.17	0.44
1:A:269:THR:HG23	1:A:270:PHE:N	2.19	0.44
1:B:104:ASP:O	1:B:108:GLN:HG3	2.18	0.44
1:B:399:VAL:HG23	1:B:400:TYR:N	2.27	0.44
1:A:404:GLY:O	1:A:408:PHE:HB2	2.18	0.44
1:A:469:ASN:HD22	1:A:507:PRO:CG	2.19	0.44
1:A:439:CYS:SG	1:A:474:ILE:HD13	2.58	0.43
1:A:583:THR:HG22	1:B:215:ALA:CB	2.47	0.43
1:A:267:GLU:O	1:A:268:LEU:HG	2.17	0.43
1:B:201:ALA:HA	2:B:621:HOH:O	2.18	0.43
1:A:524:PHE:HA	1:A:524:PHE:HD2	1.73	0.43
1:B:410:LEU:C	1:B:412:ASN:N	2.71	0.43
1:A:114:LYS:HB3	1:A:117:ASP:OD1	2.17	0.43
1:A:312:PHE:CE1	1:A:328:LYS:HB3	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:279:ALA:HB3	1:A:315:GLN:HE22	1.84	0.43
1:A:496:ASN:HD22	1:A:497:LYS:N	2.16	0.43
1:A:170:LEU:O	1:A:170:LEU:HD23	2.19	0.43
1:B:504:GLY:O	1:B:507:PRO:HD2	2.18	0.43
1:A:186:MET:SD	1:A:211:LEU:HA	2.58	0.43
1:B:548:LEU:CB	1:B:564:LEU:HD13	2.47	0.43
1:A:406:MET:O	1:A:409:ILE:HG12	2.18	0.43
1:B:496:ASN:C	1:B:498:LEU:H	2.20	0.43
1:A:279:ALA:HB2	1:A:311:LEU:HB3	2.00	0.43
1:B:505:ILE:CG2	1:B:509:VAL:HG23	2.48	0.43
1:B:445:ASN:ND2	2:B:668:HOH:O	2.52	0.43
1:A:111:ARG:HH11	1:A:111:ARG:HG3	1.83	0.43
1:A:113:LYS:HD2	1:A:113:LYS:N	2.34	0.43
1:B:558:ILE:N	1:B:558:ILE:CD1	2.80	0.43
1:A:605:GLN:NE2	1:A:605:GLN:HA	2.33	0.43
1:A:461:PHE:N	2:A:671:HOH:O	2.47	0.43
1:B:537:LEU:O	1:B:539:PRO:HD3	2.17	0.43
1:B:591:GLN:OE1	1:B:591:GLN:HA	2.17	0.43
1:A:501:ILE:O	1:A:502:TYR:C	2.56	0.43
1:B:515:LEU:HB3	1:B:527:ALA:HB2	2.01	0.43
1:A:600:LEU:HD11	1:B:194:LEU:HD12	2.00	0.43
1:A:525:ILE:CA	1:A:528:THR:HG22	2.47	0.43
1:A:558:ILE:CG1	1:A:559:ASP:N	2.82	0.43
1:B:475:LEU:CB	1:B:484:ALA:HB2	2.49	0.43
1:B:453:LEU:HD12	1:B:453:LEU:HA	1.92	0.43
1:A:404:GLY:HA3	1:A:420:PHE:CE2	2.54	0.43
1:B:520:THR:HG22	1:B:521:VAL:N	2.34	0.43
1:A:105:LYS:HD3	1:A:121:TYR:CE2	2.46	0.43
1:B:572:ALA:HB1	1:B:577:GLU:HB2	2.01	0.43
1:A:108:GLN:C	1:A:110:PHE:H	2.21	0.43
1:A:600:LEU:HD13	1:A:600:LEU:O	2.19	0.43
1:B:342:LEU:HA	1:B:342:LEU:HD23	1.88	0.43
1:B:505:ILE:HG22	1:B:505:ILE:O	2.18	0.43
1:A:285:ASN:HD21	1:A:300:LYS:HZ2	1.66	0.42
1:A:503:VAL:HG12	1:A:507:PRO:CD	2.47	0.42
1:A:390:LEU:HD21	1:A:399:VAL:CG2	2.42	0.42
1:B:437:LEU:CD2	1:B:440:LEU:HD23	2.42	0.42
1:B:295:PRO:O	1:B:297:SER:N	2.49	0.42
1:A:411:GLN:HA	1:A:413:TYR:CE2	2.54	0.42
1:B:179:LEU:HD12	1:B:179:LEU:N	2.34	0.42
1:B:345:ASP:OD1	1:B:347:LEU:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:516:THR:C	1:B:518:ASN:N	2.72	0.42
1:B:552:LYS:HG3	1:B:564:LEU:CD1	2.50	0.42
1:B:100:LEU:HD13	1:B:100:LEU:C	2.38	0.42
1:B:442:TYR:C	1:B:444:GLU:N	2.73	0.42
1:A:484:ALA:O	1:A:488:TYR:HD1	2.01	0.42
1:B:404:GLY:O	1:B:408:PHE:HB2	2.19	0.42
1:B:537:LEU:C	1:B:539:PRO:HD3	2.40	0.42
1:A:329:LEU:HD22	1:A:329:LEU:O	2.19	0.42
1:B:520:THR:H	1:B:523:ASN:HB2	1.84	0.42
1:A:410:LEU:O	1:A:412:ASN:N	2.52	0.42
1:B:362:ARG:HG2	1:B:362:ARG:HH11	1.84	0.42
1:B:552:LYS:HG3	1:B:564:LEU:HD12	2.02	0.42
1:A:263:ILE:HG12	1:A:401:TYR:CE1	2.54	0.42
1:B:565:PHE:HB3	1:B:585:ALA:HB2	2.00	0.42
1:B:139:SER:O	1:B:143:VAL:HG23	2.20	0.42
1:B:442:TYR:C	1:B:444:GLU:H	2.21	0.42
1:A:488:TYR:HE2	1:A:510:GLY:HA3	1.85	0.42
1:B:515:LEU:HD12	1:B:523:ASN:O	2.20	0.42
1:B:260:PHE:HE1	1:B:338:ILE:HD12	1.85	0.42
1:B:431:ILE:HG12	1:B:435:ILE:CD1	2.46	0.42
1:B:376:ARG:NH2	1:B:377:ASN:HB3	2.20	0.42
1:A:446:LYS:CA	1:A:446:LYS:HE2	2.49	0.42
1:B:554:GLN:C	1:B:556:GLU:N	2.73	0.42
1:B:555:GLN:HA	1:B:555:GLN:HE21	1.84	0.42
1:A:511:LYS:HD3	1:A:530:LEU:CD1	2.50	0.42
1:B:432:PHE:HD2	1:B:435:ILE:HD12	1.85	0.42
1:A:294:SER:HA	1:A:295:PRO:HD3	1.91	0.42
1:B:478:LYS:CE	1:B:478:LYS:HA	2.39	0.42
1:B:417:GLY:HA2	1:B:437:LEU:HD21	2.00	0.42
1:A:385:TYR:CD2	1:A:388:LYS:HD2	2.55	0.42
1:B:374:ALA:CB	1:B:406:MET:HE1	2.50	0.42
1:A:201:ALA:HA	1:A:204:GLU:HG2	2.02	0.42
1:A:199:ASN:O	1:A:200:ASP:HB2	2.20	0.42
1:B:550:GLN:NE2	2:B:645:HOH:O	2.52	0.42
1:A:364:ASN:HB3	1:A:368:TYR:CE2	2.54	0.41
1:A:396:ASN:ND2	1:A:398:SER:OG	2.53	0.41
1:B:360:PHE:O	1:B:361:PRO:C	2.58	0.41
1:A:326:LYS:O	1:A:330:ALA:N	2.52	0.41
1:A:574:THR:CB	1:A:577:GLU:OE2	2.68	0.41
1:A:122:TYR:O	1:A:126:LEU:HG	2.20	0.41
1:B:435:ILE:HG13	1:B:435:ILE:H	1.67	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:285:ASN:ND2	1:A:300:LYS:NZ	2.65	0.41
1:A:505:ILE:N	1:A:505:ILE:CD1	2.80	0.41
1:A:251:LEU:H	1:A:251:LEU:CD1	2.34	0.41
1:A:603:LYS:C	2:A:636:HOH:O	2.58	0.41
1:B:341:PHE:CE2	1:B:372:ILE:HA	2.54	0.41
1:A:386:PHE:O	1:A:390:LEU:HG	2.19	0.41
1:A:98:TYR:CD1	1:A:101:ALA:HB3	2.55	0.41
1:B:410:LEU:O	1:B:412:ASN:N	2.54	0.41
1:A:270:PHE:CD2	1:A:270:PHE:O	2.74	0.41
1:B:134:PHE:O	1:B:138:LEU:HB2	2.20	0.41
1:B:519:PRO:HB3	1:B:524:PHE:CZ	2.54	0.41
1:A:444:GLU:CD	2:A:656:HOH:O	2.58	0.41
1:A:603:LYS:HA	2:A:636:HOH:O	2.21	0.41
1:B:353:ILE:HD12	1:B:353:ILE:C	2.41	0.41
1:B:478:LYS:O	1:B:479:ASN:HB2	2.21	0.41
1:B:204:GLU:HB3	1:B:205:PRO:CD	2.51	0.41
1:B:370:ALA:HB1	1:B:386:PHE:CE1	2.55	0.41
1:A:531:LEU:HD13	1:A:547:GLY:HA3	2.02	0.41
1:B:465:PRO:O	1:B:468:PRO:HD2	2.19	0.41
1:B:525:ILE:CA	1:B:528:THR:HG22	2.51	0.41
1:B:131:ASP:HA	1:B:132:PRO:HD3	1.91	0.41
1:A:478:LYS:CE	1:A:478:LYS:HA	2.29	0.41
1:A:440:LEU:HD23	1:A:441:ALA:N	2.36	0.41
1:B:520:THR:HB	1:B:523:ASN:H	1.85	0.41
1:A:279:ALA:HB2	1:A:311:LEU:CB	2.50	0.41
1:A:277:ASN:HD21	1:A:315:GLN:HE22	1.68	0.41
1:A:421:ASP:O	1:A:425:GLU:HG2	2.20	0.41
1:B:493:GLU:HG3	2:B:652:HOH:O	2.19	0.41
1:A:442:TYR:C	1:A:444:GLU:N	2.74	0.41
1:A:431:ILE:HD11	1:A:467:VAL:HG23	2.02	0.41
1:A:492:ILE:HG12	1:A:507:PRO:HB2	2.03	0.41
1:B:333:LEU:HD11	1:B:355:LYS:HD2	2.03	0.41
1:B:503:VAL:HG12	1:B:507:PRO:CD	2.48	0.41
1:B:600:LEU:HD23	1:B:600:LEU:HA	1.88	0.41
1:A:565:PHE:CE1	1:A:584:PHE:HB3	2.55	0.41
1:B:253:SER:O	1:B:256:SER:OG	2.35	0.41
1:A:437:LEU:O	1:A:438:ALA:C	2.59	0.41
1:A:341:PHE:CD1	1:A:341:PHE:C	2.94	0.41
1:B:375:ASP:O	1:B:376:ARG:O	2.39	0.41
1:A:312:PHE:HB2	1:A:329:LEU:HD23	2.01	0.41
1:A:393:ASP:HB2	1:A:396:ASN:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:547:GLY:O	1:B:551:MET:HG2	2.21	0.41
1:B:500:GLY:HA3	1:B:502:TYR:HE1	1.86	0.41
1:B:502:TYR:O	1:B:504:GLY:N	2.53	0.41
1:A:420:PHE:CE1	1:A:436:GLN:HG2	2.55	0.41
1:B:109:PHE:CD1	1:B:117:ASP:HB3	2.56	0.41
1:A:529:ASN:HB3	2:A:654:HOH:O	2.21	0.41
1:B:424:LYS:HD2	1:B:434:TYR:CE2	2.55	0.41
1:A:434:TYR:O	1:A:438:ALA:HB2	2.20	0.41
1:A:503:VAL:O	1:A:504:GLY:O	2.39	0.41
1:B:341:PHE:CG	1:B:372:ILE:HG22	2.56	0.40
1:A:280:ASP:OD1	1:A:328:LYS:HD3	2.21	0.40
1:B:505:ILE:CG2	1:B:534:ALA:HB1	2.51	0.40
1:B:295:PRO:C	1:B:297:SER:N	2.75	0.40
1:B:486:LYS:HE3	2:B:614:HOH:O	2.19	0.40
1:B:549:ALA:O	1:B:553:LEU:HB2	2.20	0.40
1:B:263:ILE:H	1:B:263:ILE:HD12	1.84	0.40
1:A:464:ALA:HA	1:A:465:PRO:HD3	1.93	0.40
1:A:465:PRO:O	1:A:468:PRO:HD2	2.22	0.40
1:A:345:ASP:HA	1:A:346:PRO:HD3	1.85	0.40
1:A:204:GLU:N	1:A:205:PRO:CD	2.84	0.40
1:A:454:PHE:O	1:A:458:LYS:HB2	2.21	0.40
1:A:519:PRO:HB3	1:A:524:PHE:CZ	2.57	0.40
1:A:126:LEU:HD21	1:A:134:PHE:HB2	2.03	0.40
1:B:480:ASP:O	1:B:482:ASP:N	2.53	0.40
1:A:327:GLU:HG3	1:A:360:PHE:CD1	2.57	0.40
1:A:453:LEU:HD12	1:A:453:LEU:HA	1.94	0.40
1:B:381:GLU:OE1	1:B:384:ASN:HB3	2.20	0.40
1:B:162:LYS:HD3	1:B:165:TYR:CD2	2.56	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	483/514 (94%)	377 (78%)	81 (17%)	25 (5%)	2	15
1	B	483/514 (94%)	385 (80%)	63 (13%)	35 (7%)	1	7
All	All	966/1028 (94%)	762 (79%)	144 (15%)	60 (6%)	2	10

All (60) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	195	ASN
1	A	201	ALA
1	A	274	ASP
1	A	361	PRO
1	A	397	SER
1	A	504	GLY
1	A	597	ASP
1	B	95	LYS
1	B	274	ASP
1	B	294	SER
1	B	345	ASP
1	B	361	PRO
1	B	376	ARG
1	B	598	PRO
1	A	380	THR
1	A	495	GLU
1	A	502	TYR
1	B	195	ASN
1	B	200	ASP
1	B	252	PRO
1	B	276	SER
1	B	412	ASN
1	B	445	ASN
1	B	446	LYS
1	B	503	VAL
1	B	595	ARG
1	A	199	ASN
1	A	270	PHE
1	A	293	ARG
1	A	294	SER
1	A	438	ALA
1	A	501	ILE
1	B	277	ASN
1	B	344	ASN
1	B	481	PHE

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Mol	Chain	Res	Type
1	B	500	GLY
1	B	502	TYR
1	B	541	SER
1	A	343	LYS
1	A	345	ASP
1	A	411	GLN
1	A	427	ASP
1	A	462	PRO
1	B	113	LYS
1	B	378	ASP
1	B	413	TYR
1	B	414	ASP
1	A	268	LEU
1	A	291	TYR
1	A	296	GLU
1	B	362	ARG
1	B	394	SER
1	B	555	GLN
1	B	597	ASP
1	B	266	PRO
1	B	411	GLN
1	B	504	GLY
1	B	462	PRO
1	B	558	ILE
1	A	521	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	425/448 (95%)	380 (89%)	45 (11%)	8	31
1	B	425/448 (95%)	391 (92%)	34 (8%)	15	47
All	All	850/896 (95%)	771 (91%)	79 (9%)	11	39

All (79) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	98	TYR
1	A	100	LEU
1	A	113	LYS
1	A	116	ASP
1	A	155	SER
1	A	165	TYR
1	A	198	PHE
1	A	219	LEU
1	A	270	PHE
1	A	274	ASP
1	A	283	LEU
1	A	290	LEU
1	A	334	GLU
1	A	347	LEU
1	A	352	ASP
1	A	353	ILE
1	A	357	ILE
1	A	360	PHE
1	A	361	PRO
1	A	376	ARG
1	A	393	ASP
1	A	430	ASN
1	A	440	LEU
1	A	446	LYS
1	A	454	PHE
1	A	476	THR
1	A	478	LYS
1	A	490	LEU
1	A	495	GLU
1	A	496	ASN
1	A	499	ASP
1	A	501	ILE
1	A	502	TYR
1	A	524	PHE
1	A	532	GLU
1	A	536	LYS
1	A	540	ARG
1	A	543	GLN
1	A	555	GLN
1	A	558	ILE
1	A	566	GLU
1	A	573	ARG
1	A	574	THR

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Mol	Chain	Res	Type
1	A	600	LEU
1	A	605	GLN
1	B	98	TYR
1	B	104	ASP
1	B	116	ASP
1	B	165	TYR
1	B	212	ASN
1	B	290	LEU
1	B	316	LEU
1	B	329	LEU
1	B	331	ILE
1	B	338	ILE
1	B	345	ASP
1	B	347	LEU
1	B	352	ASP
1	B	353	ILE
1	B	361	PRO
1	B	393	ASP
1	B	396	ASN
1	B	430	ASN
1	B	439	CYS
1	B	453	LEU
1	B	454	PHE
1	B	478	LYS
1	B	488	TYR
1	B	490	LEU
1	B	495	GLU
1	B	501	ILE
1	B	514	LEU
1	B	515	LEU
1	B	538	ASP
1	B	550	GLN
1	B	553	LEU
1	B	555	GLN
1	B	558	ILE
1	B	566	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	107	ASN
1	A	123	ASN

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Mol	Chain	Res	Type
1	A	137	ASN
1	A	212	ASN
1	A	277	ASN
1	A	285	ASN
1	A	289	ASN
1	A	315	GLN
1	A	384	ASN
1	A	396	ASN
1	A	415	GLN
1	A	430	ASN
1	A	469	ASN
1	A	479	ASN
1	A	496	ASN
1	A	543	GLN
1	A	580	GLN
1	A	605	GLN
1	B	108	GLN
1	B	123	ASN
1	B	137	ASN
1	B	212	ASN
1	B	214	GLN
1	B	277	ASN
1	B	315	GLN
1	B	377	ASN
1	B	396	ASN
1	B	405	GLN
1	B	407	ASN
1	B	415	GLN
1	B	430	ASN
1	B	469	ASN
1	B	479	ASN
1	B	518	ASN
1	B	529	ASN
1	B	555	GLN
1	B	580	GLN
1	B	605	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	487/514 (94%)	-0.06	10 (2%) 67 36	40, 76, 125, 154	0
1	B	487/514 (94%)	-0.15	4 (0%) 87 67	36, 74, 123, 162	0
All	All	974/1028 (94%)	-0.11	14 (1%) 78 51	36, 75, 125, 162	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	98	TYR	5.3
1	A	195	ASN	3.7
1	A	439	CYS	3.4
1	A	438	ALA	2.8
1	A	121	TYR	2.7
1	A	276	SER	2.5
1	B	438	ALA	2.5
1	B	381	GLU	2.5
1	B	98	TYR	2.4
1	A	198	PHE	2.4
1	A	482	ASP	2.3
1	A	374	ALA	2.3
1	A	380	THR	2.2
1	B	459	ARG	2.1

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.