Full wwPDB X-ray Structure Validation Report ⓘ

Apr 27, 2023 – 07:34 pm BST

PDB ID	:	5FRR
Title	:	Structure of the Pds5-Scc1 complex and implications for cohesin function
Authors	:	Muir, K.W.; Kschonsak, M.; Li, Y.; Metz, J.; Haering, C.H.; Panne, D.
Deposited on	:	2015-12-22
Resolution	:	5.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

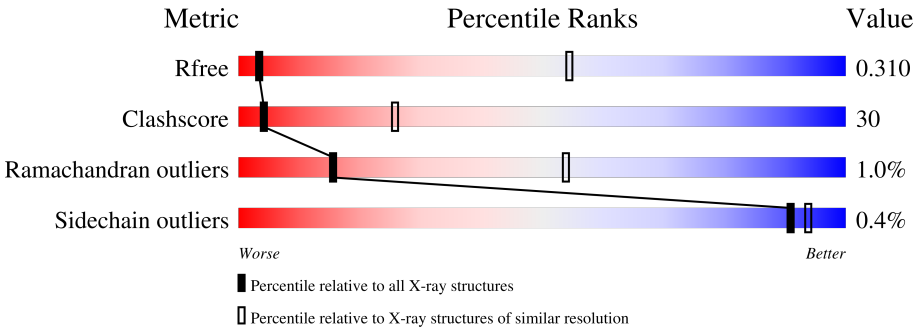
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.32.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.32.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 5.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1008 (7.70-3.86)
Clashscore	141614	1035 (7.70-3.90)
Ramachandran outliers	138981	1003 (7.70-3.86)
Sidechain outliers	138945	1006 (7.78-3.82)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Mol	Chain	Length	Quality of chain
1	A	703	47% 49%
1	B	703	46% 47% 6%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 10858 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 SISTER CHROMATID COHESION PROTEIN PDS5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	677	Total	C	N	O	S	0	0	0
			5494	3526	914	1041	13			
1	B	660	Total	C	N	O	S	0	0	0
			5364	3455	889	1009	11			

There are 4 discrepancies between the modelled and reference sequences:

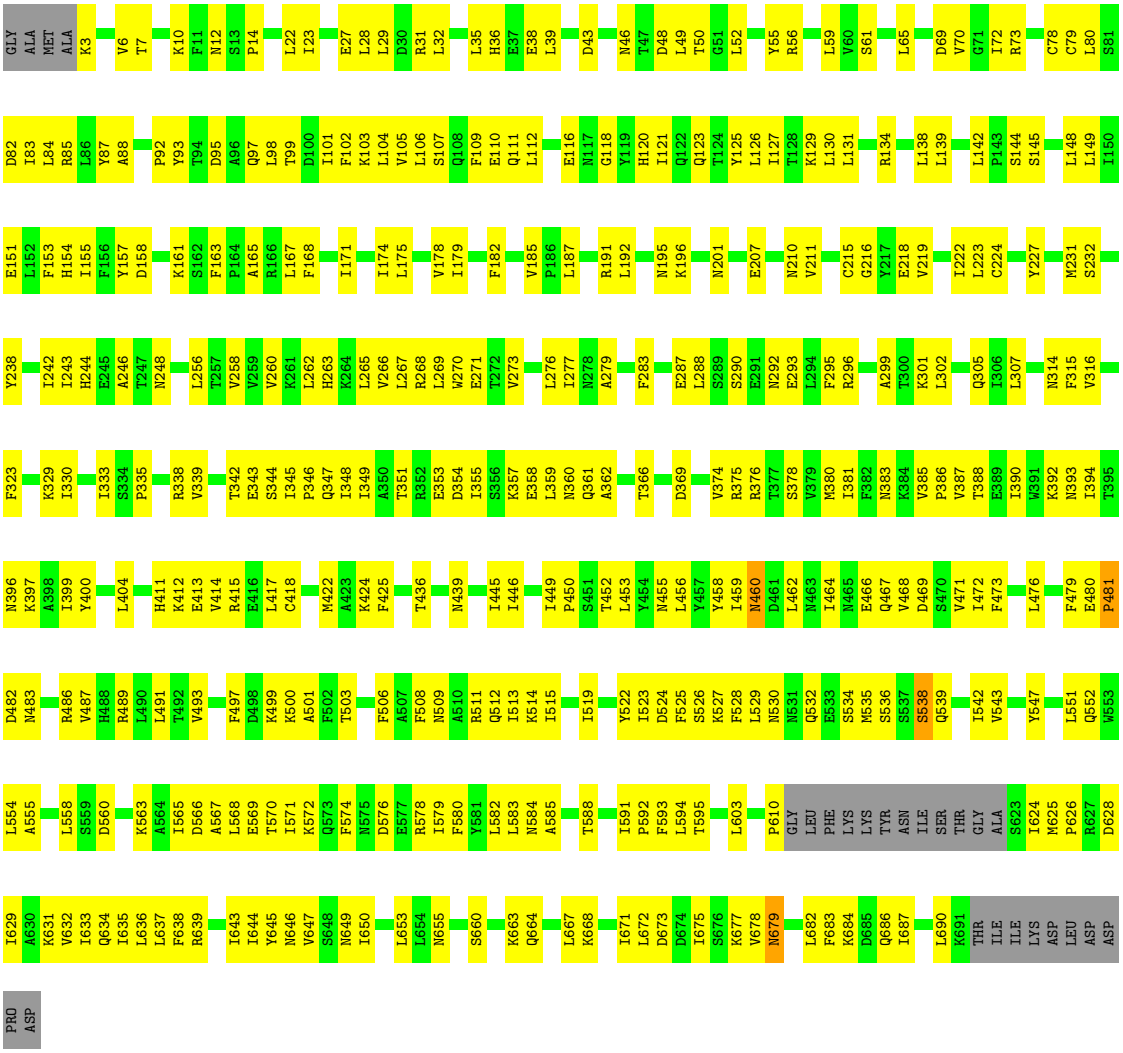
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP Q04264
A	0	ALA	-	expression tag	UNP Q04264
B	-1	GLY	-	expression tag	UNP Q04264
B	0	ALA	-	expression tag	UNP Q04264

3 Residue-property plots (i)

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

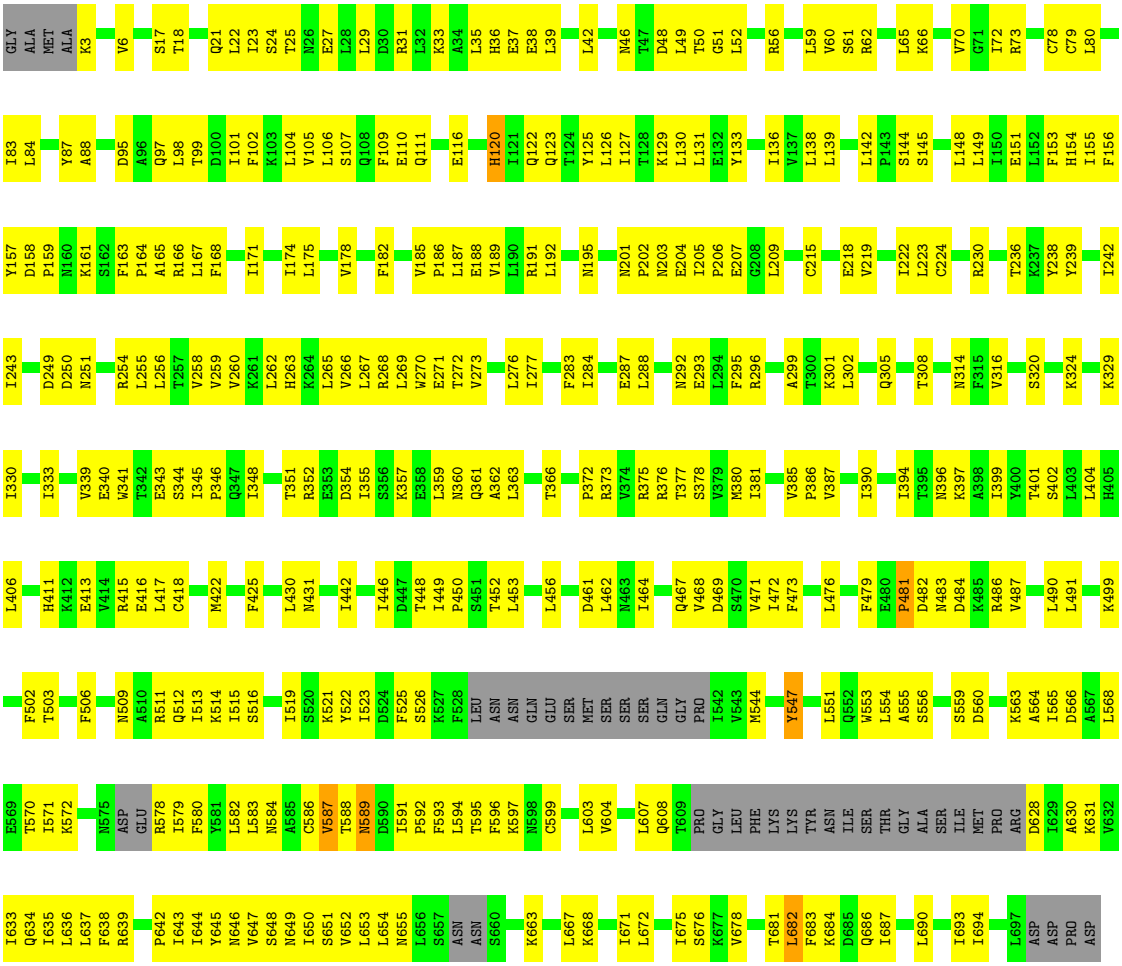
• Molecule 1: SISTER CHROMATID COHESION PROTEIN PDS5

Chain A:



• Molecule 1: SISTER CHROMATID COHESION PROTEIN PDS5

Chain B:


GLY ALA MET ALA K3 V6 S17 T18 Q21 L22 I23 S24 T25 N26 E27 L28 L29 D30 R31 L32 K33 A34 L35 H36 E37 E38 L39 L42 N46 T47 D48 L49 T50 G51 L52 R56 L59 V60 S61 R62 L65 K66 V70 G71 I72 R73 C78 C79 L80
I83 L84 Y87 A88 D95 A96 Q97 L98 T99 D100 I101 F102 K103 L104 V105 L106 S107 Q108 F109 E110 Q111 E116 H120 I121 Q122 Q123 T124 Y125 L126 I127 T128 K129 L130 L131 E132 Y133 I136 V137 L138 L139 L142 P143 S144 S145 L148 L149 I150 E151 L152 F153 H154 I155 F156
Y157 D158 P159 N160 K161 S162 F163 P164 A165 R166 L167 F168 I171 I174 L175 V178 F182 V185 P186 L187 E188 V189 L190 R191 L192 N195 N201 P202 N203 E204 I205 P206 E207 Q208 L209 C215 E218 V219 I222 L223 C224 R230 T236 K237 Y238 Y239 I242
I243 D249 D250 N251 R254 L255 L256 T257 V258 V259 V260 K261 L262 H263 K264 L265 V266 L267 R268 L269 W270 E271 T272 V273 L276 I277 F283 I284 E287 L288 N292 E293 L294 F295 R296 A299 T300 K301 L302 Q305 T308 N314 F315 V316 S320 K324 K329
I330 I333 V339 E340 W341 T342 E343 S344 I345 P346 Q347 I348 T351 R352 E353 D354 I355 S356 K357 E358 L359 N360 Q361 A362 L363 T366 P372 R373 V374 R375 R376 T377 S378 V379 M380 I381 V385 P386 V387 I390 I394 T396 N396 K397 A398 I399 Y400 T401 S402 L403 L404 H405
L406 H411 K412 E413 V414 R415 E416 L417 C418 M422 F425 L430 N431 I442 I446 D447 T448 I449 P450 S451 T452 L453 L456 D461 L462 N463 I464 Q467 V468 D469 S470 V471 I472 F473 L476 F479 E480 P481 D482 N483 D484 K485 R486 V487 L490 L491 K499
F502 T503 F506 N509 A510 R511 Q512 I513 K514 I515 S516 I519 S520 K521 Y522 I523 D524 F525 S526 K527 F528 LEU ASN ASN GLN GLU SER MET SER SER GLN GLY PRO I542 V543 M544 Y547 L551 Q552 W553 L554 A555 S556 S559 D560 K563 A564 I565 D566 A567 L568
E569 T570 I571 K572 N575 ASP GLU R578 I579 F580 Y581 L582 L583 N584 A585 C586 V587 T588 N589 D590 I591 P592 F593 L594 T595 F596 K597 N598 C599 L603 V604 L607 Q608 T609 PRO GLY LEU PHE LYS LYS TYR ASN ILE SER THR GLY ALA SER ILE MET PRO ARG D628 I629 A630 K631 V632
I633 Q634 I635 L636 L637 F638 R639 P642 I643 I644 Y645 N646 V647 S648 N649 I650 S651 V652 L653 L654 N655 L656 S657 ASN ASN S660 K663 L667 K668 I671 L672 I675 S676 K677 V678 T681 L682 F683 K684 D685 Q686 I687 L690 I693 I694 L697 ASP ASP PRO ASP

4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 4 2 2	Depositor
Cell constants a, b, c, α, β, γ	283.69Å 283.69Å 172.79Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 5.80 49.19 – 5.79	Depositor EDS
% Data completeness (in resolution range)	95.0 (50.00-5.80) 99.6 (49.19-5.79)	Depositor EDS
R_{merge}	0.02	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.73 (at 5.73Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.249 , 0.311 0.249 , 0.310	Depositor DCC
R_{free} test set	518 reflections (5.14%)	wwPDB-VP
Wilson B-factor (Å^2)	383.9	Xtriage
Anisotropy	0.013	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 403.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.84	EDS
Total number of atoms	10858	wwPDB-VP
Average B, all atoms (Å^2)	424.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.39% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.25	0/5600	0.42	0/7597
1	B	0.25	0/5464	0.41	0/7408
All	All	0.25	0/11064	0.41	0/15005

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	5494	0	5551	334	0
1	B	5364	0	5435	324	1
All	All	10858	0	10986	647	1

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 30.

All (647) 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:333:ILE:H	1:B:333:ILE:HD12	1.29	0.97
1:A:98:LEU:HD23	1:A:142:LEU:HD21	1.51	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:373:ARG:HA	1:B:376:ARG:HH12	1.36	0.91
1:B:98:LEU:HD23	1:B:142:LEU:HD21	1.52	0.89
1:B:462:LEU:HD13	1:B:559:SER:HA	1.53	0.88
1:A:333:ILE:HD12	1:A:333:ILE:H	1.39	0.86
1:A:483:ASN:HA	1:A:486:ARG:NH1	1.94	0.82
1:B:523:ILE:HD13	1:B:580:PHE:HA	1.63	0.81
1:A:70:VAL:HG12	1:A:73:ARG:HH21	1.46	0.80
1:B:70:VAL:HG12	1:B:73:ARG:HH21	1.47	0.78
1:B:372:PRO:HA	1:B:375:ARG:HE	1.49	0.78
1:B:396:ASN:HB3	1:B:399:ILE:HG12	1.65	0.78
1:A:342:THR:HA	1:A:345:ILE:HD13	1.65	0.78
1:B:308:THR:HA	1:B:351:THR:HG21	1.66	0.78
1:B:105:VAL:HG23	1:B:126:LEU:HD21	1.64	0.77
1:A:682:LEU:H	1:A:682:LEU:HD23	1.50	0.77
1:A:293:GLU:HA	1:A:296:ARG:HE	1.51	0.76
1:A:610:PRO:HG3	1:A:626:PRO:HG2	1.66	0.76
1:A:105:VAL:HG23	1:A:126:LEU:HD21	1.66	0.75
1:B:351:THR:HG22	1:B:352:ARG:HG3	1.67	0.75
1:B:111:GLN:HB2	1:B:123:GLN:HE22	1.53	0.73
1:A:396:ASN:HB3	1:A:399:ILE:HG12	1.70	0.73
1:B:483:ASN:HA	1:B:486:ARG:NH1	2.03	0.73
1:B:242:ILE:HG21	1:B:262:LEU:HD21	1.70	0.73
1:A:480:GLU:HB2	1:A:481:PRO:HA	1.70	0.72
1:A:69:ASP:HB3	1:A:72:ILE:HD13	1.72	0.72
1:A:330:ILE:HG21	1:A:362:ALA:HB1	1.70	0.72
1:A:121:ILE:HD12	1:A:121:ILE:H	1.54	0.71
1:A:154:HIS:HD2	1:A:192:LEU:HD22	1.55	0.70
1:B:633:ILE:HD12	1:B:634:GLN:N	2.07	0.70
1:B:512:GLN:HA	1:B:639:ARG:O	1.92	0.70
1:A:56:ARG:HD2	1:A:92:PRO:HB2	1.74	0.69
1:B:373:ARG:HA	1:B:376:ARG:NH1	2.07	0.69
1:A:380:MET:HA	1:A:383:ASN:HD22	1.55	0.69
1:A:111:GLN:HB2	1:A:123:GLN:HE22	1.57	0.69
1:A:381:ILE:O	1:A:385:VAL:HG12	1.91	0.69
1:B:522:TYR:OH	1:B:572:LYS:HG3	1.93	0.69
1:B:263:HIS:HB3	1:B:302:LEU:HD13	1.74	0.69
1:A:196:LYS:HE3	1:A:216:GLY:HA3	1.74	0.68
1:A:473:PHE:HB3	1:A:479:PHE:HE1	1.57	0.68
1:B:381:ILE:O	1:B:385:VAL:HG12	1.94	0.67
1:A:263:HIS:HB3	1:A:302:LEU:HD13	1.77	0.67
1:B:339:VAL:HG13	1:B:377:THR:HG21	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:513:ILE:HD12	1:B:514:LYS:N	2.10	0.67
1:A:52:LEU:O	1:A:52:LEU:HD23	1.95	0.66
1:A:201:ASN:ND2	1:A:268:ARG:HE	1.93	0.66
1:B:272:THR:HG23	1:B:273:VAL:HG22	1.76	0.66
1:A:513:ILE:HD12	1:A:514:LYS:N	2.09	0.66
1:B:522:TYR:OH	1:B:571:ILE:HG13	1.95	0.66
1:A:411:HIS:HE1	1:A:413:GLU:HB3	1.61	0.65
1:B:164:PRO:HG2	1:B:167:LEU:HD13	1.78	0.65
1:A:349:ILE:HG23	1:A:393:ASN:ND2	2.12	0.65
1:B:99:THR:HG22	1:B:142:LEU:HD13	1.79	0.65
1:B:522:TYR:CE1	1:B:568:LEU:HB3	2.32	0.65
1:B:330:ILE:HG21	1:B:362:ALA:HB1	1.79	0.65
1:A:539:GLN:O	1:A:543:VAL:HG12	1.97	0.64
1:B:604:VAL:O	1:B:608:GLN:HG3	1.98	0.64
1:A:687:ILE:HD13	1:B:687:ILE:HG12	1.78	0.64
1:A:482:ASP:CG	1:A:483:ASN:H	2.00	0.64
1:B:415:ARG:NH1	1:B:464:ILE:HD11	2.13	0.64
1:A:360:ASN:HB3	1:A:396:ASN:HB2	1.79	0.63
1:A:683:PHE:HZ	1:B:690:LEU:HB3	1.61	0.63
1:B:102:PHE:HA	1:B:105:VAL:HG12	1.80	0.63
1:A:333:ILE:HD12	1:A:333:ILE:N	2.13	0.63
1:A:683:PHE:CZ	1:B:690:LEU:HD13	2.33	0.63
1:A:79:CYS:O	1:A:83:ILE:HG12	1.98	0.63
1:A:509:ASN:OD1	1:A:644:ILE:HD11	1.99	0.63
1:B:490:LEU:O	1:B:490:LEU:HD23	1.99	0.63
1:A:551:LEU:HD12	1:A:552:GLN:N	2.14	0.63
1:B:201:ASN:O	1:B:204:GLU:HG2	1.99	0.63
1:B:267:LEU:O	1:B:271:GLU:HG3	1.99	0.63
1:B:522:TYR:HH	1:B:572:LYS:HG3	1.64	0.63
1:A:102:PHE:O	1:A:106:LEU:HG	1.99	0.62
1:B:572:LYS:NZ	1:B:572:LYS:HB3	2.14	0.62
1:B:635:ILE:HD12	1:B:636:LEU:N	2.14	0.62
1:B:449:ILE:O	1:B:453:LEU:HD13	1.99	0.62
1:A:165:ALA:HA	1:A:168:PHE:CD1	2.35	0.62
1:A:151:GLU:O	1:A:155:ILE:HG13	2.00	0.62
1:A:256:LEU:O	1:A:260:VAL:HG23	2.00	0.62
1:B:394:ILE:HD12	1:B:394:ILE:O	2.00	0.62
1:A:568:LEU:HD12	1:A:569:GLU:N	2.14	0.61
1:B:650:ILE:HD12	1:B:651:SER:N	2.14	0.61
1:A:412:LYS:NZ	1:A:412:LYS:HB3	2.15	0.61
1:A:583:LEU:HD13	1:A:633:ILE:HD11	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:283:PHE:O	1:A:287:GLU:HG3	1.99	0.61
1:A:333:ILE:H	1:A:333:ILE:CD1	2.13	0.61
1:A:394:ILE:O	1:A:394:ILE:HD12	2.00	0.61
1:B:462:LEU:HB3	1:B:559:SER:CB	2.30	0.61
1:B:18:THR:HG23	1:B:21:GLN:H	1.65	0.61
1:B:547:TYR:OH	1:B:572:LYS:HE3	2.00	0.61
1:A:686:GLN:O	1:A:690:LEU:HG	2.01	0.61
1:A:3:LYS:HB3	1:A:50:THR:HG21	1.82	0.61
1:A:387:VAL:HA	1:A:390:ILE:HD12	1.82	0.60
1:A:524:ASP:HA	1:A:527:LYS:HE2	1.83	0.60
1:B:80:LEU:HD13	1:B:101:ILE:HG23	1.83	0.60
1:A:415:ARG:NH1	1:A:464:ILE:HD11	2.16	0.60
1:B:513:ILE:HG22	1:B:589:ASN:HD21	1.65	0.60
1:A:483:ASN:HA	1:A:486:ARG:HH12	1.66	0.60
1:B:462:LEU:HB3	1:B:559:SER:HB3	1.83	0.60
1:A:201:ASN:HD22	1:A:268:ARG:HE	1.49	0.60
1:B:655:ASN:OD1	1:B:668:LYS:HD2	2.01	0.60
1:A:290:SER:O	1:A:296:ARG:HD3	2.01	0.60
1:A:288:LEU:HB3	1:A:329:LYS:HE3	1.83	0.60
1:B:151:GLU:O	1:B:155:ILE:HG13	2.02	0.60
1:B:554:LEU:HD12	1:B:555:ALA:N	2.17	0.60
1:A:635:ILE:HA	1:A:638:PHE:HD2	1.66	0.59
1:A:584:ASN:O	1:A:588:THR:HG23	2.01	0.59
1:B:355:ILE:N	1:B:355:ILE:HD12	2.17	0.59
1:B:467:GLN:O	1:B:471:VAL:HG23	2.03	0.59
1:B:628:ASP:O	1:B:631:LYS:HG2	2.01	0.59
1:A:489:ARG:O	1:A:493:VAL:HG23	2.02	0.59
1:B:648:SER:O	1:B:652:VAL:HG23	2.03	0.59
1:A:49:LEU:HD23	1:A:49:LEU:O	2.02	0.59
1:B:156:PHE:HA	1:B:163:PHE:CE2	2.38	0.59
1:B:333:ILE:H	1:B:333:ILE:CD1	2.07	0.59
1:A:418:CYS:O	1:A:422:MET:HG2	2.02	0.59
1:A:635:ILE:HA	1:A:638:PHE:CD2	2.38	0.59
1:B:70:VAL:HG12	1:B:73:ARG:NH2	2.16	0.59
1:A:70:VAL:HG12	1:A:73:ARG:NH2	2.16	0.59
1:A:673:ASP:OD1	1:A:677:LYS:HE2	2.03	0.59
1:B:676:SER:HA	1:B:682:LEU:HD11	1.84	0.59
1:B:49:LEU:O	1:B:49:LEU:HD23	2.03	0.59
1:A:456:LEU:O	1:A:459:ILE:HG13	2.02	0.59
1:B:95:ASP:O	1:B:99:THR:HG23	2.03	0.58
1:B:254:ARG:O	1:B:258:VAL:HG23	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:644:ILE:HG13	1:A:645:TYR:CD1	2.38	0.58
1:B:523:ILE:HD11	1:B:583:LEU:HD23	1.85	0.58
1:A:121:ILE:HD12	1:A:121:ILE:N	2.17	0.58
1:B:288:LEU:HB3	1:B:329:LYS:CE	2.33	0.58
1:B:314:ASN:OD1	1:B:316:VAL:HG22	2.03	0.58
1:A:110:GLU:HG3	1:A:161:LYS:NZ	2.18	0.58
1:B:288:LEU:HB3	1:B:329:LYS:HE3	1.84	0.58
1:B:139:LEU:O	1:B:139:LEU:HD23	2.04	0.58
1:B:22:LEU:HD12	1:B:22:LEU:O	2.04	0.58
1:B:333:ILE:HD12	1:B:333:ILE:N	2.11	0.58
1:B:646:ASN:OD1	1:B:647:VAL:HG13	2.03	0.58
1:A:355:ILE:HD12	1:A:355:ILE:N	2.19	0.57
1:B:116:GLU:HA	1:B:120:HIS:CE1	2.39	0.57
1:B:186:PRO:HG2	1:B:189:VAL:HG23	1.86	0.57
1:B:256:LEU:O	1:B:260:VAL:HG23	2.04	0.57
1:B:355:ILE:HG22	1:B:359:LEU:HG	1.84	0.57
1:B:554:LEU:HD11	1:B:568:LEU:HD11	1.86	0.57
1:A:139:LEU:HD23	1:A:139:LEU:O	2.04	0.57
1:B:110:GLU:HG3	1:B:161:LYS:HZ1	1.69	0.57
1:B:523:ILE:HG21	1:B:580:PHE:HB3	1.85	0.57
1:B:251:ASN:HB3	1:B:254:ARG:HB2	1.85	0.57
1:A:624:ILE:HG12	1:A:625:MET:N	2.19	0.57
1:A:571:ILE:HA	1:A:574:PHE:CD2	2.39	0.57
1:B:519:ILE:O	1:B:522:TYR:HB3	2.04	0.57
1:B:481:PRO:HG2	1:B:482:ASP:H	1.70	0.57
1:A:288:LEU:HB3	1:A:329:LYS:CE	2.35	0.57
1:A:187:LEU:HG	1:A:191:ARG:NH1	2.20	0.57
1:B:509:ASN:HD21	1:B:644:ILE:HD11	1.69	0.57
1:A:293:GLU:HA	1:A:296:ARG:NE	2.19	0.56
1:A:449:ILE:N	1:A:450:PRO:HD2	2.19	0.56
1:A:110:GLU:HG3	1:A:161:LYS:HZ1	1.69	0.56
1:A:376:ARG:O	1:A:380:MET:HG2	2.03	0.56
1:A:446:ILE:N	1:A:446:ILE:HD12	2.21	0.56
1:B:449:ILE:HB	1:B:450:PRO:HD3	1.87	0.56
1:B:633:ILE:O	1:B:637:LEU:HG	2.04	0.56
1:B:645:TYR:CE2	1:B:678:VAL:HG21	2.41	0.56
1:B:175:LEU:HD12	1:B:219:VAL:HG11	1.88	0.56
1:B:513:ILE:HG22	1:B:589:ASN:ND2	2.21	0.56
1:B:686:GLN:O	1:B:690:LEU:HG	2.04	0.56
1:A:397:LYS:NZ	1:A:445:ILE:HD11	2.21	0.56
1:B:78:CYS:SG	1:B:122:GLN:HB3	2.46	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:17:SER:HA	1:B:23:ILE:HD13	1.88	0.56
1:B:579:ILE:HG23	1:B:603:LEU:HD11	1.87	0.56
1:A:560:ASP:OD1	1:A:563:LYS:HB2	2.06	0.56
1:B:62:ARG:NH1	1:B:66:LYS:HD2	2.21	0.56
1:B:187:LEU:O	1:B:187:LEU:HD23	2.06	0.56
1:B:273:VAL:HB	1:B:276:LEU:HD13	1.86	0.56
1:A:453:LEU:HA	1:A:456:LEU:HD13	1.86	0.55
1:B:23:ILE:N	1:B:23:ILE:HD12	2.22	0.55
1:A:14:PRO:HG2	1:A:31:ARG:NH1	2.21	0.55
1:B:110:GLU:HG3	1:B:161:LYS:NZ	2.21	0.55
1:B:584:ASN:HA	1:B:587:VAL:HG12	1.88	0.55
1:A:22:LEU:C	1:A:23:ILE:HD12	2.27	0.55
1:A:633:ILE:O	1:A:637:LEU:HG	2.07	0.55
1:B:386:PRO:O	1:B:390:ILE:HG13	2.06	0.55
1:A:459:ILE:HD12	1:A:460:ASN:N	2.21	0.55
1:A:95:ASP:O	1:A:99:THR:HG23	2.07	0.55
1:B:131:LEU:HB2	1:B:174:ILE:HD11	1.89	0.55
1:B:283:PHE:O	1:B:287:GLU:HG3	2.07	0.55
1:A:565:ILE:HG13	1:A:566:ASP:OD1	2.06	0.55
1:B:592:PRO:O	1:B:595:THR:HG22	2.07	0.55
1:A:568:LEU:HA	1:A:571:ILE:HD12	1.88	0.55
1:A:664:GLN:HG2	1:A:668:LYS:HE3	1.88	0.55
1:B:219:VAL:O	1:B:223:LEU:HD13	2.07	0.55
1:B:663:LYS:O	1:B:667:LEU:HD13	2.07	0.55
1:B:188:GLU:O	1:B:192:LEU:HG	2.08	0.54
1:A:270:TRP:HE3	1:A:277:ILE:HG13	1.73	0.54
1:B:102:PHE:O	1:B:106:LEU:HG	2.08	0.54
1:B:288:LEU:HD12	1:B:299:ALA:HB1	1.89	0.54
1:B:654:LEU:C	1:B:655:ASN:HD22	2.11	0.54
1:A:335:PRO:HA	1:A:338:ARG:HD2	1.90	0.54
1:A:628:ASP:O	1:A:632:VAL:HG23	2.07	0.54
1:B:372:PRO:HB3	1:B:375:ARG:HH21	1.71	0.54
1:A:219:VAL:O	1:A:223:LEU:HD13	2.08	0.54
1:B:102:PHE:O	1:B:105:VAL:HG12	2.08	0.54
1:B:238:TYR:O	1:B:242:ILE:HG12	2.07	0.54
1:B:418:CYS:O	1:B:422:MET:HG2	2.08	0.54
1:B:453:LEU:HD22	1:B:476:LEU:HD21	1.90	0.54
1:B:560:ASP:OD1	1:B:563:LYS:HG3	2.07	0.54
1:A:690:LEU:HD13	1:B:683:PHE:CE2	2.43	0.54
1:B:376:ARG:O	1:B:380:MET:HG2	2.08	0.54
1:A:668:LYS:O	1:A:672:LEU:HD13	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:683:PHE:CZ	1:B:690:LEU:HB3	2.43	0.54
1:A:22:LEU:O	1:A:22:LEU:HD12	2.08	0.54
1:A:467:GLN:O	1:A:471:VAL:HG23	2.07	0.54
1:A:509:ASN:CG	1:A:644:ILE:HD11	2.29	0.53
1:B:165:ALA:HA	1:B:168:PHE:CD1	2.43	0.53
1:B:205:ILE:N	1:B:206:PRO:CD	2.71	0.53
1:B:316:VAL:HG11	1:B:355:ILE:HD11	1.90	0.53
1:A:157:TYR:HB2	1:A:192:LEU:HD21	1.89	0.53
1:A:585:ALA:O	1:A:591:ILE:HD13	2.07	0.53
1:B:396:ASN:HB3	1:B:399:ILE:CG1	2.37	0.53
1:B:411:HIS:HE1	1:B:413:GLU:HB3	1.72	0.53
1:A:23:ILE:HD12	1:A:23:ILE:N	2.23	0.53
1:A:84:LEU:O	1:A:88:ALA:HB2	2.08	0.53
1:A:635:ILE:HD12	1:A:636:LEU:N	2.24	0.53
1:B:156:PHE:HA	1:B:163:PHE:HE2	1.73	0.53
1:A:215:CYS:O	1:A:219:VAL:HG23	2.08	0.53
1:B:22:LEU:C	1:B:23:ILE:HD12	2.29	0.53
1:B:292:ASN:HB3	1:B:295:PHE:HD2	1.73	0.53
1:B:344:SER:O	1:B:348:ILE:HG13	2.09	0.53
1:B:516:SER:OG	1:B:587:VAL:HG22	2.09	0.53
1:A:154:HIS:O	1:A:158:ASP:HB2	2.09	0.53
1:A:646:ASN:OD1	1:A:647:VAL:HG13	2.09	0.53
1:B:479:PHE:HB3	1:B:597:LYS:HD3	1.90	0.53
1:A:571:ILE:HA	1:A:574:PHE:HD2	1.72	0.53
1:A:624:ILE:HG12	1:A:625:MET:H	1.73	0.53
1:B:205:ILE:O	1:B:207:GLU:HG2	2.09	0.53
1:A:380:MET:SD	1:A:417:LEU:HD21	2.49	0.52
1:A:411:HIS:CE1	1:A:413:GLU:HB3	2.43	0.52
1:A:673:ASP:O	1:A:677:LYS:HG3	2.09	0.52
1:B:566:ASP:O	1:B:570:THR:HG23	2.08	0.52
1:B:671:ILE:HG22	1:B:675:ILE:HD11	1.90	0.52
1:A:664:GLN:O	1:A:668:LYS:HG3	2.09	0.52
1:B:84:LEU:O	1:B:88:ALA:HB2	2.10	0.52
1:B:589:ASN:HA	1:B:642:PRO:HG3	1.91	0.52
1:A:339:VAL:O	1:A:343:GLU:HG3	2.09	0.52
1:A:449:ILE:O	1:A:453:LEU:HD13	2.09	0.52
1:A:551:LEU:HD22	1:A:568:LEU:HD11	1.91	0.52
1:B:254:ARG:HE	1:B:254:ARG:HA	1.74	0.52
1:B:643:ILE:HD12	1:B:643:ILE:N	2.25	0.52
1:A:72:ILE:N	1:A:72:ILE:HD12	2.25	0.52
1:A:644:ILE:HG13	1:A:645:TYR:HD1	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:521:LYS:HB3	1:B:525:PHE:CE2	2.44	0.52
1:B:3:LYS:HE3	1:B:50:THR:HG21	1.91	0.52
1:B:380:MET:SD	1:B:417:LEU:HD21	2.50	0.52
1:B:565:ILE:HG13	1:B:566:ASP:OD1	2.09	0.52
1:A:262:LEU:O	1:A:266:VAL:HG23	2.08	0.52
1:A:527:LYS:HA	1:A:530:ASN:OD1	2.10	0.52
1:A:121:ILE:H	1:A:121:ILE:CD1	2.20	0.52
1:A:99:THR:HG22	1:A:142:LEU:HD13	1.92	0.52
1:A:238:TYR:O	1:A:242:ILE:HG12	2.10	0.52
1:A:396:ASN:HB3	1:A:399:ILE:CG1	2.40	0.52
1:A:355:ILE:HG22	1:A:359:LEU:HG	1.92	0.51
1:A:27:GLU:O	1:A:31:ARG:HG3	2.10	0.51
1:A:523:ILE:HG23	1:A:580:PHE:HD2	1.75	0.51
1:B:649:ASN:O	1:B:653:LEU:HG	2.10	0.51
1:A:314:ASN:OD1	1:A:316:VAL:HG22	2.11	0.51
1:A:643:ILE:N	1:A:643:ILE:HD12	2.25	0.51
1:B:464:ILE:O	1:B:468:VAL:HG23	2.10	0.51
1:A:301:LYS:O	1:A:305:GLN:HG3	2.10	0.51
1:A:459:ILE:HD12	1:A:459:ILE:C	2.31	0.51
1:A:506:PHE:HA	1:A:509:ASN:HD22	1.74	0.51
1:B:215:CYS:O	1:B:219:VAL:HG23	2.11	0.51
1:B:607:LEU:HD23	1:B:633:ILE:HG12	1.92	0.51
1:B:693:ILE:HD12	1:B:694:ILE:N	2.26	0.51
1:A:87:TYR:HB3	1:A:92:PRO:HD3	1.92	0.51
1:A:265:LEU:O	1:A:269:LEU:HG	2.11	0.51
1:A:634:GLN:HG2	1:A:638:PHE:CE2	2.46	0.51
1:B:136:ILE:HG12	1:B:174:ILE:HG23	1.90	0.51
1:A:528:PHE:CE2	1:A:543:VAL:HG11	2.45	0.51
1:B:270:TRP:HE3	1:B:277:ILE:HG13	1.74	0.51
1:B:526:SER:CB	1:B:572:LYS:HE2	2.40	0.51
1:A:105:VAL:HG22	1:A:109:PHE:CE2	2.46	0.51
1:A:388:THR:O	1:A:392:LYS:HG2	2.10	0.51
1:A:576:ASP:OD2	1:A:578:ARG:HB3	2.10	0.51
1:B:415:ARG:HH11	1:B:464:ILE:HD11	1.74	0.51
1:A:663:LYS:O	1:A:667:LEU:HD13	2.11	0.51
1:B:360:ASN:HB3	1:B:396:ASN:HB2	1.92	0.51
1:B:397:LYS:HE3	1:B:401:THR:HG21	1.93	0.51
1:A:357:LYS:HB3	1:A:358:GLU:OE1	2.11	0.51
1:A:59:LEU:O	1:A:80:LEU:HD21	2.11	0.50
1:A:116:GLU:HG2	1:A:118:GLY:H	1.75	0.50
1:A:529:LEU:N	1:A:529:LEU:HD12	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:56:ARG:HD3	1:A:87:TYR:CE2	2.45	0.50
1:A:479:PHE:HA	1:A:593:PHE:HZ	1.75	0.50
1:A:523:ILE:HG23	1:A:580:PHE:CD2	2.46	0.50
1:B:97:GLN:O	1:B:101:ILE:HG13	2.11	0.50
1:A:273:VAL:HB	1:A:276:LEU:HD13	1.94	0.50
1:A:566:ASP:O	1:A:570:THR:HG23	2.12	0.50
1:A:650:ILE:HG21	1:B:650:ILE:HD13	1.93	0.50
1:B:339:VAL:O	1:B:343:GLU:HG3	2.11	0.50
1:B:430:LEU:HD12	1:B:431:ASN:OD1	2.11	0.50
1:B:578:ARG:NE	1:B:582:LEU:HD11	2.27	0.50
1:B:584:ASN:O	1:B:587:VAL:HG12	2.11	0.50
1:A:592:PRO:HB2	1:A:595:THR:HG22	1.93	0.50
1:A:366:THR:HG22	1:A:378:SER:OG	2.11	0.50
1:A:487:VAL:O	1:A:491:LEU:HG	2.12	0.50
1:A:211:VAL:HG22	1:A:211:VAL:O	2.12	0.50
1:B:51:GLY:C	1:B:52:LEU:HD12	2.32	0.50
1:A:72:ILE:HD12	1:A:72:ILE:H	1.77	0.50
1:A:387:VAL:HG23	1:A:425:PHE:CE1	2.47	0.50
1:A:635:ILE:HD12	1:A:635:ILE:C	2.32	0.50
1:B:209:LEU:N	1:B:209:LEU:HD12	2.26	0.50
1:B:262:LEU:O	1:B:266:VAL:HG23	2.12	0.50
1:A:468:VAL:O	1:A:472:ILE:HG13	2.12	0.50
1:B:105:VAL:HG22	1:B:109:PHE:CE2	2.47	0.50
1:B:167:LEU:O	1:B:171:ILE:HG13	2.12	0.50
1:B:354:ASP:HB3	1:B:355:ILE:HD12	1.94	0.50
1:B:690:LEU:O	1:B:694:ILE:HG13	2.12	0.50
1:A:134:ARG:HG2	1:A:134:ARG:HH11	1.76	0.49
1:A:390:ILE:O	1:A:394:ILE:HG13	2.11	0.49
1:A:526:SER:C	1:A:528:PHE:H	2.14	0.49
1:B:6:VAL:CG1	1:B:46:ASN:HD21	2.24	0.49
1:B:572:LYS:HB3	1:B:572:LYS:HZ3	1.77	0.49
1:A:102:PHE:HA	1:A:105:VAL:HG12	1.93	0.49
1:B:482:ASP:O	1:B:486:ARG:HG3	2.12	0.49
1:A:683:PHE:HZ	1:B:690:LEU:HD13	1.78	0.49
1:B:265:LEU:O	1:B:269:LEU:HG	2.11	0.49
1:A:508:PHE:HE1	1:A:639:ARG:HG2	1.77	0.49
1:B:154:HIS:O	1:B:158:ASP:HB2	2.11	0.49
1:B:366:THR:HG22	1:B:378:SER:OG	2.13	0.49
1:A:628:ASP:HA	1:A:631:LYS:HG2	1.94	0.49
1:A:97:GLN:O	1:A:101:ILE:HG13	2.12	0.49
1:A:102:PHE:HZ	1:A:138:LEU:HB2	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:145:SER:HB3	1:B:182:PHE:HZ	1.76	0.49
1:B:579:ILE:HG23	1:B:603:LEU:CD1	2.43	0.49
1:A:515:ILE:HD12	1:A:639:ARG:O	2.13	0.49
1:B:301:LYS:HD3	1:B:340:GLU:OE2	2.12	0.49
1:A:52:LEU:HD22	1:A:87:TYR:HE1	1.78	0.49
1:A:276:LEU:HD12	1:A:276:LEU:N	2.27	0.49
1:A:678:VAL:O	1:A:679:ASN:CB	2.61	0.49
1:A:687:ILE:HA	1:A:690:LEU:HD12	1.95	0.49
1:B:276:LEU:N	1:B:276:LEU:HD12	2.28	0.49
1:B:25:THR:O	1:B:29:LEU:HG	2.13	0.49
1:B:387:VAL:HG23	1:B:425:PHE:CE1	2.48	0.49
1:B:515:ILE:HG22	1:B:519:ILE:HD13	1.93	0.49
1:A:292:ASN:HB3	1:A:295:PHE:HD2	1.77	0.48
1:A:534:SER:OG	1:A:538:SER:HB3	2.13	0.48
1:B:461:ASP:HB3	1:B:464:ILE:HB	1.95	0.48
1:B:588:THR:HG22	1:B:588:THR:O	2.13	0.48
1:B:218:GLU:O	1:B:222:ILE:HG13	2.13	0.48
1:B:442:ILE:HG22	1:B:446:ILE:HD13	1.94	0.48
1:B:523:ILE:CD1	1:B:583:LEU:HD23	2.43	0.48
1:A:6:VAL:HG13	1:A:7:THR:HG23	1.94	0.48
1:A:515:ILE:HG22	1:A:519:ILE:HD13	1.94	0.48
1:B:452:THR:O	1:B:456:LEU:HG	2.14	0.48
1:B:582:LEU:HD23	1:B:599:CYS:O	2.13	0.48
1:A:266:VAL:HG13	1:A:277:ILE:HD12	1.96	0.48
1:B:144:SER:O	1:B:148:LEU:HD13	2.13	0.48
1:B:165:ALA:HA	1:B:168:PHE:CE1	2.48	0.48
1:A:357:LYS:HG2	1:A:361:GLN:HE21	1.77	0.48
1:A:473:PHE:CE2	1:A:638:PHE:HB3	2.49	0.48
1:B:56:ARG:HD3	1:B:87:TYR:CE2	2.48	0.48
1:B:166:ARG:HG3	1:B:167:LEU:CD1	2.43	0.48
1:A:354:ASP:HB3	1:A:355:ILE:HD12	1.96	0.48
1:A:511:ARG:O	1:A:515:ILE:HG13	2.14	0.48
1:A:102:PHE:CZ	1:A:138:LEU:HB2	2.48	0.48
1:A:131:LEU:HB2	1:A:174:ILE:HD11	1.95	0.48
1:A:523:ILE:CD1	1:A:584:ASN:HB2	2.44	0.48
1:B:515:ILE:O	1:B:519:ILE:HD13	2.13	0.48
1:B:468:VAL:O	1:B:472:ILE:HG13	2.13	0.48
1:B:513:ILE:HD12	1:B:513:ILE:C	2.34	0.48
1:B:681:THR:HA	1:B:684:LYS:HE3	1.96	0.48
1:A:104:LEU:C	1:A:104:LEU:HD23	2.34	0.48
1:A:104:LEU:HD23	1:A:104:LEU:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:452:THR:HA	1:A:455:ASN:HD22	1.79	0.48
1:A:109:PHE:HE1	1:A:127:ILE:HB	1.79	0.48
1:A:464:ILE:O	1:A:468:VAL:HG23	2.14	0.48
1:B:411:HIS:CE1	1:B:413:GLU:HB3	2.49	0.48
1:B:676:SER:CB	1:B:682:LEU:HD11	2.44	0.48
1:A:107:SER:O	1:A:111:GLN:HG3	2.14	0.47
1:B:153:PHE:CE1	1:B:175:LEU:HB3	2.49	0.47
1:B:293:GLU:HA	1:B:296:ARG:HD2	1.95	0.47
1:B:650:ILE:HD12	1:B:650:ILE:C	2.33	0.47
1:A:551:LEU:HB2	1:A:568:LEU:HD21	1.96	0.47
1:B:635:ILE:HD12	1:B:635:ILE:C	2.34	0.47
1:A:569:GLU:O	1:A:572:LYS:HB3	2.14	0.47
1:B:487:VAL:O	1:B:491:LEU:HG	2.15	0.47
1:B:509:ASN:ND2	1:B:644:ILE:HD11	2.28	0.47
1:A:436:THR:HG23	1:A:439:ASN:HD21	1.80	0.47
1:B:448:THR:O	1:B:452:THR:HG23	2.14	0.47
1:B:564:ALA:O	1:B:568:LEU:HG	2.15	0.47
1:B:402:SER:O	1:B:406:LEU:HG	2.15	0.47
1:B:582:LEU:H	1:B:582:LEU:HD12	1.79	0.47
1:A:565:ILE:O	1:A:569:GLU:HB2	2.15	0.47
1:A:682:LEU:H	1:A:682:LEU:CD2	2.25	0.47
1:B:60:VAL:HA	1:B:65:LEU:HD11	1.96	0.47
1:B:131:LEU:HB2	1:B:174:ILE:CD1	2.45	0.47
1:B:149:LEU:HD22	1:B:182:PHE:CE2	2.50	0.47
1:B:201:ASN:ND2	1:B:268:ARG:HE	2.13	0.47
1:B:314:ASN:HD21	1:B:352:ARG:HH22	1.63	0.47
1:A:567:ALA:O	1:A:571:ILE:HG13	2.15	0.47
1:B:48:ASP:C	1:B:50:THR:H	2.18	0.47
1:B:404:LEU:N	1:B:404:LEU:HD12	2.29	0.47
1:A:36:HIS:CE1	1:A:78:CYS:HB3	2.50	0.47
1:A:218:GLU:O	1:A:222:ILE:HG13	2.15	0.47
1:A:569:GLU:OE2	1:A:572:LYS:HD3	2.15	0.47
1:B:607:LEU:CD2	1:B:633:ILE:HG12	2.45	0.47
1:A:157:TYR:HB3	1:A:192:LEU:HD11	1.98	0.47
1:A:232:SER:OG	1:A:279:ALA:HB2	2.15	0.47
1:A:513:ILE:HD12	1:A:513:ILE:C	2.35	0.47
1:A:690:LEU:HD13	1:B:683:PHE:CD2	2.50	0.47
1:B:36:HIS:CE1	1:B:78:CYS:HB3	2.50	0.47
1:B:647:VAL:O	1:B:650:ILE:HG13	2.15	0.47
1:A:80:LEU:HD13	1:A:101:ILE:HG23	1.96	0.46
1:A:369:ASP:HB3	1:A:374:VAL:HG21	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:126:LEU:O	1:B:130:LEU:HG	2.15	0.46
1:B:416:GLU:HB3	1:B:467:GLN:HE22	1.80	0.46
1:B:594:LEU:HD13	1:B:594:LEU:C	2.35	0.46
1:A:112:LEU:HD21	1:A:167:LEU:HD13	1.97	0.46
1:A:386:PRO:O	1:A:390:ILE:HG13	2.14	0.46
1:A:592:PRO:O	1:A:595:THR:HG22	2.15	0.46
1:B:59:LEU:O	1:B:80:LEU:HD21	2.15	0.46
1:B:107:SER:O	1:B:111:GLN:HG3	2.14	0.46
1:B:630:ALA:O	1:B:634:GLN:HG3	2.15	0.46
1:A:462:LEU:HD13	1:A:558:LEU:O	2.15	0.46
1:B:109:PHE:HE1	1:B:127:ILE:HB	1.80	0.46
1:B:174:ILE:O	1:B:178:VAL:HG23	2.15	0.46
1:A:167:LEU:O	1:A:171:ILE:HG13	2.15	0.46
1:A:246:ALA:CB	1:A:258:VAL:HG21	2.46	0.46
1:A:243:ILE:HD11	1:A:262:LEU:HD12	1.97	0.46
1:A:539:GLN:C	1:A:543:VAL:HG12	2.36	0.46
1:A:678:VAL:HG23	1:A:679:ASN:N	2.30	0.46
1:B:104:LEU:HD23	1:B:104:LEU:C	2.36	0.46
1:B:582:LEU:HD12	1:B:582:LEU:N	2.30	0.46
1:A:10:LYS:HB2	1:A:38:GLU:OE2	2.15	0.46
1:A:153:PHE:HB3	1:A:192:LEU:HD23	1.95	0.46
1:A:267:LEU:O	1:A:271:GLU:HG3	2.16	0.46
1:B:102:PHE:HZ	1:B:138:LEU:HB2	1.80	0.46
1:B:345:ILE:HD13	1:B:363:LEU:HD21	1.97	0.46
1:B:357:LYS:O	1:B:361:GLN:HG3	2.15	0.46
1:A:404:LEU:N	1:A:404:LEU:HD12	2.30	0.46
1:B:476:LEU:HD12	1:B:476:LEU:N	2.29	0.46
1:B:526:SER:OG	1:B:572:LYS:HG2	2.15	0.46
1:B:687:ILE:HA	1:B:690:LEU:HD12	1.97	0.46
1:A:131:LEU:HB2	1:A:174:ILE:CD1	2.45	0.46
1:A:207:GLU:HG2	1:A:210:ASN:OD1	2.16	0.46
1:A:523:ILE:HD12	1:A:584:ASN:HB2	1.97	0.46
1:B:693:ILE:HD12	1:B:693:ILE:C	2.36	0.46
1:A:453:LEU:HD22	1:A:476:LEU:HD21	1.98	0.46
1:A:512:GLN:HA	1:A:639:ARG:O	2.16	0.46
1:B:166:ARG:NH1	1:B:167:LEU:HD11	2.31	0.46
1:A:288:LEU:HD12	1:A:299:ALA:HB1	1.97	0.45
1:A:532:GLN:HE22	1:A:535:MET:HB2	1.81	0.45
1:B:24:SER:HB3	1:B:27:GLU:HG3	1.98	0.45
1:A:125:TYR:CZ	1:A:129:LYS:HG3	2.51	0.45
1:A:168:PHE:CE2	1:A:215:CYS:HA	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:49:LEU:CA	1:B:52:LEU:HD13	2.46	0.45
1:B:292:ASN:O	1:B:296:ARG:HG3	2.17	0.45
1:A:83:ILE:HG21	1:A:93:TYR:OH	2.16	0.45
1:A:390:ILE:HG22	1:A:394:ILE:HD11	1.97	0.45
1:A:476:LEU:N	1:A:476:LEU:HD12	2.31	0.45
1:A:542:ILE:HG13	1:A:543:VAL:N	2.31	0.45
1:B:263:HIS:CG	1:B:302:LEU:HD22	2.51	0.45
1:A:145:SER:HB3	1:A:182:PHE:HZ	1.81	0.45
1:A:116:GLU:HA	1:A:120:HIS:NE2	2.32	0.45
1:A:629:ILE:O	1:A:633:ILE:HG22	2.16	0.45
1:A:165:ALA:HA	1:A:168:PHE:CE1	2.52	0.45
1:B:256:LEU:O	1:B:259:VAL:HG12	2.16	0.45
1:B:284:ILE:O	1:B:288:LEU:HD13	2.15	0.45
1:B:79:CYS:O	1:B:83:ILE:HD13	2.17	0.45
1:B:268:ARG:O	1:B:272:THR:HG22	2.16	0.45
1:B:586:CYS:HG	1:B:599:CYS:HG	1.63	0.45
1:B:635:ILE:HA	1:B:638:PHE:HD2	1.82	0.45
1:A:400:TYR:HB3	1:A:445:ILE:HG21	1.98	0.45
1:B:129:LYS:HD2	1:B:133:TYR:CE2	2.52	0.45
1:B:301:LYS:O	1:B:305:GLN:HG3	2.17	0.45
1:B:238:TYR:CE1	1:B:242:ILE:HD11	2.52	0.45
1:A:347:GLN:O	1:A:351:THR:HG23	2.17	0.44
1:A:411:HIS:CE1	1:A:414:VAL:HG23	2.52	0.44
1:A:519:ILE:O	1:A:522:TYR:HB3	2.17	0.44
1:A:558:LEU:HD13	1:A:632:VAL:HG13	2.00	0.44
1:A:149:LEU:HD22	1:A:182:PHE:CE2	2.52	0.44
1:A:191:ARG:HB3	1:A:195:ASN:HD21	1.82	0.44
1:A:594:LEU:C	1:A:594:LEU:HD13	2.37	0.44
1:B:61:SER:O	1:B:65:LEU:HD13	2.18	0.44
1:B:243:ILE:HG23	1:B:255:LEU:HD11	1.99	0.44
1:A:153:PHE:CE1	1:A:175:LEU:HB3	2.52	0.44
1:A:174:ILE:O	1:A:178:VAL:HG23	2.16	0.44
1:A:519:ILE:HD12	1:A:519:ILE:N	2.33	0.44
1:A:28:LEU:O	1:A:32:LEU:HG	2.18	0.44
1:A:345:ILE:HD12	1:A:345:ILE:N	2.32	0.44
1:B:345:ILE:HB	1:B:346:PRO:HD3	2.00	0.44
1:B:676:SER:CA	1:B:682:LEU:HD11	2.48	0.44
1:A:52:LEU:HD22	1:A:87:TYR:CE1	2.52	0.44
1:A:436:THR:OG1	1:A:439:ASN:ND2	2.51	0.44
1:B:387:VAL:HA	1:B:390:ILE:HD12	2.00	0.44
1:A:29:LEU:C	1:A:29:LEU:HD23	2.37	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:43:ASP:HB2	1:A:46:ASN:OD1	2.18	0.44
1:B:29:LEU:HD23	1:B:72:ILE:HD13	1.98	0.44
1:B:482:ASP:OD1	1:B:484:ASP:HB2	2.17	0.44
1:B:589:ASN:N	1:B:591:ILE:HD11	2.32	0.44
1:B:646:ASN:OD1	1:B:647:VAL:N	2.50	0.44
1:A:273:VAL:O	1:A:273:VAL:HG23	2.17	0.44
1:A:358:GLU:OE1	1:A:358:GLU:N	2.48	0.44
1:A:374:VAL:HG23	1:A:375:ARG:N	2.32	0.44
1:B:239:TYR:CE1	1:B:243:ILE:HD11	2.53	0.44
1:B:645:TYR:CD2	1:B:678:VAL:HG21	2.52	0.44
1:A:35:LEU:O	1:A:39:LEU:HG	2.18	0.44
1:A:646:ASN:OD1	1:A:647:VAL:N	2.51	0.44
1:A:683:PHE:CZ	1:B:690:LEU:HD22	2.52	0.44
1:B:551:LEU:C	1:B:551:LEU:HD23	2.37	0.44
1:A:506:PHE:HA	1:A:509:ASN:ND2	2.33	0.44
1:A:528:PHE:HB3	1:A:529:LEU:HD12	2.00	0.44
1:A:554:LEU:HD12	1:A:554:LEU:C	2.39	0.44
1:B:644:ILE:HG13	1:B:645:TYR:CD1	2.53	0.44
1:A:529:LEU:HD11	1:A:572:LYS:HE3	1.98	0.43
1:B:514:LYS:HE2	1:B:553:TRP:CZ2	2.53	0.43
1:A:139:LEU:HD23	1:A:139:LEU:C	2.38	0.43
1:B:201:ASN:OD1	1:B:203:ASN:ND2	2.51	0.43
1:B:446:ILE:N	1:B:446:ILE:HD12	2.33	0.43
1:A:48:ASP:O	1:A:49:LEU:HB3	2.18	0.43
1:A:224:CYS:O	1:A:276:LEU:HD11	2.17	0.43
1:A:227:TYR:O	1:A:231:MET:HG2	2.18	0.43
1:A:567:ALA:CB	1:A:629:ILE:HG12	2.48	0.43
1:B:522:TYR:CZ	1:B:568:LEU:HD22	2.53	0.43
1:B:544:MET:HE3	1:B:544:MET:O	2.19	0.43
1:B:672:LEU:N	1:B:672:LEU:HD12	2.33	0.43
1:A:582:LEU:N	1:A:582:LEU:HD12	2.34	0.43
1:B:35:LEU:O	1:B:39:LEU:HG	2.18	0.43
1:B:589:ASN:C	1:B:591:ILE:HD12	2.37	0.43
1:A:126:LEU:O	1:A:130:LEU:HG	2.18	0.43
1:B:341:TRP:CZ3	1:B:345:ILE:HD11	2.53	0.43
1:B:582:LEU:H	1:B:582:LEU:CD1	2.32	0.43
1:A:72:ILE:H	1:A:72:ILE:CD1	2.31	0.43
1:A:355:ILE:CG2	1:A:359:LEU:HG	2.49	0.43
1:B:104:LEU:HD23	1:B:104:LEU:O	2.17	0.43
1:B:499:LYS:O	1:B:503:THR:HG23	2.17	0.43
1:B:591:ILE:HD12	1:B:591:ILE:N	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:157:TYR:CD2	1:A:192:LEU:HG	2.54	0.43
1:B:33:LYS:O	1:B:37:GLU:HG3	2.19	0.43
1:B:442:ILE:O	1:B:446:ILE:HD13	2.19	0.43
1:B:593:PHE:O	1:B:596:PHE:HB3	2.19	0.43
1:A:82:ASP:O	1:A:85:ARG:HB3	2.18	0.43
1:A:99:THR:O	1:A:103:LYS:HB2	2.18	0.43
1:A:116:GLU:HA	1:A:120:HIS:CD2	2.54	0.43
1:A:263:HIS:CG	1:A:302:LEU:HD22	2.54	0.43
1:A:482:ASP:CG	1:A:483:ASN:N	2.70	0.43
1:A:567:ALA:HB1	1:A:629:ILE:HG23	2.00	0.43
1:B:249:ASP:C	1:B:251:ASN:H	2.22	0.43
1:B:355:ILE:CG2	1:B:359:LEU:HG	2.47	0.43
1:B:80:LEU:O	1:B:84:LEU:HG	2.19	0.42
1:B:139:LEU:HD23	1:B:139:LEU:C	2.38	0.42
1:B:273:VAL:HG23	1:B:273:VAL:O	2.18	0.42
1:B:686:GLN:OE1	1:B:686:GLN:N	2.47	0.42
1:A:179:ILE:HG13	1:A:185:VAL:HG21	2.01	0.42
1:A:667:LEU:O	1:A:671:ILE:HG13	2.19	0.42
1:B:320:SER:O	1:B:324:LYS:HG3	2.19	0.42
1:A:48:ASP:C	1:A:50:THR:H	2.22	0.42
1:A:508:PHE:O	1:A:512:GLN:HG3	2.20	0.42
1:A:522:TYR:OH	1:A:568:LEU:HB2	2.18	0.42
1:A:671:ILE:HG22	1:A:675:ILE:HD11	2.02	0.42
1:B:292:ASN:HB3	1:B:295:PHE:CD2	2.51	0.42
1:A:383:ASN:OD1	1:A:424:LYS:HE2	2.19	0.42
1:A:480:GLU:HB2	1:A:481:PRO:CA	2.46	0.42
1:B:52:LEU:HD12	1:B:52:LEU:N	2.34	0.42
1:A:650:ILE:HD13	1:B:650:ILE:HB	2.01	0.42
1:B:249:ASP:O	1:B:250:ASP:HB3	2.20	0.42
1:B:554:LEU:HD12	1:B:554:LEU:C	2.39	0.42
1:A:307:LEU:HD21	1:A:315:PHE:HD2	1.84	0.42
1:A:539:GLN:HB3	1:A:542:ILE:HG13	2.01	0.42
1:B:652:VAL:HG12	1:B:672:LEU:HD11	2.02	0.42
1:A:497:PHE:CD2	1:A:501:ALA:HB1	2.55	0.42
1:A:525:PHE:O	1:A:528:PHE:HB2	2.19	0.42
1:B:49:LEU:HD23	1:B:49:LEU:C	2.40	0.42
1:B:481:PRO:HG2	1:B:482:ASP:N	2.33	0.42
1:A:112:LEU:HD21	1:A:167:LEU:CD1	2.49	0.42
1:A:292:ASN:HB3	1:A:295:PHE:CD2	2.54	0.42
1:A:462:LEU:O	1:A:466:GLU:HG3	2.19	0.42
1:A:499:LYS:O	1:A:503:THR:HG23	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:678:VAL:O	1:A:679:ASN:HB2	2.19	0.42
1:B:376:ARG:NH1	1:B:376:ARG:HB3	2.35	0.42
1:A:345:ILE:HB	1:A:346:PRO:HD3	2.02	0.42
1:A:568:LEU:HD12	1:A:568:LEU:C	2.40	0.42
1:A:671:ILE:O	1:A:675:ILE:HG13	2.20	0.42
1:A:678:VAL:O	1:A:679:ASN:ND2	2.52	0.42
1:B:154:HIS:CD2	1:B:192:LEU:HD11	2.54	0.42
1:B:509:ASN:O	1:B:512:GLN:HB3	2.19	0.42
1:B:511:ARG:HG2	1:B:515:ILE:HG13	2.00	0.42
1:A:191:ARG:HB3	1:A:195:ASN:ND2	2.34	0.42
1:A:376:ARG:HG2	1:A:376:ARG:HH11	1.85	0.41
1:A:671:ILE:HG22	1:A:675:ILE:CD1	2.49	0.41
1:B:48:ASP:O	1:B:49:LEU:HB3	2.20	0.41
1:B:224:CYS:O	1:B:276:LEU:HD11	2.20	0.41
1:B:49:LEU:HA	1:B:52:LEU:HD13	2.01	0.41
1:B:125:TYR:CZ	1:B:129:LYS:HG3	2.55	0.41
1:B:164:PRO:CG	1:B:167:LEU:HD13	2.46	0.41
1:B:191:ARG:HB2	1:B:195:ASN:ND2	2.35	0.41
1:B:230:ARG:HG3	1:B:230:ARG:HH11	1.85	0.41
1:A:3:LYS:HB3	1:A:50:THR:CG2	2.48	0.41
1:A:411:HIS:ND1	1:A:414:VAL:HG23	2.36	0.41
1:A:529:LEU:CD1	1:A:572:LYS:HE3	2.50	0.41
1:A:591:ILE:H	1:A:646:ASN:HD21	1.67	0.41
1:B:185:VAL:HG13	1:B:186:PRO:HD2	2.01	0.41
1:B:236:THR:HG23	1:B:283:PHE:CE2	2.56	0.41
1:B:270:TRP:HB2	1:B:277:ILE:HG13	2.01	0.41
1:B:523:ILE:HD13	1:B:580:PHE:CA	2.43	0.41
1:A:394:ILE:HD12	1:A:394:ILE:C	2.41	0.41
1:A:458:TYR:CE2	1:A:500:LYS:HB3	2.55	0.41
1:A:649:ASN:O	1:A:653:LEU:HB2	2.19	0.41
1:B:145:SER:HB3	1:B:182:PHE:CZ	2.54	0.41
1:B:157:TYR:O	1:B:159:PRO:HD3	2.21	0.41
1:B:523:ILE:CD1	1:B:580:PHE:HA	2.40	0.41
1:A:92:PRO:HG2	1:A:93:TYR:H	1.86	0.41
1:A:154:HIS:CD2	1:A:192:LEU:HD22	2.44	0.41
1:B:65:LEU:O	1:B:73:ARG:HG2	2.21	0.41
1:B:588:THR:O	1:B:589:ASN:HB2	2.20	0.41
1:B:390:ILE:CG2	1:B:394:ILE:HD11	2.51	0.41
1:A:49:LEU:HD23	1:A:49:LEU:C	2.41	0.41
1:A:144:SER:O	1:A:148:LEU:HG	2.21	0.41
1:A:161:LYS:HB3	1:A:163:PHE:CE1	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:335:PRO:HA	1:A:338:ARG:CD	2.50	0.41
1:A:353:GLU:HG2	1:A:353:GLU:O	2.19	0.41
1:A:579:ILE:HG23	1:A:603:LEU:HD11	2.01	0.41
1:A:686:GLN:CD	1:A:686:GLN:H	2.24	0.41
1:B:522:TYR:OH	1:B:568:LEU:O	2.37	0.41
1:B:671:ILE:O	1:B:675:ILE:HG13	2.21	0.41
1:A:46:ASN:OD1	1:A:46:ASN:O	2.39	0.41
1:A:61:SER:O	1:A:65:LEU:HD13	2.21	0.41
1:B:38:GLU:O	1:B:42:LEU:HG	2.21	0.41
1:B:348:ILE:O	1:B:351:THR:HB	2.21	0.41
1:A:316:VAL:HG12	1:A:323:PHE:CD1	2.55	0.40
1:A:554:LEU:HD12	1:A:555:ALA:N	2.36	0.40
1:B:27:GLU:O	1:B:31:ARG:HG3	2.20	0.40
1:B:166:ARG:C	1:B:167:LEU:HD12	2.42	0.40
1:B:502:PHE:HB3	1:B:506:PHE:CE2	2.56	0.40
1:A:12:ASN:HA	1:A:55:TYR:OH	2.21	0.40
1:A:347:GLN:H	1:A:347:GLN:CD	2.24	0.40
1:A:647:VAL:HG12	1:B:654:LEU:HD13	2.04	0.40
1:B:416:GLU:CB	1:B:467:GLN:HE22	2.34	0.40
1:A:145:SER:HB3	1:A:182:PHE:CZ	2.56	0.40
1:A:244:HIS:CE1	1:A:248:ASN:ND2	2.90	0.40
1:A:344:SER:O	1:A:348:ILE:HG13	2.21	0.40
1:A:412:LYS:HB3	1:A:412:LYS:HZ2	1.86	0.40
1:B:272:THR:HG23	1:B:273:VAL:N	2.36	0.40
1:B:551:LEU:HD23	1:B:551:LEU:O	2.21	0.40
1:A:385:VAL:CG2	1:A:386:PRO:HD2	2.51	0.40
1:A:385:VAL:HG23	1:A:386:PRO:HD2	2.04	0.40
1:B:473:PHE:CE2	1:B:638:PHE:HB3	2.56	0.40
1:B:584:ASN:HA	1:B:587:VAL:CG1	2.50	0.40
1:A:560:ASP:CG	1:A:563:LYS:HB2	2.42	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:556:SER:CB	1:B:556:SER:CB[7_555]	2.12	0.08

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	673/703 (96%)	601 (89%)	64 (10%)	8 (1%)	13 49
1	B	650/703 (92%)	582 (90%)	63 (10%)	5 (1%)	19 60
All	All	1323/1406 (94%)	1183 (89%)	127 (10%)	13 (1%)	15 54

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	536	SER
1	A	538	SER
1	A	679	ASN
1	B	682	LEU
1	A	655	ASN
1	A	460	ASN
1	A	660	SER
1	A	684	LYS
1	B	481	PRO
1	B	589	ASN
1	B	587	VAL
1	B	202	PRO
1	A	481	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	629/650 (97%)	627 (100%)	2 (0%)	92 94

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	611/650 (94%)	608 (100%)	3 (0%)	88 93
All	All	1240/1300 (95%)	1235 (100%)	5 (0%)	91 94

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	469	ASP
1	A	547	TYR
1	B	120	HIS
1	B	469	ASP
1	B	547	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	ASN
1	A	123	GLN
1	A	154	HIS
1	A	195	ASN
1	A	201	ASN
1	A	244	HIS
1	A	248	ASN
1	A	252	ASN
1	A	347	GLN
1	A	361	GLN
1	A	393	ASN
1	A	428	ASN
1	A	439	ASN
1	A	455	ASN
1	A	509	ASN
1	A	549	GLN
1	A	575	ASN
1	A	598	ASN
1	A	655	ASN
1	B	36	HIS
1	B	117	ASN
1	B	123	GLN
1	B	154	HIS
1	B	195	ASN
1	B	244	HIS
1	B	460	ASN

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Mol	Chain	Res	Type
1	B	467	GLN
1	B	509	ASN
1	B	589	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers

Unable to reproduce the depositors R factor - this section is therefore empty.