Full wwPDB X-ray Structure Validation Report ⓘ

Nov 13, 2023 – 01:23 PM JST

PDB ID	:	5XAM
Title	:	Crystal structure of SecDF in I form at 4 A resolution
Authors	:	Tsukazaki, T.; Tanaka, Y.; Furukwa, A.
Deposited on	:	2017-03-14
Resolution	:	4.00 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
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:

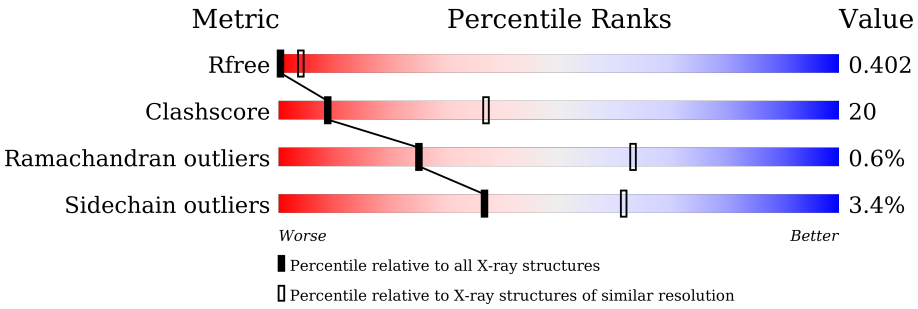
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 4.00 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}	130704	1087 (4.30-3.70)
Clashscore	141614	1148 (4.30-3.70)
Ramachandran outliers	138981	1108 (4.30-3.70)
Sidechain outliers	138945	1099 (4.30-3.70)

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	750	62% 33%
1	B	750	54% 36% 9%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 9852 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 Protein translocase subunit SecD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	727	Total	C	N	O	S	0	0	0
			5000	3215	830	947	8			
1	B	684	Total	C	N	O	S	0	0	0
			4852	3140	801	900	11			

There are 18 discrepancies between the modelled and reference sequences:

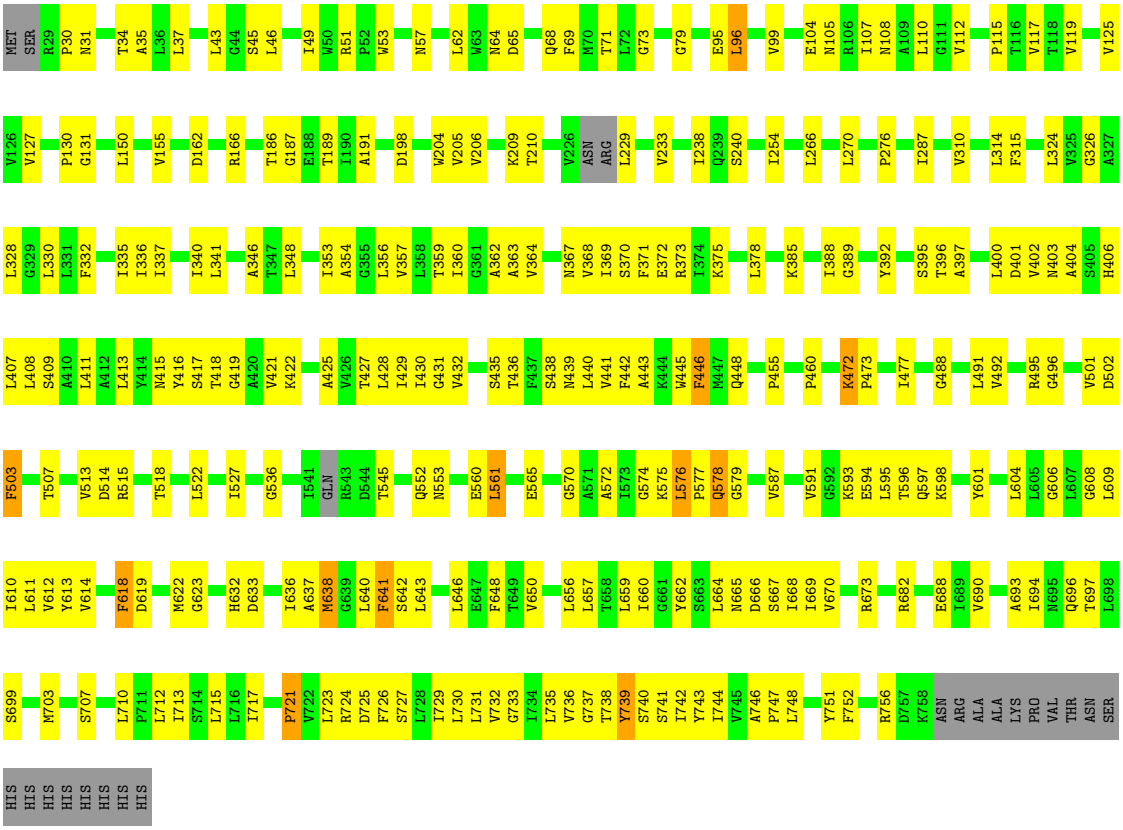
Chain	Residue	Modelled	Actual	Comment	Reference
A	27	MET	-	expression tag	UNP Q9RTE3
A	769	HIS	-	expression tag	UNP Q9RTE3
A	770	HIS	-	expression tag	UNP Q9RTE3
A	771	HIS	-	expression tag	UNP Q9RTE3
A	772	HIS	-	expression tag	UNP Q9RTE3
A	773	HIS	-	expression tag	UNP Q9RTE3
A	774	HIS	-	expression tag	UNP Q9RTE3
A	775	HIS	-	expression tag	UNP Q9RTE3
A	776	HIS	-	expression tag	UNP Q9RTE3
B	27	MET	-	expression tag	UNP Q9RTE3
B	769	HIS	-	expression tag	UNP Q9RTE3
B	770	HIS	-	expression tag	UNP Q9RTE3
B	771	HIS	-	expression tag	UNP Q9RTE3
B	772	HIS	-	expression tag	UNP Q9RTE3
B	773	HIS	-	expression tag	UNP Q9RTE3
B	774	HIS	-	expression tag	UNP Q9RTE3
B	775	HIS	-	expression tag	UNP Q9RTE3
B	776	HIS	-	expression tag	UNP Q9RTE3

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.

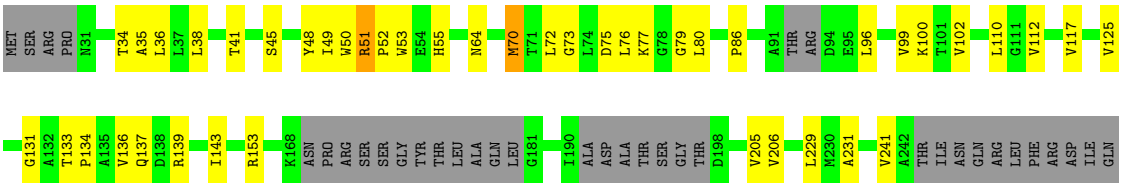
• Molecule 1: Protein translocase subunit SecD

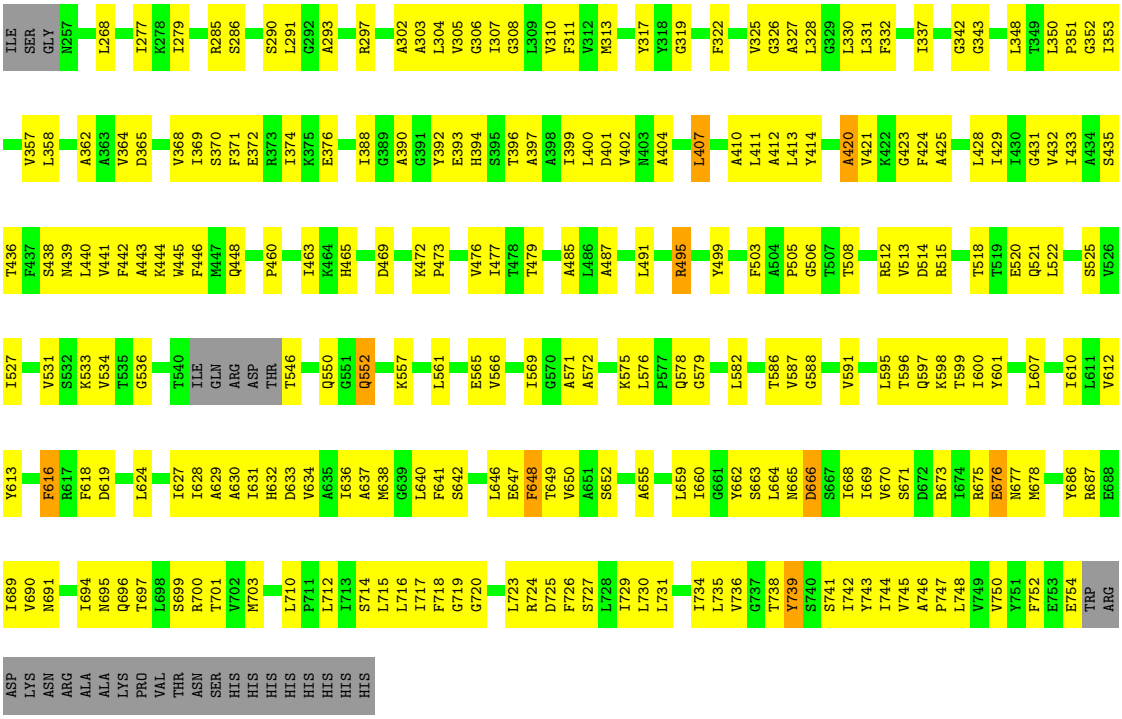
Chain A:



• Molecule 1: Protein translocase subunit SecD

Chain B:




ILE SER GLY N257 L268 I277 K278 I279 R285 S286 S290 L291 G292 A293 R297 A302 A303 L304 V305 G306 I307 G308 L309 V310 F311 V312 M313 Y317 Y318 G319 F322 V325 G326 A327 L328 G329 L330 L331 F332 I337 G342 G343 L348 T349 L350 P351 G352 I353
V357 L358 A362 A363 V364 D365 V368 I369 S370 F371 E372 R373 I374 K375 E376 I388 G389 A390 G391 Y392 E393 H394 S395 T396 A397 A398 I399 L400 D401 V402 N403 A404 L407 A410 L411 A412 L413 Y414 A420 V421 K422 G423 F424 A425 L428 I429 I430 G431 V432 I433 A434 S435
T436 F437 S438 M439 L440 V441 F442 A443 K444 W445 F446 M447 Q448 P460 I463 K464 H465 D469 K472 P473 V476 I477 T478 T479 A485 L486 A487 L491 R495 Y499 F503 A504 P505 G506 T507 T508 R512 V513 D514 R515 T518 T519 E520 Q521 L522 S525 V526
I527 V531 S532 K533 V534 T535 G536 T540 ILE GLN ARG ASP THR T546 Q550 G551 Q552 K557 L561 E565 V566 I569 G570 A571 A572 K575 L576 P577 Q578 G579 L582 T586 V587 G588 V591 L595 T596 Q597 K598 T599 I600 Y601 L607 I610 L611 V612
Y613 F616 R617 F618 D619 L624 I627 I628 A629 A630 I631 H632 D633 V634 A635 I636 A637 M638 G639 L640 F641 S642 L646 E647 F648 T649 V650 A651 S652 A655 L659 I660 G661 Y662 S663 L664 N665 D666 S667 I668 I669 V670 S671 D672 R673 I674 R675 E676 N677 M678 Y686 R687 E688
I689 V690 N691 I694 N695 Q696 T697 L698 S699 R700 T701 V702 M703 L710 P711 L712 I713 S714 L715 L716 I717 F718 G719 G720 L723 R724 D725 F726 S727 L728 I729 L730 L731 I734 L735 V736 G737 T738 Y739 S740 S741 I742 Y743 I744 V745 A746 P747 L748 V749 V750 Y751 F752 E753 E754 TRP ARG
ASP LYS ASN ARG ALA ALA LYS PRO VAL THR ASN SER HIS HIS HIS HIS HIS HIS HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	93.32Å 62.26Å 181.71Å 90.00° 101.71° 90.00°	Depositor
Resolution (Å)	47.98 – 4.00 47.99 – 3.92	Depositor EDS
% Data completeness (in resolution range)	96.6 (47.98-4.00) 93.3 (47.99-3.92)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.95 (at 3.88Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, R_{free}	0.333 , 0.402 0.333 , 0.402	Depositor DCC
R_{free} test set	1762 reflections (10.02%)	wwPDB-VP
Wilson B-factor (Å^2)	150.3	Xtriage
Anisotropy	0.356	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.19 , 176.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.39$, $< L^2 > = 0.22$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.79	EDS
Total number of atoms	9852	wwPDB-VP
Average B, all atoms (Å^2)	242.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.44% 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	0.27	1/5071 (0.0%)	0.48	1/6964 (0.0%)
1	B	0.26	0/4926	0.48	0/6735
All	All	0.27	1/9997 (0.0%)	0.48	1/13699 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	51	ARG	C-N	7.32	1.48	1.34

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	576	LEU	CA-CB-CG	5.41	127.75	115.30

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	5000	0	4921	195	0
1	B	4852	0	4894	208	0
All	All	9852	0	9815	403	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 20.

All (403) 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:30:PRO:HG2	1:A:448:GLN:HG2	1.48	0.92
1:B:690:VAL:HG21	1:B:750:VAL:HG11	1.60	0.83
1:B:561:LEU:HB2	1:B:565:GLU:HB3	1.61	0.82
1:A:34:THR:HA	1:A:37:LEU:HB3	1.60	0.82
1:A:404:ALA:HA	1:A:407:LEU:HB2	1.62	0.80
1:B:438:SER:HA	1:B:442:PHE:HB3	1.62	0.80
1:B:531:VAL:HB	1:B:534:VAL:HG12	1.63	0.79
1:A:368:VAL:O	1:A:372:GLU:N	2.13	0.78
1:B:619:ASP:HB3	1:B:675:ARG:HH22	1.48	0.76
1:A:591:VAL:HA	1:A:594:GLU:HB2	1.68	0.75
1:B:618:PHE:HZ	1:B:668:ILE:HA	1.52	0.74
1:A:641:PHE:HE2	1:A:648:PHE:HB3	1.52	0.74
1:B:35:ALA:HB2	1:B:445:TRP:CH2	2.24	0.73
1:A:561:LEU:HB2	1:A:565:GLU:HG3	1.71	0.73
1:B:531:VAL:HG12	1:B:533:LYS:H	1.52	0.73
1:B:137:GLN:NE2	1:B:286:SER:OG	2.22	0.72
1:B:741:SER:HA	1:B:745:VAL:HB	1.73	0.71
1:B:368:VAL:O	1:B:372:GLU:N	2.21	0.71
1:B:100:LYS:HG2	1:B:117:VAL:HG21	1.72	0.71
1:B:70:MET:HG3	1:B:342:GLY:HA3	1.72	0.70
1:A:205:VAL:HG12	1:A:206:VAL:H	1.56	0.70
1:A:641:PHE:CE2	1:A:648:PHE:HB3	2.26	0.70
1:B:399:ILE:HD11	1:B:439:ASN:HB3	1.71	0.70
1:A:662:TYR:O	1:A:665:ASN:ND2	2.24	0.69
1:B:472:LYS:HG3	1:B:473:PRO:HD3	1.74	0.69
1:B:712:LEU:HD12	1:B:731:LEU:HB3	1.74	0.69
1:A:673:ARG:NH2	1:A:693:ALA:O	2.26	0.68
1:A:513:VAL:HB	1:A:579:GLY:HA3	1.76	0.68
1:B:719:GLY:HA2	1:B:723:LEU:HD22	1.76	0.68
1:A:396:THR:O	1:A:400:LEU:N	2.16	0.68
1:A:618:PHE:HE1	1:A:668:ILE:HG12	1.59	0.67
1:A:491:LEU:HA	1:A:495:ARG:HB3	1.76	0.67
1:B:401:ASP:OD1	1:B:613:TYR:OH	2.13	0.67
1:B:368:VAL:HA	1:B:371:PHE:HB3	1.75	0.67
1:A:402:VAL:O	1:A:406:HIS:ND1	2.29	0.66
1:B:134:PRO:HA	1:B:137:GLN:HB3	1.78	0.65
1:A:611:LEU:HA	1:A:614:VAL:HG12	1.79	0.65
1:B:720:GLY:H	1:B:723:LEU:HD13	1.62	0.64
1:B:231:ALA:HA	1:B:241:VAL:HG21	1.78	0.64
1:B:476:VAL:HA	1:B:479:THR:HG22	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:744:ILE:HG23	1:A:748:LEU:HD22	1.80	0.64
1:A:604:LEU:O	1:A:608:GLY:N	2.29	0.63
1:A:561:LEU:HD13	1:A:565:GLU:HB2	1.80	0.63
1:B:96:LEU:HB2	1:B:125:VAL:HG21	1.81	0.62
1:B:319:GLY:HA2	1:B:460:PRO:HD2	1.81	0.62
1:B:628:ILE:O	1:B:632:HIS:N	2.28	0.62
1:B:374:ILE:HD12	1:B:388:ILE:HA	1.82	0.62
1:B:51:ARG:HH21	1:B:343:GLY:HA3	1.64	0.62
1:A:57:ASN:HD22	1:A:64:ASN:HB2	1.64	0.61
1:A:742:ILE:HG23	1:A:743:TYR:HD1	1.65	0.61
1:B:86:PRO:HB3	1:B:277:ILE:HG21	1.82	0.61
1:A:30:PRO:HG2	1:A:448:GLN:CG	2.27	0.61
1:B:630:ALA:HB1	1:B:660:ILE:HD12	1.82	0.61
1:B:428:LEU:O	1:B:432:VAL:HG12	2.00	0.61
1:A:618:PHE:CE1	1:A:668:ILE:HG12	2.35	0.60
1:A:403:ASN:O	1:A:407:LEU:N	2.35	0.60
1:B:527:ILE:HD12	1:B:536:GLY:HA2	1.83	0.60
1:A:666:ASP:OD1	1:A:741:SER:OG	2.14	0.59
1:A:735:LEU:O	1:A:739:TYR:HB3	2.01	0.59
1:A:664:LEU:O	1:A:668:ILE:HG13	2.02	0.59
1:A:413:LEU:HD23	1:A:657:LEU:HD11	1.85	0.59
1:B:513:VAL:HG11	1:B:576:LEU:HD23	1.83	0.59
1:A:45:SER:OG	1:A:335:ILE:O	2.21	0.59
1:B:691:ASN:O	1:B:695:ASN:ND2	2.36	0.59
1:B:506:GLY:N	1:B:587:VAL:HG11	2.18	0.59
1:A:513:VAL:HG21	1:A:576:LEU:HG	1.83	0.58
1:B:435:SER:OG	1:B:439:ASN:ND2	2.36	0.58
1:A:407:LEU:O	1:A:411:LEU:N	2.36	0.58
1:B:633:ASP:OD2	1:B:663:SER:OG	2.22	0.58
1:A:186:THR:OG1	1:A:189:THR:OG1	2.17	0.58
1:B:374:ILE:HG21	1:B:388:ILE:HG22	1.86	0.58
1:A:673:ARG:HH21	1:A:697:THR:HG23	1.69	0.57
1:B:325:VAL:HG22	1:B:446:PHE:HE2	1.70	0.57
1:B:72:LEU:HB2	1:B:77:LYS:HD3	1.86	0.57
1:B:404:ALA:HA	1:B:407:LEU:HB2	1.86	0.57
1:B:724:ARG:HA	1:B:727:SER:HB3	1.85	0.57
1:A:369:ILE:O	1:A:373:ARG:N	2.34	0.57
1:A:360:ILE:O	1:A:364:VAL:HG22	2.04	0.57
1:A:367:ASN:HA	1:A:439:ASN:OD1	2.03	0.56
1:A:610:ILE:O	1:A:614:VAL:N	2.26	0.56
1:B:508:THR:HG22	1:B:557:LYS:HG2	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:514:ASP:HB3	1:B:578:GLN:HB2	1.88	0.56
1:A:418:THR:HG22	1:A:419:GLY:H	1.70	0.56
1:B:546:THR:HA	1:B:720:GLY:HA2	1.86	0.56
1:B:719:GLY:O	1:B:724:ARG:NH1	2.38	0.56
1:A:186:THR:HG1	1:A:189:THR:HG1	1.51	0.56
1:B:440:LEU:HG	1:B:441:VAL:HG13	1.87	0.56
1:B:505:PRO:HA	1:B:587:VAL:HG21	1.86	0.56
1:B:701:THR:HG21	1:B:742:ILE:HD11	1.88	0.56
1:B:424:PHE:O	1:B:428:LEU:HG	2.05	0.55
1:B:566:VAL:O	1:B:569:ILE:HG13	2.06	0.55
1:A:667:SER:HA	1:A:670:VAL:HG12	1.88	0.55
1:A:477:ILE:HG13	1:A:743:TYR:CD2	2.41	0.55
1:B:473:PRO:HB2	1:B:477:ILE:HG13	1.88	0.55
1:A:96:LEU:HB2	1:A:125:VAL:HG21	1.89	0.55
1:B:421:VAL:HG21	1:B:650:VAL:HB	1.89	0.55
1:A:736:VAL:HG22	1:A:740:SER:HB3	1.89	0.55
1:B:736:VAL:HA	1:B:739:TYR:CD1	2.42	0.55
1:B:76:LEU:HD11	1:B:350:LEU:HG	1.89	0.54
1:B:669:ILE:HG21	1:B:700:ARG:HB3	1.89	0.54
1:A:356:LEU:O	1:A:359:THR:OG1	2.21	0.54
1:A:371:PHE:O	1:A:375:LYS:NZ	2.40	0.54
1:A:408:LEU:HD11	1:A:609:LEU:HB3	1.90	0.54
1:A:340:ILE:HD13	1:A:430:ILE:HG13	1.89	0.54
1:A:673:ARG:NH2	1:A:697:THR:HG23	2.22	0.54
1:B:308:GLY:HA2	1:B:311:PHE:CE2	2.42	0.54
1:B:390:ALA:HA	1:B:393:GLU:HB2	1.89	0.54
1:B:677:ASN:HB3	1:B:689:ILE:HD11	1.89	0.54
1:B:694:ILE:CG2	1:B:742:ILE:HG23	2.38	0.54
1:A:31:ASN:OD1	1:A:31:ASN:N	2.38	0.54
1:A:370:SER:HG	1:A:392:TYR:HE1	1.54	0.54
1:A:609:LEU:O	1:A:613:TYR:N	2.41	0.54
1:B:715:LEU:HD23	1:B:727:SER:HB2	1.90	0.54
1:A:738:THR:O	1:A:742:ILE:HG22	2.08	0.53
1:A:57:ASN:N	1:A:57:ASN:OD1	2.41	0.53
1:B:322:PHE:HB3	1:B:371:PHE:CE2	2.43	0.53
1:A:593:LYS:HA	1:A:596:THR:HG22	1.89	0.53
1:B:627:ILE:O	1:B:631:ILE:HG12	2.09	0.53
1:A:477:ILE:HG21	1:A:743:TYR:HB3	1.91	0.53
1:A:503:PHE:HE1	1:A:650:VAL:HG22	1.74	0.53
1:B:720:GLY:N	1:B:723:LEU:HD13	2.23	0.53
1:A:666:ASP:HA	1:A:669:ILE:HB	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:51:ARG:HH11	1:B:53:TRP:HE1	1.56	0.53
1:B:413:LEU:HB3	1:B:425:ALA:HB2	1.90	0.53
1:A:513:VAL:HG13	1:A:514:ASP:H	1.73	0.53
1:A:577:PRO:O	1:A:578:GLN:HB2	2.09	0.52
1:A:614:VAL:O	1:A:618:PHE:HB2	2.09	0.52
1:A:491:LEU:O	1:A:642:SER:OG	2.23	0.52
1:B:697:THR:HA	1:B:700:ARG:HG3	1.90	0.52
1:A:502:ASP:HB3	1:A:595:LEU:HD13	1.91	0.52
1:B:357:VAL:HG11	1:B:715:LEU:HD22	1.90	0.52
1:B:513:VAL:HA	1:B:579:GLY:HA2	1.90	0.52
1:B:607:LEU:HA	1:B:610:ILE:HG12	1.89	0.52
1:B:624:LEU:HA	1:B:627:ILE:HB	1.89	0.52
1:A:477:ILE:HG13	1:A:743:TYR:HD2	1.74	0.52
1:A:598:LYS:HA	1:A:601:TYR:HD2	1.74	0.52
1:B:396:THR:HA	1:B:399:ILE:HG22	1.90	0.52
1:A:341:LEU:HD11	1:A:427:THR:HG22	1.91	0.52
1:B:86:PRO:HA	1:B:279:ILE:HG22	1.91	0.52
1:B:641:PHE:CD2	1:B:729:ILE:HD11	2.45	0.52
1:B:368:VAL:HG11	1:B:703:MET:HB3	1.92	0.52
1:A:609:LEU:HA	1:A:612:VAL:HB	1.92	0.52
1:A:637:ALA:HB1	1:A:656:LEU:HD22	1.91	0.52
1:A:507:THR:HG23	1:A:560:GLU:HA	1.92	0.52
1:A:513:VAL:HG11	1:A:576:LEU:HG	1.91	0.51
1:A:95:GLU:O	1:A:99:VAL:HG23	2.10	0.51
1:B:399:ILE:CD1	1:B:439:ASN:HB3	2.38	0.51
1:A:406:HIS:HE1	1:A:665:ASN:HB2	1.76	0.51
1:B:362:ALA:HA	1:B:365:ASP:HB3	1.93	0.51
1:B:400:LEU:O	1:B:404:ALA:N	2.41	0.51
1:B:512:ARG:NH2	1:B:550:GLN:HG2	2.26	0.51
1:A:117:VAL:HG13	1:A:127:VAL:HG22	1.92	0.51
1:B:463:ILE:HD11	1:B:465:HIS:HD2	1.75	0.51
1:B:557:LYS:NZ	1:B:647:GLU:OE1	2.43	0.51
1:A:359:THR:O	1:A:363:ALA:N	2.41	0.51
1:A:513:VAL:HG13	1:A:514:ASP:N	2.26	0.51
1:B:306:GLY:HA2	1:B:714:SER:HB3	1.93	0.51
1:B:670:VAL:HG11	1:B:746:ALA:HB2	1.92	0.50
1:B:304:LEU:O	1:B:308:GLY:N	2.44	0.50
1:B:655:ALA:HB2	1:B:726:PHE:HB3	1.93	0.50
1:B:739:TYR:O	1:B:743:TYR:HB2	2.12	0.50
1:B:515:ARG:HA	1:B:552:GLN:HG3	1.93	0.50
1:B:96:LEU:HA	1:B:99:VAL:HG12	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:364:VAL:O	1:B:368:VAL:HG23	2.11	0.50
1:B:673:ARG:HA	1:B:676:GLU:OE2	2.11	0.50
1:A:353:ILE:HD12	1:A:354:ALA:N	2.25	0.50
1:B:36:LEU:H	1:B:36:LEU:HD12	1.76	0.50
1:B:319:GLY:HA3	1:B:322:PHE:HB2	1.94	0.50
1:B:619:ASP:HB3	1:B:675:ARG:NH2	2.23	0.50
1:A:659:LEU:HD11	1:A:733:GLY:HA3	1.92	0.50
1:A:690:VAL:O	1:A:694:ILE:HG12	2.12	0.50
1:A:742:ILE:HG23	1:A:743:TYR:CD1	2.46	0.50
1:B:641:PHE:HZ	1:B:648:PHE:HA	1.76	0.50
1:A:746:ALA:HB3	1:A:747:PRO:HD3	1.93	0.50
1:A:638:MET:O	1:A:642:SER:N	2.45	0.50
1:A:752:PHE:O	1:A:756:ARG:N	2.36	0.50
1:B:330:LEU:HD12	1:B:331:LEU:N	2.27	0.50
1:B:438:SER:O	1:B:443:ALA:N	2.43	0.50
1:A:673:ARG:NH1	1:A:696:GLN:HB3	2.26	0.49
1:B:75:ASP:OD1	1:B:75:ASP:N	2.41	0.49
1:B:499:TYR:CB	1:B:648:PHE:HB2	2.42	0.49
1:B:597:GLN:HG2	1:B:601:TYR:CD2	2.47	0.49
1:A:736:VAL:HA	1:A:739:TYR:HD2	1.77	0.49
1:B:45:SER:O	1:B:49:ILE:HG22	2.12	0.49
1:B:469:ASP:HB3	1:B:472:LYS:HE3	1.94	0.49
1:B:518:THR:HG22	1:B:520:GLU:H	1.78	0.49
1:A:712:LEU:HD21	1:A:727:SER:O	2.13	0.49
1:B:307:ILE:HD11	1:B:330:LEU:HD13	1.93	0.49
1:B:410:ALA:HB1	1:B:429:ILE:HG12	1.95	0.49
1:B:302:ALA:HB1	1:B:715:LEU:HA	1.95	0.49
1:B:370:SER:O	1:B:374:ILE:HG12	2.12	0.49
1:A:595:LEU:HD12	1:A:596:THR:N	2.28	0.49
1:A:640:LEU:O	1:A:643:LEU:HG	2.13	0.48
1:A:732:VAL:O	1:A:736:VAL:HG12	2.13	0.48
1:A:35:ALA:HB2	1:A:445:TRP:CZ2	2.49	0.48
1:A:440:LEU:HD23	1:A:441:VAL:HG23	1.95	0.48
1:A:729:ILE:HD12	1:A:730:LEU:N	2.28	0.48
1:B:358:LEU:HD13	1:B:730:LEU:HD21	1.95	0.48
1:A:502:ASP:HB3	1:A:595:LEU:CD1	2.44	0.48
1:B:664:LEU:O	1:B:668:ILE:HG13	2.14	0.48
1:A:359:THR:HA	1:A:362:ALA:HB3	1.93	0.48
1:A:359:THR:HG23	1:A:428:LEU:HD23	1.96	0.48
1:B:51:ARG:O	1:B:55:HIS:NE2	2.47	0.48
1:A:45:SER:O	1:A:49:ILE:HG13	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:308:GLY:HA2	1:B:311:PHE:CZ	2.49	0.48
1:B:322:PHE:HB3	1:B:371:PHE:HE2	1.79	0.48
1:A:439:ASN:O	1:A:443:ALA:HB3	2.14	0.48
1:A:502:ASP:C	1:A:595:LEU:HD11	2.34	0.48
1:A:633:ASP:OD2	1:A:737:GLY:HA2	2.14	0.48
1:B:34:THR:O	1:B:38:LEU:N	2.39	0.48
1:B:50:TRP:O	1:B:52:PRO:HD3	2.13	0.48
1:B:64:ASN:H	1:B:64:ASN:HD22	1.62	0.48
1:B:73:GLY:N	1:B:348:LEU:O	2.46	0.48
1:B:411:LEU:HD12	1:B:412:ALA:N	2.29	0.48
1:B:666:ASP:OD2	1:B:701:THR:HG23	2.14	0.48
1:A:570:GLY:O	1:A:574:GLY:N	2.45	0.48
1:A:608:GLY:O	1:A:611:LEU:HG	2.13	0.48
1:B:699:SER:O	1:B:703:MET:HG2	2.13	0.48
1:A:105:ASN:HA	1:A:108:ASN:HD22	1.78	0.47
1:A:310:VAL:HG13	1:A:314:LEU:HD12	1.96	0.47
1:A:332:PHE:O	1:A:336:ILE:HG13	2.14	0.47
1:B:485:ALA:HA	1:B:636:ILE:HG12	1.94	0.47
1:A:43:LEU:HD23	1:A:46:LEU:HD12	1.96	0.47
1:A:364:VAL:HG23	1:A:707:SER:HB2	1.95	0.47
1:B:512:ARG:HH22	1:B:550:GLN:H	1.60	0.47
1:A:712:LEU:CD2	1:A:731:LEU:HB2	2.44	0.47
1:B:38:LEU:O	1:B:41:THR:OG1	2.30	0.47
1:B:522:LEU:HD13	1:B:576:LEU:HD22	1.95	0.47
1:A:744:ILE:O	1:A:748:LEU:HB2	2.14	0.47
1:B:432:VAL:O	1:B:436:THR:HG23	2.14	0.47
1:A:435:SER:O	1:A:438:SER:OG	2.32	0.47
1:B:376:GLU:OE2	1:B:696:GLN:NE2	2.47	0.47
1:B:746:ALA:HB3	1:B:747:PRO:HD3	1.96	0.47
1:A:150:LEU:HB3	1:A:187:GLY:HA2	1.96	0.47
1:A:62:LEU:HD11	1:A:68:GLN:O	2.14	0.47
1:B:410:ALA:HA	1:B:428:LEU:HD13	1.97	0.47
1:B:686:TYR:HE1	1:B:754:GLU:HB2	1.80	0.47
1:A:354:ALA:HA	1:A:357:VAL:HG22	1.97	0.47
1:A:406:HIS:HB3	1:A:432:VAL:HG11	1.95	0.47
1:B:513:VAL:HG12	1:B:514:ASP:OD1	2.15	0.47
1:B:586:THR:HG22	1:B:587:VAL:H	1.80	0.47
1:B:638:MET:O	1:B:642:SER:N	2.48	0.47
1:B:744:ILE:O	1:B:748:LEU:N	2.45	0.47
1:A:155:VAL:HG21	1:A:229:LEU:HD12	1.96	0.47
1:B:503:PHE:HB2	1:B:596:THR:HB	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:646:LEU:HD21	1:B:725:ASP:HB3	1.96	0.47
1:B:34:THR:HG23	1:B:445:TRP:CE3	2.50	0.47
1:B:717:ILE:HG13	1:B:718:PHE:CD2	2.50	0.47
1:A:364:VAL:O	1:A:368:VAL:N	2.48	0.46
1:B:205:VAL:HG12	1:B:206:VAL:H	1.79	0.46
1:B:487:ALA:O	1:B:491:LEU:HG	2.14	0.46
1:B:317:TYR:HE2	1:B:703:MET:SD	2.38	0.46
1:B:697:THR:O	1:B:701:THR:N	2.48	0.46
1:A:712:LEU:HD21	1:A:731:LEU:HB2	1.97	0.46
1:B:491:LEU:HB3	1:B:495:ARG:HD2	1.97	0.46
1:A:191:ALA:HB1	1:A:209:LYS:O	2.15	0.46
1:A:324:LEU:HD11	1:A:328:LEU:HD12	1.97	0.46
1:B:332:PHE:HD2	1:B:438:SER:HB2	1.80	0.46
1:B:350:LEU:O	1:B:353:ILE:HG22	2.16	0.46
1:B:618:PHE:CE2	1:B:671:SER:HB3	2.51	0.46
1:A:233:VAL:HG22	1:A:238:ILE:HG12	1.97	0.46
1:A:392:TYR:O	1:A:396:THR:HG23	2.16	0.46
1:A:606:GLY:O	1:A:610:ILE:HB	2.16	0.46
1:A:660:ILE:O	1:A:664:LEU:N	2.39	0.46
1:B:291:LEU:H	1:B:582:LEU:HD21	1.80	0.46
1:B:337:ILE:HD11	1:B:431:GLY:HA2	1.98	0.46
1:B:624:LEU:HD12	1:B:627:ILE:HB	1.98	0.46
1:A:415:ASN:OD1	1:A:416:TYR:N	2.49	0.46
1:A:488:GLY:HA2	1:A:491:LEU:HB2	1.97	0.46
1:A:632:HIS:O	1:A:636:ILE:HG12	2.16	0.46
1:A:96:LEU:H	1:A:96:LEU:HD23	1.80	0.46
1:A:189:THR:OG1	1:A:189:THR:O	2.32	0.46
1:B:80:LEU:HB2	1:B:285:ARG:O	2.16	0.46
1:B:472:LYS:HG3	1:B:473:PRO:CD	2.44	0.46
1:A:233:VAL:HG22	1:A:238:ILE:HG23	1.98	0.46
1:B:229:LEU:HD13	1:B:229:LEU:O	2.16	0.46
1:B:313:MET:HE1	1:B:317:TYR:CD2	2.50	0.46
1:B:591:VAL:O	1:B:595:LEU:HB2	2.16	0.46
1:B:634:VAL:HA	1:B:637:ALA:HB3	1.97	0.46
1:A:337:ILE:HD11	1:A:431:GLY:HA2	1.98	0.45
1:A:619:ASP:HB2	1:A:622:MET:HB3	1.98	0.45
1:A:240:SER:OG	1:A:254:ILE:HD12	2.16	0.45
1:A:417:SER:OG	1:A:421:VAL:HG23	2.16	0.45
1:B:328:LEU:HD21	1:B:446:PHE:CD2	2.52	0.45
1:A:364:VAL:CG2	1:A:707:SER:HB2	2.46	0.45
1:A:401:ASP:OD1	1:A:668:ILE:HG21	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:133:THR:HB	1:B:136:VAL:HG23	1.98	0.45
1:B:326:GLY:O	1:B:330:LEU:N	2.48	0.45
1:A:501:VAL:O	1:A:587:VAL:HG21	2.16	0.45
1:B:293:ALA:O	1:B:297:ARG:HG2	2.17	0.45
1:B:433:ILE:O	1:B:436:THR:OG1	2.28	0.45
1:B:599:THR:OG1	1:B:600:ILE:N	2.50	0.45
1:B:734:ILE:O	1:B:738:THR:HG23	2.17	0.45
1:B:358:LEU:HD21	1:B:662:TYR:HE2	1.82	0.45
1:B:518:THR:HB	1:B:521:GLN:HB2	1.98	0.45
1:B:525:SER:OG	1:B:572:ALA:HB1	2.17	0.45
1:A:79:GLY:N	1:A:131:GLY:H	2.15	0.45
1:A:397:ALA:HA	1:A:400:LEU:HB3	1.99	0.45
1:A:656:LEU:HD23	1:A:729:ILE:HD13	1.99	0.45
1:A:492:VAL:O	1:A:496:GLY:HA2	2.16	0.44
1:A:699:SER:O	1:A:703:MET:HG2	2.17	0.44
1:B:139:ARG:O	1:B:143:ILE:HG12	2.17	0.44
1:A:515:ARG:HA	1:A:552:GLN:N	2.32	0.44
1:B:392:TYR:O	1:B:396:THR:N	2.50	0.44
1:A:721:PRO:O	1:A:724:ARG:N	2.51	0.44
1:A:392:TYR:HA	1:A:395:SER:HB3	1.99	0.44
1:B:472:LYS:CG	1:B:473:PRO:HD3	2.45	0.44
1:B:634:VAL:HG12	1:B:659:LEU:HD23	1.98	0.44
1:A:64:ASN:OD1	1:A:65:ASP:N	2.48	0.44
1:B:305:VAL:HA	1:B:308:GLY:HA3	1.99	0.44
1:B:110:LEU:HB3	1:B:112:VAL:HG23	1.98	0.44
1:A:328:LEU:HB3	1:A:446:PHE:CZ	2.53	0.44
1:B:735:LEU:O	1:B:738:THR:OG1	2.31	0.44
1:A:310:VAL:HG22	1:A:710:LEU:HD12	2.00	0.43
1:A:593:LYS:O	1:A:597:GLN:HG3	2.18	0.43
1:A:715:LEU:HD11	1:A:723:LEU:HG	2.00	0.43
1:B:268:LEU:HD23	1:B:268:LEU:HA	1.74	0.43
1:B:303:ALA:O	1:B:307:ILE:N	2.48	0.43
1:B:669:ILE:H	1:B:669:ILE:HG13	1.55	0.43
1:B:99:VAL:HA	1:B:102:VAL:HG22	2.01	0.43
1:B:310:VAL:HG22	1:B:710:LEU:HB2	2.00	0.43
1:B:332:PHE:CD2	1:B:438:SER:HB2	2.53	0.43
1:B:597:GLN:O	1:B:601:TYR:HB2	2.18	0.43
1:B:629:ALA:HA	1:B:632:HIS:HB3	2.01	0.43
1:A:335:ILE:HD12	1:A:335:ILE:HA	1.92	0.43
1:A:403:ASN:OD1	1:A:404:ALA:N	2.51	0.43
1:A:266:LEU:O	1:A:270:LEU:HG	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:618:PHE:CD2	1:A:623:GLY:HA2	2.53	0.43
1:B:290:SER:HB2	1:B:582:LEU:HD21	2.00	0.43
1:A:402:VAL:HG23	1:A:669:ILE:HD11	2.00	0.43
1:A:408:LEU:HD13	1:A:613:TYR:HB2	2.01	0.43
1:B:38:LEU:HD13	1:B:445:TRP:CD1	2.53	0.43
1:A:79:GLY:O	1:A:287:ILE:HD12	2.18	0.43
1:A:107:ILE:HD11	1:A:115:PRO:HG3	2.01	0.43
1:B:665:ASN:HA	1:B:668:ILE:HD12	1.99	0.43
1:A:117:VAL:HG22	1:A:127:VAL:HG13	2.00	0.43
1:A:425:ALA:O	1:A:429:ILE:HG13	2.19	0.42
1:B:369:ILE:HG12	1:B:402:VAL:HG21	2.01	0.42
1:A:388:ILE:HG13	1:A:389:GLY:N	2.35	0.42
1:A:400:LEU:HA	1:A:403:ASN:HD21	1.84	0.42
1:A:403:ASN:HB3	1:A:436:THR:HG21	2.02	0.42
1:A:545:THR:HG22	1:A:553:ASN:N	2.35	0.42
1:B:595:LEU:HD12	1:B:598:LYS:HD3	2.01	0.42
1:B:716:LEU:HD23	1:B:724:ARG:HG2	2.01	0.42
1:A:162:ASP:O	1:A:166:ARG:N	2.53	0.42
1:A:725:ASP:O	1:A:729:ILE:HG13	2.19	0.42
1:B:641:PHE:CE2	1:B:646:LEU:HD23	2.54	0.42
1:A:49:ILE:HD11	1:A:335:ILE:O	2.19	0.42
1:A:572:ALA:HA	1:A:575:LYS:NZ	2.34	0.42
1:B:64:ASN:H	1:B:64:ASN:ND2	2.17	0.42
1:A:119:VAL:HA	1:A:125:VAL:HA	2.02	0.42
1:B:34:THR:HG23	1:B:445:TRP:HE3	1.84	0.42
1:B:441:VAL:O	1:B:445:TRP:N	2.52	0.42
1:B:48:TYR:HA	1:B:51:ARG:HD3	2.01	0.42
1:A:71:THR:HB	1:A:346:ALA:O	2.19	0.42
1:A:359:THR:HG21	1:A:431:GLY:HA3	2.02	0.42
1:A:375:LYS:O	1:A:378:LEU:HG	2.19	0.42
1:A:713:ILE:O	1:A:717:ILE:HG13	2.19	0.42
1:A:422:LYS:O	1:A:425:ALA:HB3	2.20	0.42
1:A:503:PHE:CE1	1:A:650:VAL:HG22	2.54	0.42
1:A:712:LEU:HA	1:A:715:LEU:HB3	2.01	0.42
1:A:721:PRO:O	1:A:724:ARG:HG2	2.20	0.42
1:B:351:PRO:HG3	1:B:420:ALA:HB1	2.02	0.42
1:B:612:VAL:O	1:B:616:PHE:N	2.50	0.42
1:B:352:GLY:HA2	1:B:423:GLY:C	2.40	0.41
1:A:104:GLU:HG2	1:A:117:VAL:HG21	2.02	0.41
1:B:561:LEU:HB2	1:B:565:GLU:CB	2.43	0.41
1:A:443:ALA:HA	1:A:446:PHE:CD2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:662:TYR:CA	1:A:665:ASN:HD22	2.33	0.41
1:B:629:ALA:HB2	1:B:745:VAL:HG21	2.01	0.41
1:B:649:THR:O	1:B:652:SER:HB2	2.20	0.41
1:A:191:ALA:HB1	1:A:210:THR:HA	2.02	0.41
1:A:518:THR:HA	1:A:522:LEU:HD12	2.01	0.41
1:A:730:LEU:HD12	1:A:730:LEU:HA	1.95	0.41
1:B:641:PHE:HD2	1:B:729:ILE:HD11	1.83	0.41
1:A:375:LYS:HA	1:A:375:LYS:HD3	1.86	0.41
1:B:327:ALA:O	1:B:331:LEU:HB2	2.20	0.41
1:B:390:ALA:O	1:B:394:HIS:N	2.43	0.41
1:B:397:ALA:O	1:B:401:ASP:N	2.54	0.41
1:B:231:ALA:HA	1:B:241:VAL:HG11	2.03	0.41
1:A:328:LEU:HD13	1:A:446:PHE:CD1	2.56	0.41
1:B:370:SER:HB3	1:B:399:ILE:HD12	2.02	0.41
1:B:571:ALA:O	1:B:575:LYS:HD3	2.21	0.41
1:A:472:LYS:HB2	1:A:473:PRO:HD3	2.02	0.41
1:A:665:ASN:CG	1:A:666:ASP:N	2.73	0.41
1:B:420:ALA:O	1:B:423:GLY:N	2.43	0.41
1:B:441:VAL:HA	1:B:444:LYS:HB3	2.03	0.41
1:A:79:GLY:HA3	1:A:130:PRO:HA	2.03	0.41
1:A:662:TYR:C	1:A:665:ASN:HD22	2.21	0.41
1:A:712:LEU:HD11	1:A:730:LEU:HB3	2.03	0.41
1:B:79:GLY:HA2	1:B:131:GLY:HA2	2.02	0.41
1:B:636:ILE:HG22	1:B:640:LEU:HD13	2.03	0.40
1:A:34:THR:HG23	1:A:37:LEU:HD23	2.03	0.40
1:A:73:GLY:HA2	1:A:348:LEU:O	2.21	0.40
1:A:406:HIS:HA	1:A:409:SER:HG	1.86	0.40
1:B:631:ILE:HA	1:B:634:VAL:HG22	2.03	0.40
1:A:110:LEU:HD22	1:A:112:VAL:HG22	2.03	0.40
1:A:326:GLY:O	1:A:330:LEU:HD13	2.22	0.40
1:A:527:ILE:HG21	1:A:536:GLY:HA2	2.03	0.40
1:B:495:ARG:CZ	1:B:642:SER:HB3	2.52	0.40
1:B:587:VAL:HG22	1:B:588:GLY:H	1.85	0.40
1:A:646:LEU:HD12	1:A:646:LEU:HA	1.93	0.40
1:A:488:GLY:O	1:A:492:VAL:N	2.55	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	721/750 (96%)	656 (91%)	59 (8%)	6 (1%)	19	58
1	B	672/750 (90%)	622 (93%)	47 (7%)	3 (0%)	34	71
All	All	1393/1500 (93%)	1278 (92%)	106 (8%)	9 (1%)	25	63

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	578	GLN
1	A	721	PRO
1	B	51	ARG
1	A	446	PHE
1	B	420	ALA
1	A	276	PRO
1	B	153	ARG
1	A	460	PRO
1	A	455	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	481/603 (80%)	462 (96%)	19 (4%)	31	57
1	B	484/603 (80%)	470 (97%)	14 (3%)	42	65
All	All	965/1206 (80%)	932 (97%)	33 (3%)	37	61

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	53	TRP
1	A	69	PHE
1	A	96	LEU
1	A	198	ASP
1	A	204	TRP
1	A	315	PHE
1	A	385	LYS
1	A	442	PHE
1	A	472	LYS
1	A	503	PHE
1	A	561	LEU
1	A	618	PHE
1	A	638	MET
1	A	641	PHE
1	A	682	ARG
1	A	688	GLU
1	A	726	PHE
1	A	739	TYR
1	A	751	TYR
1	B	70	MET
1	B	407	LEU
1	B	414	TYR
1	B	448	GLN
1	B	495	ARG
1	B	552	GLN
1	B	616	PHE
1	B	648	PHE
1	B	666	ASP
1	B	676	GLU
1	B	678	MET
1	B	687	ARG
1	B	739	TYR
1	B	752	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	66	GLN
1	A	108	ASN
1	B	31	ASN
1	B	137	GLN

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Mol	Chain	Res	Type
1	B	448	GLN
1	B	465	HIS

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.