



Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 07:31 am BST

PDB ID : 1KFX
Title : Crystal Structure of Human m-Calpain Form I
Authors : Strobl, S.; Fernandez-Catalan, C.; Braun, M.; Huber, R.; Masumoto, H.; Nakagawa, K.; Irie, A.; Sorimachi, H.; Bourenkow, G.; Bartunik, H.; Suzuki, K.; Bode, W.
Deposited on : 2001-11-23
Resolution : 3.15 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

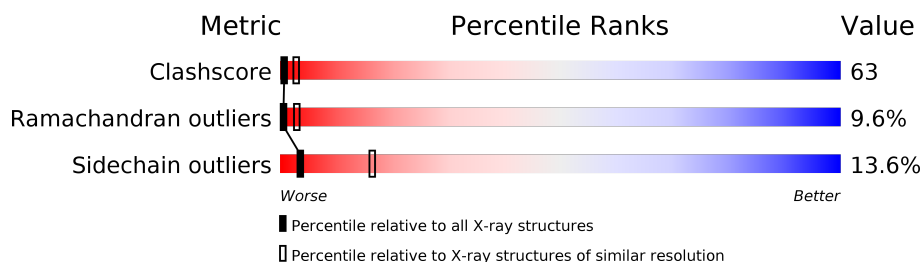
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.15 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))
Clashscore	141614	1804 (3.20-3.12)
Ramachandran outliers	138981	1770 (3.20-3.12)
Sidechain outliers	138945	1769 (3.20-3.12)

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 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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	L	699	
2	S	184	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6826 atoms, of which 1 is hydrogen 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 M-CALPAIN LARGE SUBUNIT.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	L	640	Total	C	H	N	O	S	209	0	0
			5156	3284	1	873	973	25			

- Molecule 2 is a protein called M-CALPAIN SMALL SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	S	176	Total	C	N	O	S	47	0	0
			1426	895	244	276	11			

- Molecule 3 is water.

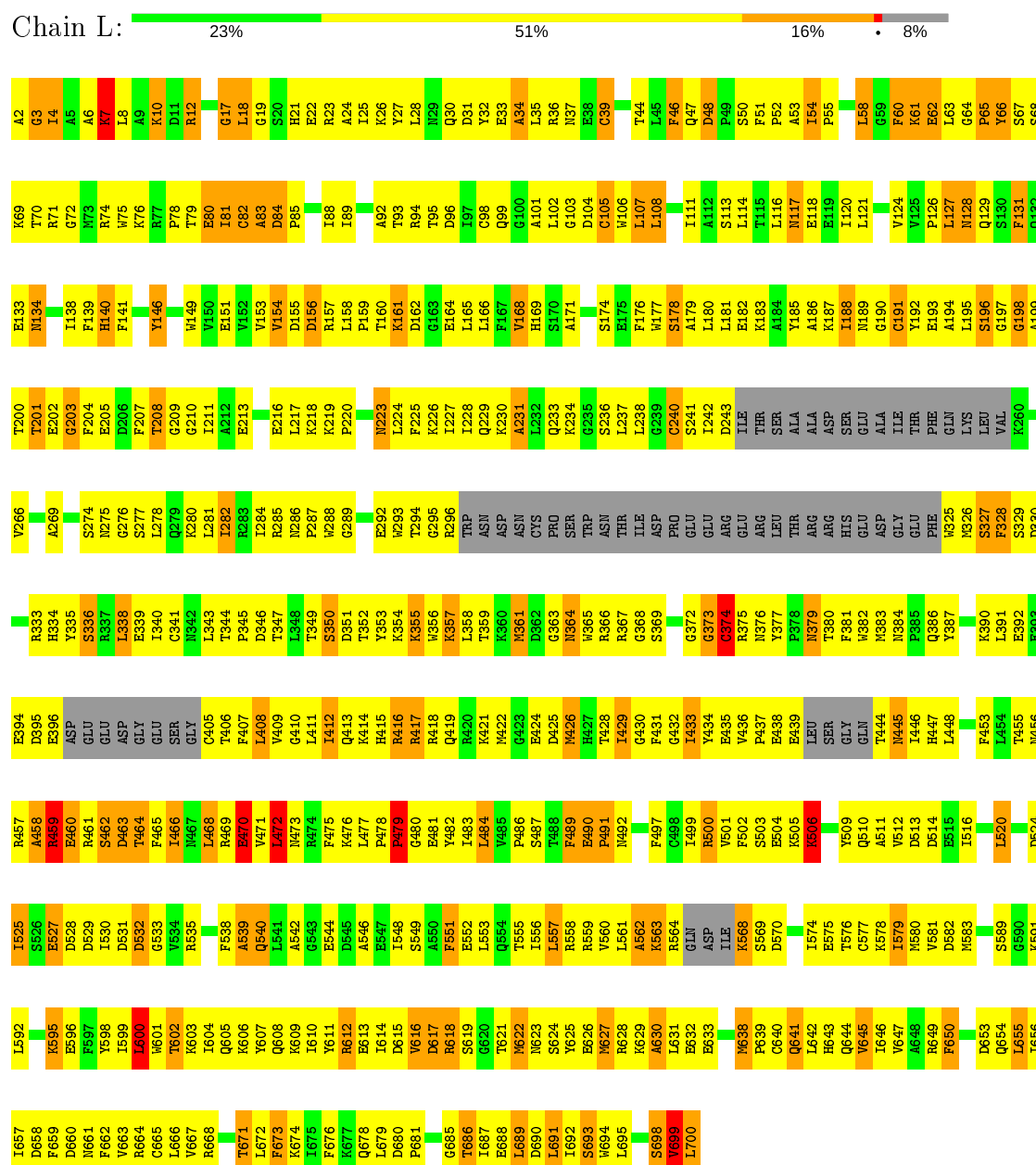
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	L	197	Total	O	0	0
			197	197		
3	S	47	Total	O	0	0
			47	47		

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 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.

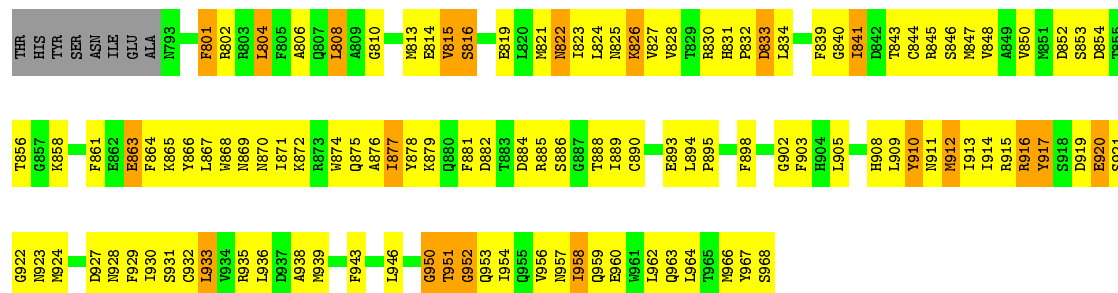
Note EDS was not executed.

• Molecule 1: M-CALPAIN LARGE SUBUNIT



● Molecule 2: M-CALPAIN SMALL SUBUNIT

Chain S:



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	64.78Å 133.25Å 77.53Å 90.00° 102.07° 90.00°	Depositor
Resolution (Å)	30.00 – 3.15	Depositor
% Data completeness (in resolution range)	(Not available) (30.00-3.15)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.243 , 0.318	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6826	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

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	L	0.55	1/5265 (0.0%)	0.79	5/7099 (0.1%)
2	S	0.51	0/1453	0.72	0/1954
All	All	0.54	1/6718 (0.0%)	0.77	5/9053 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	S	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	700	LEU	C-O	-6.97	1.10	1.23

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	612	ARG	NE-CZ-NH2	6.99	123.80	120.30
1	L	472	LEU	CA-CB-CG	6.17	129.48	115.30
1	L	107	LEU	CA-CB-CG	5.36	127.63	115.30
1	L	650	PHE	N-CA-C	5.09	124.75	111.00
1	L	60	PHE	N-CA-C	-5.07	97.31	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	S	917	TYR	Sidechain

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	L	5155	1	5044	659	0
2	S	1426	0	1367	143	0
3	L	197	0	0	3	0
3	S	47	0	0	1	0
All	All	6825	1	6411	783	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 63.

All (783) 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:L:638:MET:HG3	1:L:643:HIS:NE2	1.66	1.09
1:L:99:GLN:OE1	1:L:103:GLY:HA3	1.56	1.05
1:L:361:MET:HB2	1:L:509:TYR:CE1	1.93	1.04
1:L:4:ILE:HD13	1:L:4:ILE:H	1.23	1.00
2:S:877:ILE:H	2:S:877:ILE:HD12	1.29	0.98
2:S:890:CYS:HB3	2:S:893:GLU:HB2	1.46	0.97
1:L:577:CYS:HA	1:L:580:MET:HG3	1.44	0.97
1:L:373:GLY:H	1:L:384:ASN:HD21	1.02	0.96
1:L:638:MET:HG3	1:L:643:HIS:HE2	1.31	0.95
1:L:638:MET:HG3	1:L:643:HIS:CD2	2.01	0.94
1:L:355:LYS:H	1:L:355:LYS:HE2	1.30	0.94
1:L:211:ILE:HB	1:L:502:PHE:CE1	2.04	0.93
1:L:30:GLN:HE22	1:L:187:LYS:NZ	1.67	0.93
1:L:405:CYS:SG	1:L:504:GLU:HB2	2.11	0.91
1:L:369:SER:HB2	1:L:647:VAL:HG21	1.53	0.91
1:L:406:THR:OG1	1:L:504:GLU:HG3	1.72	0.88
1:L:4:ILE:N	1:L:4:ILE:HD13	1.89	0.88
1:L:386:GLN:HB3	1:L:512:VAL:HB	1.55	0.87
1:L:204:PHE:O	1:L:208:THR:HG23	1.75	0.87
1:L:598:TYR:O	1:L:602:THR:HG22	1.75	0.87
1:L:99:GLN:HE21	1:L:168:VAL:HG23	1.39	0.86
1:L:52:PRO:HB2	1:L:54:ILE:CG1	2.06	0.86
1:L:552:GLU:O	1:L:556:ILE:HG12	1.76	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:825:ASN:HD21	2:S:839:PHE:H	1.23	0.85
1:L:31:ASP:HB3	1:L:34:ALA:HB3	1.57	0.85
1:L:383:MET:SD	1:L:625:TYR:HD2	2.01	0.84
2:S:917:TYR:HB3	2:S:928:ASN:HB3	1.60	0.84
1:L:621:THR:HB	1:L:656:ILE:HG21	1.60	0.84
1:L:679:LEU:C	1:L:681:PRO:HD3	1.98	0.83
1:L:592:LEU:HD22	1:L:596:GLU:HG3	1.59	0.83
1:L:85:PRO:HB3	1:L:176:PHE:CE1	2.14	0.82
1:L:387:TYR:HA	1:L:511:ALA:HA	1.62	0.82
1:L:373:GLY:HA2	1:L:487:SER:HB2	1.62	0.82
1:L:22:GLU:H	1:L:22:GLU:CD	1.82	0.81
1:L:74:ARG:HD3	1:L:76:LYS:HE3	1.63	0.80
1:L:4:ILE:CD1	1:L:4:ILE:H	1.94	0.80
1:L:211:ILE:HD13	1:L:408:LEU:HD12	1.62	0.80
1:L:444:THR:HG23	1:L:445:ASN:H	1.47	0.80
1:L:281:LEU:HD21	1:L:296:ARG:HH21	1.46	0.80
1:L:373:GLY:N	1:L:384:ASN:HD21	1.80	0.80
1:L:364:ASN:HB3	1:L:366:ARG:HH12	1.47	0.80
1:L:217:LEU:O	1:L:220:PRO:HD3	1.82	0.79
1:L:238:LEU:HB2	1:L:266:VAL:HB	1.63	0.79
1:L:373:GLY:H	1:L:384:ASN:ND2	1.78	0.79
2:S:915:ARG:O	2:S:916:ARG:HB2	1.80	0.79
1:L:209:GLY:HA3	1:L:343:LEU:HD23	1.63	0.79
1:L:561:LEU:HD12	1:L:563:LYS:HD3	1.63	0.79
1:L:201:THR:HG22	1:L:338:LEU:HD23	1.64	0.79
2:S:877:ILE:CD1	2:S:877:ILE:H	1.95	0.78
1:L:373:GLY:O	1:L:374:CYS:HB2	1.83	0.78
1:L:84:ASP:N	1:L:85:PRO:HD3	1.98	0.78
1:L:379:ASN:HB3	3:L:735:HOH:O	1.84	0.78
1:L:687:ILE:O	1:L:687:ILE:HG13	1.81	0.78
1:L:114:LEU:HD23	1:L:120:ILE:HG22	1.64	0.77
1:L:355:LYS:HE2	1:L:355:LYS:N	1.99	0.77
1:L:458:ALA:O	1:L:459:ARG:HB2	1.83	0.77
1:L:102:LEU:HD22	1:L:166:LEU:HD12	1.66	0.77
1:L:484:LEU:H	1:L:484:LEU:HD23	1.49	0.77
1:L:242:ILE:HA	1:L:335:TYR:HB3	1.66	0.77
1:L:562:ALA:H	1:L:563:LYS:HD2	1.47	0.77
1:L:412:ILE:HA	1:L:470:GLU:HA	1.66	0.77
1:L:448:LEU:HG	1:L:512:VAL:HG11	1.66	0.76
1:L:368:GLY:HA3	1:L:655:LEU:HD22	1.67	0.76
1:L:411:LEU:HD23	1:L:429:ILE:HG13	1.67	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:220:PRO:HB2	1:L:224:LEU:HD22	1.69	0.75
1:L:406:THR:HG22	1:L:476:LYS:HG3	1.68	0.75
2:S:815:VAL:HG22	2:S:819:GLU:HB3	1.66	0.75
1:L:99:GLN:NE2	1:L:168:VAL:HG23	2.02	0.75
2:S:888:THR:O	2:S:889:ILE:HG13	1.87	0.75
1:L:643:HIS:O	1:L:647:VAL:HG23	1.87	0.74
2:S:962:LEU:O	2:S:966:MET:HB2	1.87	0.74
1:L:484:LEU:N	1:L:484:LEU:HD23	2.02	0.74
1:L:195:LEU:HD12	1:L:195:LEU:N	2.02	0.74
1:L:394:GLU:HA	1:L:405:CYS:HB2	1.68	0.74
1:L:102:LEU:HD22	1:L:166:LEU:CD1	2.18	0.74
1:L:392:GLU:O	1:L:479:PRO:HB3	1.88	0.74
1:L:344:THR:HG21	1:L:356:TRP:O	1.88	0.73
2:S:819:GLU:O	2:S:823:ILE:HG12	1.87	0.73
1:L:60:PHE:O	1:L:193:GLU:OE2	2.05	0.73
2:S:878:TYR:HB2	2:S:929:PHE:CD2	2.23	0.73
1:L:341:CYS:HB3	1:L:356:TRP:NE1	2.04	0.73
1:L:436:VAL:HB	1:L:481:GLU:HG3	1.70	0.73
1:L:199:ALA:HB3	1:L:202:GLU:HG3	1.71	0.73
1:L:549:SER:H	1:L:552:GLU:HB3	1.53	0.73
1:L:679:LEU:O	1:L:681:PRO:HD3	1.89	0.73
1:L:405:CYS:N	1:L:477:LEU:O	2.22	0.72
1:L:52:PRO:HB2	1:L:54:ILE:HG13	1.71	0.72
1:L:411:LEU:HD12	1:L:499:ILE:HG12	1.70	0.72
1:L:366:ARG:NE	2:S:856:THR:HG22	2.05	0.72
2:S:919:ASP:O	2:S:922:GLY:N	2.21	0.72
1:L:470:GLU:HG3	1:L:471:VAL:N	2.04	0.72
1:L:168:VAL:HG12	1:L:179:ALA:HA	1.72	0.71
1:L:54:ILE:HG22	1:L:55:PRO:HD3	1.72	0.71
1:L:233:GLN:HG2	1:L:354:LYS:HD3	1.71	0.71
2:S:951:THR:O	2:S:953:GLN:N	2.24	0.71
1:L:500:ARG:HH11	1:L:500:ARG:HG3	1.54	0.71
1:L:621:THR:HB	1:L:656:ILE:CG2	2.21	0.71
1:L:85:PRO:HB3	1:L:176:PHE:HE1	1.52	0.71
1:L:31:ASP:HB3	1:L:34:ALA:CB	2.19	0.71
1:L:105:CYS:HA	1:L:108:LEU:HD22	1.71	0.70
1:L:532:ASP:HA	1:L:535:ARG:HB3	1.73	0.70
2:S:877:ILE:HD12	2:S:877:ILE:N	2.06	0.70
1:L:358:LEU:HG	1:L:359:THR:N	2.06	0.70
1:L:52:PRO:HB2	1:L:54:ILE:HD11	1.72	0.70
1:L:95:THR:O	1:L:96:ASP:HB3	1.92	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:432:GLY:HA2	1:L:461:ARG:HG3	1.72	0.70
1:L:528:ASP:CG	1:L:529:ASP:H	1.94	0.70
1:L:197:GLY:O	1:L:198:GLY:O	2.10	0.70
1:L:52:PRO:HB2	1:L:54:ILE:CD1	2.21	0.70
1:L:563:LYS:HD2	1:L:563:LYS:N	2.07	0.69
1:L:30:GLN:HE22	1:L:187:LYS:HZ1	1.41	0.69
1:L:646:ILE:O	1:L:650:PHE:HB2	1.91	0.69
1:L:486:PRO:HB3	1:L:499:ILE:HD11	1.75	0.69
1:L:654:GLN:O	1:L:655:LEU:HB2	1.93	0.69
1:L:94:ARG:HA	1:L:287:PRO:O	1.93	0.69
2:S:917:TYR:HB2	2:S:924:MET:CE	2.24	0.68
1:L:373:GLY:HA2	1:L:487:SER:CB	2.23	0.68
2:S:825:ASN:ND2	2:S:839:PHE:H	1.91	0.68
1:L:281:LEU:HD21	1:L:296:ARG:NH2	2.07	0.67
1:L:60:PHE:O	1:L:61:LYS:C	2.32	0.67
1:L:234:LYS:O	1:L:353:TYR:HB3	1.94	0.67
1:L:583:MET:HA	1:L:671:THR:HG23	1.75	0.67
1:L:641:GLN:HA	1:L:644:GLN:HE21	1.57	0.67
1:L:406:THR:HG22	1:L:476:LYS:CG	2.23	0.67
1:L:375:ARG:NH1	1:L:457:ARG:NH1	2.43	0.67
1:L:520:LEU:HD22	1:L:520:LEU:H	1.57	0.67
2:S:874:TRP:C	2:S:876:ALA:H	1.96	0.67
1:L:54:ILE:HD12	1:L:54:ILE:H	1.60	0.66
1:L:364:ASN:HB3	1:L:366:ARG:NH1	2.10	0.66
1:L:688:GLU:H	1:L:688:GLU:CD	1.97	0.66
1:L:113:SER:O	1:L:117:ASN:OD1	2.13	0.66
1:L:688:GLU:HB2	2:S:953:GLN:HE21	1.60	0.66
1:L:568:LYS:HA	1:L:568:LYS:HE3	1.76	0.66
1:L:459:ARG:O	1:L:460:GLU:HB3	1.96	0.66
1:L:662:PHE:CZ	1:L:666:LEU:HD11	2.31	0.66
1:L:230:LYS:HA	1:L:233:GLN:HB3	1.77	0.66
1:L:553:LEU:O	1:L:557:LEU:HB2	1.96	0.66
1:L:676:PHE:CZ	1:L:687:ILE:HG23	2.31	0.66
1:L:478:PRO:HG2	1:L:482:TYR:OH	1.96	0.66
1:L:286:ASN:HD22	1:L:289:GLY:N	1.94	0.66
1:L:209:GLY:HA3	1:L:343:LEU:CD2	2.25	0.65
1:L:525:ILE:HD13	1:L:525:ILE:O	1.96	0.65
1:L:631:LEU:HD13	1:L:638:MET:HE3	1.77	0.65
1:L:579:ILE:HA	1:L:582:ASP:HB2	1.78	0.65
1:L:363:GLY:HA3	1:L:497:PHE:CZ	2.31	0.65
1:L:366:ARG:HE	2:S:856:THR:HG22	1.60	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:959:GLN:O	2:S:963:GLN:HG3	1.97	0.65
1:L:649:ARG:O	1:L:649:ARG:HG3	1.95	0.65
2:S:890:CYS:CB	2:S:893:GLU:HB2	2.26	0.65
1:L:380:THR:O	1:L:383:MET:HB2	1.96	0.65
1:L:341:CYS:HB3	1:L:356:TRP:HE1	1.62	0.64
1:L:631:LEU:HD13	1:L:638:MET:CE	2.27	0.64
1:L:198:GLY:CA	1:L:422:MET:HE2	2.27	0.64
1:L:293:TRP:HZ2	1:L:325:TRP:O	1.81	0.64
1:L:269:ALA:HB1	1:L:281:LEU:O	1.97	0.64
1:L:343:LEU:HD13	1:L:345:PRO:HG2	1.80	0.64
1:L:434:TYR:N	1:L:483:ILE:O	2.30	0.64
1:L:361:MET:HB2	1:L:509:TYR:HE1	1.58	0.64
1:L:613:GLU:O	1:L:614:ILE:HD12	1.98	0.64
1:L:367:ARG:HG2	1:L:655:LEU:HD11	1.77	0.63
1:L:284:ILE:HD12	1:L:326:MET:SD	2.38	0.63
1:L:328:PHE:C	1:L:330:ASP:H	2.01	0.63
1:L:464:THR:HG22	1:L:465:PHE:N	2.13	0.63
1:L:527:GLU:HG2	1:L:527:GLU:O	1.96	0.63
1:L:186:ALA:HA	1:L:195:LEU:HD11	1.81	0.63
1:L:433:ILE:HA	1:L:483:ILE:O	1.99	0.63
1:L:242:ILE:HD11	1:L:334:HIS:ND1	2.14	0.63
1:L:352:THR:O	1:L:353:TYR:HB2	1.99	0.63
1:L:478:PRO:O	1:L:480:GLY:N	2.32	0.63
2:S:801:PHE:CZ	2:S:827:VAL:HG21	2.34	0.63
1:L:88:ILE:HD13	1:L:127:LEU:HD11	1.80	0.62
1:L:146:TYR:CD2	1:L:414:LYS:HA	2.34	0.62
1:L:355:LYS:H	1:L:355:LYS:CE	2.10	0.62
1:L:405:CYS:SG	1:L:406:THR:N	2.72	0.62
1:L:618:ARG:O	1:L:618:ARG:HD2	1.99	0.62
1:L:698:SER:HB3	2:S:939:MET:HG3	1.81	0.62
1:L:133:GLU:O	1:L:134:ASN:HB2	1.98	0.62
1:L:562:ALA:N	1:L:563:LYS:HD2	2.13	0.62
1:L:583:MET:HG2	1:L:583:MET:O	1.99	0.62
1:L:63:LEU:O	1:L:70:THR:HG21	1.99	0.62
2:S:868:TRP:O	2:S:871:ILE:HB	1.99	0.62
1:L:162:ASP:O	1:L:164:GLU:HG2	1.99	0.62
1:L:236:SER:OG	1:L:341:CYS:HA	2.00	0.62
1:L:428:THR:HA	1:L:466:ILE:O	2.00	0.62
1:L:410:GLY:HA2	1:L:471:VAL:O	2.00	0.61
1:L:432:GLY:CA	1:L:461:ARG:HG3	2.29	0.61
1:L:65:PRO:O	1:L:67:SER:N	2.28	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:114:LEU:CD2	1:L:120:ILE:HG22	2.31	0.61
1:L:375:ARG:HH12	1:L:457:ARG:NH1	1.98	0.61
2:S:832:PRO:C	2:S:834:LEU:H	2.04	0.61
2:S:908:HIS:HD1	2:S:908:HIS:H	1.48	0.61
2:S:843:THR:HG23	2:S:931:SER:HB2	1.83	0.61
1:L:220:PRO:CB	1:L:224:LEU:HD22	2.31	0.61
1:L:227:ILE:O	1:L:231:ALA:N	2.30	0.61
1:L:78:PRO:HG2	1:L:131:PHE:HE2	1.65	0.61
1:L:282:ILE:CG2	1:L:284:ILE:HG13	2.31	0.61
1:L:286:ASN:ND2	1:L:289:GLY:N	2.48	0.61
1:L:386:GLN:CB	1:L:512:VAL:HB	2.28	0.61
1:L:366:ARG:HG2	1:L:644:GLN:OE1	1.99	0.61
1:L:416:ARG:HG2	1:L:416:ARG:HH11	1.65	0.61
1:L:457:ARG:O	1:L:458:ALA:HB2	2.00	0.61
1:L:131:PHE:N	1:L:131:PHE:CD1	2.68	0.60
1:L:556:ILE:O	1:L:560:VAL:HG23	2.01	0.60
1:L:391:LEU:HD11	1:L:407:PHE:HE2	1.66	0.60
2:S:958:ILE:CD1	2:S:962:LEU:HG	2.31	0.60
1:L:225:PHE:C	1:L:227:ILE:H	2.04	0.60
1:L:198:GLY:HA3	1:L:422:MET:HE2	1.84	0.60
1:L:463:ASP:O	1:L:464:THR:HB	2.01	0.60
1:L:640:CYS:O	1:L:644:GLN:HG3	2.02	0.60
1:L:657:ILE:HD12	1:L:657:ILE:N	2.16	0.60
1:L:699:VAL:O	1:L:699:VAL:HG22	2.01	0.60
2:S:943:PHE:CZ	2:S:954:ILE:HG23	2.37	0.60
1:L:233:GLN:HG3	1:L:354:LYS:NZ	2.17	0.60
1:L:84:ASP:N	1:L:85:PRO:CD	2.64	0.59
2:S:816:SER:H	2:S:819:GLU:HB2	1.67	0.59
1:L:700:LEU:HD22	2:S:916:ARG:NE	2.17	0.59
2:S:958:ILE:HD13	2:S:958:ILE:O	2.02	0.59
1:L:205:GLU:HG2	1:L:210:GLY:O	2.03	0.59
1:L:48:ASP:OD2	1:L:154:VAL:HA	2.02	0.59
1:L:80:GLU:O	1:L:81:ILE:HG23	2.01	0.59
1:L:192:TYR:O	1:L:195:LEU:HD13	2.02	0.59
1:L:230:LYS:CA	1:L:233:GLN:HB3	2.32	0.59
1:L:327:SER:C	1:L:329:SER:H	2.04	0.59
1:L:628:ARG:HG3	1:L:643:HIS:CE1	2.38	0.59
1:L:74:ARG:HH11	1:L:74:ARG:HG3	1.66	0.59
1:L:181:LEU:C	1:L:181:LEU:HD23	2.22	0.59
1:L:27:TYR:CE2	1:L:28:LEU:HG	2.37	0.59
1:L:82:CYS:O	1:L:83:ALA:CB	2.51	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:463:ASP:O	1:L:464:THR:CB	2.51	0.59
1:L:373:GLY:CA	1:L:487:SER:HB2	2.31	0.59
1:L:500:ARG:NH1	1:L:500:ARG:HG3	2.17	0.59
1:L:6:ALA:C	1:L:8:LEU:H	2.04	0.58
1:L:105:CYS:HA	1:L:108:LEU:CD2	2.32	0.58
1:L:107:LEU:CD1	1:L:182:GLU:HG3	2.33	0.58
1:L:209:GLY:CA	1:L:343:LEU:HD23	2.33	0.58
2:S:874:TRP:HB2	2:S:930:ILE:CD1	2.32	0.58
1:L:10:LYS:HD3	1:L:10:LYS:O	2.03	0.58
1:L:60:PHE:O	1:L:61:LYS:O	2.21	0.58
1:L:61:LYS:O	1:L:193:GLU:OE1	2.22	0.58
1:L:213:GLU:HG3	1:L:339:GLU:HG3	1.86	0.58
1:L:528:ASP:O	1:L:530:ILE:HG23	2.02	0.58
1:L:638:MET:O	1:L:643:HIS:NE2	2.35	0.58
1:L:233:GLN:CG	1:L:354:LYS:HD3	2.34	0.58
1:L:286:ASN:HD22	1:L:289:GLY:H	1.50	0.58
2:S:903:PHE:CE2	2:S:936:LEU:HD23	2.38	0.58
2:S:847:MET:CE	2:S:871:ILE:HD11	2.33	0.58
2:S:929:PHE:O	2:S:933:LEU:HD12	2.04	0.58
1:L:386:GLN:O	1:L:512:VAL:N	2.33	0.58
1:L:468:LEU:HD12	1:L:468:LEU:O	2.03	0.58
1:L:81:ILE:O	1:L:82:CYS:HB2	2.03	0.58
2:S:915:ARG:O	2:S:916:ARG:CB	2.52	0.58
2:S:841:ILE:HG13	2:S:841:ILE:O	2.03	0.57
1:L:576:THR:O	1:L:579:ILE:N	2.36	0.57
1:L:579:ILE:HG23	1:L:667:VAL:HG11	1.86	0.57
1:L:181:LEU:HD23	1:L:181:LEU:O	2.05	0.57
1:L:357:LYS:HB3	1:L:503:SER:OG	2.04	0.57
1:L:673:PHE:O	1:L:676:PHE:N	2.38	0.57
2:S:943:PHE:CE1	2:S:954:ILE:HG23	2.39	0.57
1:L:28:LEU:HD12	1:L:50:SER:HB3	1.85	0.57
1:L:32:TYR:CE2	1:L:36:ARG:NH2	2.72	0.57
1:L:238:LEU:N	1:L:238:LEU:HD12	2.20	0.57
1:L:30:GLN:HE22	1:L:187:LYS:HZ3	1.49	0.57
2:S:917:TYR:HB2	2:S:924:MET:HE1	1.85	0.57
1:L:623:ASN:ND2	1:L:623:ASN:H	2.02	0.57
2:S:846:SER:HB3	2:S:935:ARG:HD3	1.86	0.57
1:L:82:CYS:HB3	1:L:85:PRO:HG3	1.86	0.57
2:S:878:TYR:HB2	2:S:929:PHE:CE2	2.40	0.57
2:S:954:ILE:C	2:S:954:ILE:HD12	2.25	0.57
1:L:211:ILE:HB	1:L:502:PHE:HE1	1.63	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:641:GLN:HA	1:L:644:GLN:NE2	2.20	0.56
1:L:217:LEU:HD12	1:L:334:HIS:C	2.26	0.56
1:L:79:THR:O	1:L:81:ILE:N	2.38	0.56
1:L:326:MET:C	1:L:328:PHE:H	2.08	0.56
1:L:380:THR:HA	1:L:383:MET:HE2	1.87	0.56
1:L:577:CYS:HA	1:L:580:MET:CG	2.27	0.56
2:S:874:TRP:C	2:S:876:ALA:N	2.59	0.56
1:L:293:TRP:CZ2	1:L:325:TRP:O	2.58	0.56
1:L:18:LEU:H	1:L:23:ARG:CZ	2.18	0.56
1:L:368:GLY:HA2	1:L:625:TYR:CE1	2.40	0.56
1:L:558:ARG:C	1:L:560:VAL:H	2.07	0.56
1:L:655:LEU:C	1:L:656:ILE:HD12	2.26	0.56
1:L:528:ASP:OD2	1:L:529:ASP:N	2.38	0.56
1:L:416:ARG:CG	1:L:416:ARG:HH11	2.18	0.56
1:L:58:LEU:HD13	1:L:75:TRP:CZ2	2.40	0.56
1:L:599:ILE:O	1:L:602:THR:HG23	2.05	0.56
1:L:62:GLU:C	1:L:64:GLY:H	2.09	0.56
1:L:368:GLY:HA3	1:L:655:LEU:CD2	2.36	0.56
1:L:484:LEU:N	1:L:484:LEU:CD2	2.69	0.56
2:S:828:VAL:HG12	2:S:875:GLN:NE2	2.21	0.55
1:L:217:LEU:HD12	1:L:334:HIS:O	2.05	0.55
2:S:894:LEU:HB2	2:S:895:PRO:HD3	1.88	0.55
1:L:126:PRO:O	1:L:128:ASN:N	2.39	0.55
1:L:234:LYS:C	1:L:353:TYR:HB3	2.26	0.55
1:L:99:GLN:HG3	1:L:104:ASP:O	2.07	0.55
1:L:343:LEU:CD1	1:L:345:PRO:HG2	2.36	0.55
2:S:844:CYS:O	2:S:848:VAL:HG23	2.07	0.55
1:L:61:LYS:O	1:L:62:GLU:HB2	2.07	0.55
1:L:25:ILE:HG22	1:L:26:LYS:N	2.22	0.55
1:L:327:SER:C	1:L:329:SER:N	2.59	0.55
1:L:464:THR:CG2	1:L:465:PHE:N	2.69	0.55
1:L:492:ASN:ND2	1:L:625:TYR:OH	2.39	0.55
1:L:530:ILE:C	1:L:532:ASP:H	2.07	0.55
1:L:64:GLY:O	1:L:67:SER:HB3	2.07	0.55
1:L:387:TYR:HB3	1:L:510:GLN:O	2.07	0.55
1:L:574:ILE:HG23	1:L:575:GLU:N	2.21	0.55
1:L:575:GLU:O	1:L:578:LYS:HB3	2.06	0.55
2:S:819:GLU:HA	2:S:822:ASN:HD21	1.72	0.55
2:S:884:ASP:OD1	2:S:886:SER:N	2.39	0.54
2:S:885:ARG:O	2:S:885:ARG:HG2	2.07	0.54
1:L:358:LEU:HD13	1:L:502:PHE:CE2	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:433:ILE:HA	1:L:484:LEU:HA	1.90	0.54
1:L:616:VAL:O	1:L:617:ASP:OD1	2.25	0.54
2:S:910:TYR:O	2:S:911:ASN:C	2.46	0.54
2:S:874:TRP:HB2	2:S:930:ILE:HD11	1.89	0.54
1:L:216:GLU:HG3	1:L:218:LYS:HG2	1.90	0.54
1:L:282:ILE:HG22	1:L:282:ILE:O	2.06	0.54
1:L:486:PRO:O	1:L:487:SER:HB3	2.07	0.54
1:L:338:LEU:N	1:L:338:LEU:HD12	2.22	0.54
1:L:455:THR:HG22	1:L:456:ASN:N	2.22	0.54
1:L:530:ILE:HD12	1:L:535:ARG:CB	2.37	0.54
1:L:286:ASN:ND2	1:L:288:TRP:N	2.56	0.54
1:L:27:TYR:CD2	1:L:28:LEU:HG	2.43	0.54
1:L:406:THR:HA	1:L:476:LYS:HA	1.90	0.54
1:L:528:ASP:CG	1:L:529:ASP:N	2.60	0.54
1:L:161:LYS:O	1:L:162:ASP:HB2	2.08	0.54
1:L:201:THR:HG22	1:L:338:LEU:CD2	2.34	0.54
1:L:602:THR:O	1:L:605:GLN:HB2	2.08	0.54
1:L:689:LEU:HD12	2:S:954:ILE:HD11	1.88	0.54
2:S:898:PHE:CE2	2:S:913:ILE:HG21	2.42	0.54
1:L:168:VAL:O	1:L:179:ALA:HB2	2.08	0.54
1:L:228:ILE:O	1:L:231:ALA:HB3	2.08	0.54
1:L:188:ILE:O	1:L:188:ILE:HD13	2.08	0.53
1:L:236:SER:C	1:L:237:LEU:HD23	2.29	0.53
1:L:54:ILE:CD1	1:L:54:ILE:H	2.18	0.53
1:L:107:LEU:HD12	1:L:182:GLU:HG3	1.89	0.53
1:L:419:GLN:HG2	1:L:425:ASP:HB2	1.89	0.53
1:L:520:LEU:HD22	1:L:520:LEU:N	2.23	0.53
1:L:659:PHE:O	1:L:662:PHE:HB3	2.08	0.53
1:L:95:THR:O	1:L:96:ASP:CB	2.56	0.53
2:S:875:GLN:HG2	2:S:875:GLN:O	2.08	0.53
2:S:821:MET:HB2	2:S:844:CYS:SG	2.49	0.53
2:S:814:GLU:HG2	2:S:858:LYS:HB3	1.91	0.53
1:L:438:GLU:HG2	1:L:438:GLU:O	2.08	0.53
2:S:876:ALA:O	2:S:877:ILE:C	2.47	0.53
2:S:890:CYS:HB3	2:S:893:GLU:CB	2.27	0.53
1:L:113:SER:HB2	1:L:204:PHE:CZ	2.43	0.53
1:L:281:LEU:CD2	1:L:296:ARG:HE	2.21	0.53
1:L:366:ARG:HE	2:S:856:THR:CG2	2.21	0.53
1:L:531:ASP:O	1:L:533:GLY:N	2.34	0.53
1:L:58:LEU:HD13	1:L:75:TRP:HZ2	1.74	0.53
1:L:193:GLU:O	1:L:193:GLU:CG	2.56	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:806:ALA:O	2:S:810:GLY:HA2	2.09	0.53
2:S:890:CYS:SG	2:S:893:GLU:HG3	2.49	0.53
1:L:627:MET:O	1:L:631:LEU:HG	2.09	0.52
1:L:656:ILE:HD12	1:L:656:ILE:N	2.24	0.52
2:S:825:ASN:O	2:S:826:LYS:HB2	2.09	0.52
1:L:6:ALA:C	1:L:8:LEU:N	2.61	0.52
1:L:356:TRP:HE3	1:L:503:SER:O	1.92	0.52
1:L:639:PRO:HD2	1:L:642:LEU:HD23	1.90	0.52
1:L:411:LEU:HD11	1:L:486:PRO:CB	2.40	0.52
1:L:198:GLY:HA2	1:L:422:MET:HE2	1.90	0.52
2:S:802:ARG:HA	2:S:861:PHE:CE2	2.45	0.52
2:S:864:PHE:CD2	2:S:864:PHE:C	2.82	0.52
2:S:889:ILE:CG2	2:S:894:LEU:HD23	2.40	0.52
1:L:111:ILE:O	1:L:114:LEU:HB2	2.10	0.52
1:L:138:ILE:HD11	1:L:153:VAL:HG13	1.92	0.52
1:L:530:ILE:HB	1:L:535:ARG:HB2	1.92	0.52
1:L:409:VAL:HG22	1:L:501:VAL:HG22	1.92	0.52
2:S:852:ASP:HB3	2:S:967:TYR:HE2	1.75	0.52
1:L:2:ALA:O	1:L:3:GLY:O	2.26	0.52
1:L:530:ILE:HD12	1:L:535:ARG:HB2	1.91	0.52
2:S:801:PHE:HZ	2:S:827:VAL:HG21	1.75	0.52
2:S:894:LEU:N	2:S:895:PRO:CD	2.72	0.52
1:L:211:ILE:O	1:L:211:ILE:CG2	2.58	0.51
1:L:114:LEU:HD23	1:L:120:ILE:CG2	2.35	0.51
1:L:124:VAL:HG22	1:L:207:PHE:O	2.10	0.51
1:L:349:THR:O	1:L:350:SER:CB	2.58	0.51
1:L:102:LEU:CD1	1:L:102:LEU:N	2.74	0.51
1:L:349:THR:O	1:L:350:SER:HB2	2.10	0.51
1:L:237:LEU:C	1:L:238:LEU:HD12	2.31	0.51
1:L:538:PHE:CG	1:L:539:ALA:N	2.78	0.51
1:L:527:GLU:CG	1:L:527:GLU:O	2.59	0.51
1:L:286:ASN:HD21	1:L:288:TRP:HB2	1.75	0.51
1:L:444:THR:C	1:L:446:ILE:H	2.14	0.51
1:L:497:PHE:C	1:L:497:PHE:CD1	2.83	0.51
1:L:561:LEU:O	1:L:562:ALA:HB2	2.10	0.51
1:L:615:ASP:O	1:L:617:ASP:N	2.35	0.51
1:L:638:MET:CG	1:L:643:HIS:HE2	2.12	0.51
1:L:674:LYS:O	1:L:678:GLN:HG2	2.11	0.51
1:L:195:LEU:H	1:L:195:LEU:HD12	1.74	0.51
1:L:626:GLU:HA	1:L:626:GLU:OE1	2.11	0.51
1:L:668:ARG:CZ	1:L:700:LEU:HD12	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:815:VAL:HG22	2:S:819:GLU:CB	2.40	0.51
2:S:847:MET:HE2	2:S:871:ILE:HD11	1.93	0.51
1:L:113:SER:HB2	1:L:204:PHE:HZ	1.76	0.51
1:L:343:LEU:O	1:L:346:ASP:OD2	2.28	0.51
1:L:428:THR:HG22	1:L:465:PHE:HB3	1.93	0.51
1:L:357:LYS:HE3	1:L:505:LYS:HA	1.93	0.51
1:L:196:SER:O	1:L:421:LYS:HD3	2.10	0.50
1:L:660:ASP:O	1:L:663:VAL:HG22	2.11	0.50
2:S:839:PHE:HD1	2:S:843:THR:HG21	1.76	0.50
1:L:121:LEU:O	1:L:121:LEU:HD23	2.11	0.50
1:L:155:ASP:C	1:L:155:ASP:OD2	2.50	0.50
1:L:228:ILE:HG23	1:L:238:LEU:CD2	2.41	0.50
1:L:31:ASP:O	1:L:35:LEU:HD13	2.11	0.50
1:L:413:GLN:HE21	1:L:429:ILE:HD12	1.76	0.50
1:L:629:LYS:O	1:L:632:GLU:HB3	2.12	0.50
2:S:946:LEU:HD11	2:S:964:LEU:HD11	1.91	0.50
1:L:75:TRP:CH2	1:L:159:PRO:HG3	2.47	0.50
1:L:98:CYS:SG	1:L:169:HIS:CE1	3.04	0.50
1:L:229:GLN:O	1:L:233:GLN:CB	2.60	0.50
1:L:455:THR:O	1:L:456:ASN:C	2.50	0.50
1:L:381:PHE:HE2	1:L:453:PHE:CD2	2.30	0.50
1:L:383:MET:SD	1:L:625:TYR:CD2	2.93	0.50
2:S:910:TYR:O	2:S:913:ILE:N	2.44	0.50
1:L:131:PHE:N	1:L:131:PHE:HD1	2.09	0.50
1:L:579:ILE:O	1:L:579:ILE:HD13	2.12	0.50
2:S:876:ALA:O	2:S:879:LYS:N	2.45	0.50
1:L:194:ALA:O	1:L:422:MET:HG3	2.12	0.50
2:S:830:ARG:HG2	2:S:831:HIS:N	2.27	0.50
1:L:24:ALA:HB1	1:L:149:TRP:O	2.12	0.50
1:L:277:SER:O	1:L:278:LEU:HB3	2.12	0.50
1:L:375:ARG:HG2	1:L:376:ASN:OD1	2.12	0.50
1:L:436:VAL:HG22	1:L:483:ILE:HG12	1.94	0.50
1:L:195:LEU:CD1	1:L:195:LEU:N	2.73	0.50
1:L:568:LYS:HG3	1:L:619:SER:O	2.12	0.50
2:S:850:VAL:CG1	2:S:938:ALA:HB2	2.42	0.50
2:S:850:VAL:HG11	2:S:938:ALA:HB2	1.93	0.50
1:L:293:TRP:CH2	1:L:326:MET:HG2	2.46	0.49
1:L:116:LEU:HD11	1:L:287:PRO:HA	1.94	0.49
1:L:161:LYS:O	1:L:162:ASP:CB	2.60	0.49
1:L:176:PHE:O	1:L:177:TRP:C	2.50	0.49
1:L:447:HIS:HB2	1:L:513:ASP:HA	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:433:ILE:HG23	1:L:460:GLU:O	2.11	0.49
1:L:382:TRP:CE2	1:L:383:MET:HG3	2.47	0.49
1:L:35:LEU:O	1:L:39:CYS:HB2	2.12	0.49
1:L:412:ILE:HG13	1:L:413:GLN:N	2.28	0.49
1:L:600:LEU:HD12	1:L:604:ILE:HG12	1.94	0.49
1:L:198:GLY:HA3	1:L:422:MET:CE	2.42	0.49
1:L:685:GLY:O	2:S:957:ASN:HA	2.13	0.49
2:S:824:LEU:O	2:S:828:VAL:HG22	2.13	0.49
2:S:909:LEU:O	2:S:912:MET:HB2	2.11	0.49
1:L:416:ARG:O	1:L:417:ARG:C	2.51	0.49
1:L:430:GLY:HA3	1:L:465:PHE:CD1	2.48	0.49
1:L:53:ALA:HB1	1:L:75:TRP:CD2	2.47	0.49
1:L:292:GLU:O	1:L:293:TRP:HB3	2.12	0.49
1:L:168:VAL:HG13	1:L:178:SER:OG	2.13	0.49
1:L:415:HIS:O	1:L:416:ARG:HG3	2.12	0.48
1:L:504:GLU:C	1:L:505:LYS:HD2	2.34	0.48
1:L:576:THR:O	1:L:577:CYS:C	2.51	0.48
1:L:577:CYS:O	1:L:581:VAL:HG23	2.13	0.48
1:L:608:GLN:HA	1:L:659:PHE:CE2	2.47	0.48
1:L:230:LYS:C	1:L:233:GLN:HB3	2.33	0.48
1:L:409:VAL:O	1:L:472:LEU:HA	2.13	0.48
1:L:514:ASP:O	1:L:639:PRO:HG3	2.13	0.48
1:L:595:LYS:O	1:L:599:ILE:HG13	2.13	0.48
1:L:662:PHE:CE2	1:L:666:LEU:HD11	2.48	0.48
1:L:89:ILE:HD12	1:L:89:ILE:O	2.14	0.48
1:L:17:GLY:N	1:L:23:ARG:NH1	2.61	0.48
1:L:364:ASN:CB	1:L:366:ARG:NH1	2.75	0.48
1:L:387:TYR:HH	1:L:497:PHE:HZ	1.62	0.48
1:L:225:PHE:O	1:L:227:ILE:N	2.44	0.48
1:L:374:CYS:HB2	1:L:489:PHE:O	2.12	0.48
1:L:37:ASN:N	1:L:37:ASN:HD22	2.09	0.48
1:L:395:ASP:OD2	1:L:405:CYS:SG	2.64	0.48
1:L:447:HIS:HA	1:L:512:VAL:HG12	1.95	0.48
1:L:121:LEU:HD11	1:L:177:TRP:CH2	2.49	0.48
1:L:188:ILE:CG2	1:L:189:ASN:N	2.77	0.48
1:L:195:LEU:O	1:L:197:GLY:N	2.47	0.48
1:L:460:GLU:HG3	1:L:475:PHE:HE2	1.78	0.48
1:L:561:LEU:HD12	1:L:563:LYS:CD	2.39	0.48
1:L:698:SER:O	1:L:700:LEU:N	2.46	0.48
1:L:613:GLU:OE1	1:L:613:GLU:HA	2.13	0.48
1:L:592:LEU:CD2	1:L:596:GLU:HG3	2.37	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:700:LEU:N	2:S:935:ARG:HH22	2.12	0.48
2:S:903:PHE:CZ	2:S:936:LEU:HD23	2.49	0.48
1:L:668:ARG:O	1:L:672:LEU:HD23	2.14	0.48
1:L:78:PRO:HG2	1:L:131:PHE:CE2	2.47	0.48
2:S:881:PHE:CD2	2:S:881:PHE:N	2.82	0.47
2:S:898:PHE:HE2	2:S:913:ILE:HG21	1.77	0.47
1:L:281:LEU:HD21	1:L:296:ARG:HE	1.77	0.47
1:L:79:THR:C	1:L:81:ILE:H	2.17	0.47
1:L:200:THR:O	1:L:204:PHE:HB2	2.15	0.47
2:S:844:CYS:HA	2:S:847:MET:SD	2.53	0.47
1:L:476:LYS:O	1:L:477:LEU:HD23	2.14	0.47
1:L:623:ASN:HD22	1:L:623:ASN:H	1.62	0.47
1:L:230:LYS:O	1:L:233:GLN:HB3	2.15	0.47
1:L:47:GLN:HA	1:L:157:ARG:NH1	2.30	0.47
1:L:286:ASN:ND2	1:L:289:GLY:H	2.09	0.47
1:L:412:ILE:HA	1:L:470:GLU:CA	2.39	0.47
1:L:55:PRO:O	1:L:58:LEU:HB2	2.14	0.47
1:L:650:PHE:CE1	1:L:665:CYS:HB2	2.49	0.47
1:L:83:ALA:C	1:L:85:PRO:HD3	2.34	0.47
1:L:6:ALA:O	1:L:8:LEU:N	2.47	0.47
1:L:551:PHE:CD1	1:L:551:PHE:N	2.76	0.47
1:L:54:ILE:HB	1:L:55:PRO:CD	2.44	0.47
2:S:832:PRO:O	2:S:834:LEU:N	2.47	0.47
1:L:106:TRP:CH2	1:L:203:GLY:HA3	2.50	0.47
1:L:367:ARG:HG3	1:L:492:ASN:HB3	1.96	0.47
1:L:126:PRO:O	1:L:127:LEU:C	2.54	0.47
1:L:375:ARG:HG2	1:L:376:ASN:N	2.30	0.47
1:L:158:LEU:HD21	1:L:180:LEU:HD23	1.97	0.46
1:L:190:GLY:O	1:L:191:CYS:HB3	2.15	0.46
1:L:340:ILE:O	1:L:340:ILE:HG23	2.15	0.46
1:L:595:LYS:O	1:L:598:TYR:HB3	2.15	0.46
2:S:881:PHE:HD2	2:S:881:PHE:N	2.12	0.46
2:S:930:ILE:HA	2:S:933:LEU:HD12	1.96	0.46
1:L:102:LEU:CD2	1:L:166:LEU:HD12	2.41	0.46
1:L:242:ILE:HG12	1:L:335:TYR:H	1.80	0.46
1:L:459:ARG:O	1:L:460:GLU:CB	2.62	0.46
1:L:676:PHE:CD1	1:L:676:PHE:C	2.88	0.46
1:L:691:LEU:HD11	1:L:695:LEU:HD11	1.97	0.46
2:S:935:ARG:HH11	2:S:968:SER:HB2	1.80	0.46
1:L:274:SER:C	1:L:276:GLY:H	2.19	0.46
1:L:444:THR:HG23	1:L:445:ASN:N	2.23	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:664:ARG:HH22	2:S:916:ARG:HH21	1.63	0.46
1:L:157:ARG:NH2	3:L:708:HOH:O	2.47	0.46
1:L:286:ASN:HD21	1:L:288:TRP:CA	2.28	0.46
1:L:477:LEU:HB3	1:L:478:PRO:HD2	1.98	0.46
1:L:66:TYR:O	1:L:71:ARG:NH1	2.48	0.46
1:L:129:GLN:OE1	1:L:139:PHE:HB3	2.15	0.46
1:L:426:MET:HE2	1:L:426:MET:CA	2.46	0.46
1:L:530:ILE:C	1:L:532:ASP:N	2.68	0.46
1:L:700:LEU:HD22	2:S:916:ARG:HE	1.81	0.46
1:L:193:GLU:O	1:L:193:GLU:HG2	2.15	0.46
1:L:395:ASP:C	1:L:396:GLU:HG3	2.35	0.46
1:L:643:HIS:CD2	1:L:643:HIS:H	2.34	0.46
2:S:943:PHE:CE2	2:S:954:ILE:HG13	2.51	0.46
1:L:350:SER:O	1:L:351:ASP:HB2	2.16	0.46
1:L:445:ASN:O	1:L:445:ASN:CG	2.54	0.46
1:L:688:GLU:HB2	2:S:953:GLN:NE2	2.29	0.46
1:L:10:LYS:CD	1:L:10:LYS:O	2.63	0.45
1:L:413:GLN:HE21	1:L:429:ILE:CD1	2.29	0.45
1:L:600:LEU:HD11	1:L:604:ILE:HD11	1.97	0.45
1:L:74:ARG:HG3	1:L:74:ARG:NH1	2.29	0.45
1:L:19:GLY:N	1:L:23:ARG:O	2.47	0.45
1:L:391:LEU:HD11	1:L:407:PHE:CE2	2.49	0.45
1:L:365:TRP:CE2	1:L:487:SER:HA	2.51	0.45
2:S:804:LEU:O	2:S:808:LEU:HD12	2.16	0.45
1:L:530:ILE:O	1:L:531:ASP:HB2	2.16	0.45
1:L:99:GLN:NE2	1:L:168:VAL:CA	2.80	0.45
1:L:99:GLN:NE2	1:L:168:VAL:CG2	2.75	0.45
1:L:99:GLN:HE22	1:L:168:VAL:CA	2.29	0.45
1:L:455:THR:HG22	1:L:456:ASN:H	1.81	0.45
1:L:629:LYS:O	1:L:632:GLU:N	2.47	0.45
1:L:65:PRO:C	1:L:67:SER:H	2.19	0.45
1:L:240:CYS:HA	1:L:336:SER:O	2.17	0.45
1:L:281:LEU:HD21	1:L:296:ARG:NE	2.32	0.45
1:L:416:ARG:NH1	1:L:416:ARG:CG	2.79	0.45
1:L:516:ILE:HD12	1:L:516:ILE:H	1.81	0.45
2:S:832:PRO:C	2:S:834:LEU:N	2.69	0.45
2:S:841:ILE:O	2:S:845:ARG:HG3	2.16	0.45
2:S:916:ARG:NH1	2:S:916:ARG:O	2.50	0.45
2:S:962:LEU:O	2:S:966:MET:CB	2.60	0.45
1:L:233:GLN:HG3	1:L:354:LYS:HZ3	1.81	0.45
1:L:375:ARG:CG	1:L:376:ASN:N	2.79	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:444:THR:O	1:L:446:ILE:N	2.50	0.45
1:L:564:ARG:N	1:L:564:ARG:HD2	2.32	0.45
1:L:570:ASP:C	1:L:570:ASP:OD2	2.55	0.45
2:S:951:THR:O	2:S:952:GLY:C	2.53	0.45
1:L:99:GLN:HE22	1:L:168:VAL:CB	2.30	0.45
1:L:580:MET:HB3	1:L:600:LEU:HD21	1.98	0.45
1:L:78:PRO:CG	1:L:131:PHE:HE2	2.27	0.45
1:L:21:HIS:O	1:L:22:GLU:C	2.53	0.45
1:L:32:TYR:O	1:L:33:GLU:C	2.54	0.45
1:L:395:ASP:HA	1:L:505:LYS:NZ	2.32	0.45
1:L:377:TYR:CE2	1:L:491:PRO:HD3	2.52	0.45
1:L:609:LYS:O	1:L:613:GLU:HB2	2.17	0.45
2:S:841:ILE:O	2:S:841:ILE:HG23	2.16	0.45
2:S:864:PHE:CD2	2:S:865:LYS:N	2.84	0.45
2:S:865:LYS:O	2:S:866:TYR:C	2.55	0.45
1:L:126:PRO:HD2	1:L:140:HIS:O	2.17	0.45
1:L:78:PRO:HD3	1:L:156:ASP:HB2	1.98	0.45
1:L:412:ILE:HD11	1:L:469:ARG:NE	2.32	0.45
1:L:407:PHE:CE1	1:L:475:PHE:HB2	2.52	0.45
2:S:854:ASP:O	2:S:856:THR:HG23	2.17	0.45
1:L:155:ASP:OD2	1:L:183:LYS:NZ	2.50	0.45
1:L:390:LYS:HE2	1:L:481:GLU:HB3	1.97	0.45
1:L:434:TYR:CD1	1:L:434:TYR:N	2.85	0.45
1:L:4:ILE:O	1:L:8:LEU:HB2	2.17	0.45
2:S:911:ASN:O	2:S:912:MET:C	2.55	0.45
1:L:411:LEU:HD11	1:L:486:PRO:HB2	1.98	0.44
1:L:54:ILE:CB	1:L:55:PRO:CD	2.95	0.44
1:L:673:PHE:CZ	2:S:962:LEU:HD11	2.52	0.44
1:L:223:ASN:HD22	1:L:223:ASN:HA	1.55	0.44
1:L:561:LEU:HA	1:L:563:LYS:HE3	1.98	0.44
1:L:433:ILE:CA	1:L:483:ILE:O	2.65	0.44
1:L:592:LEU:HB3	1:L:596:GLU:HG3	1.98	0.44
1:L:686:THR:HA	2:S:956:VAL:O	2.17	0.44
1:L:102:LEU:CD1	1:L:102:LEU:H	2.29	0.44
1:L:106:TRP:CE2	1:L:107:LEU:HD22	2.52	0.44
1:L:377:TYR:CD1	1:L:377:TYR:N	2.85	0.44
1:L:525:ILE:HD13	1:L:525:ILE:N	2.32	0.44
1:L:606:LYS:O	1:L:607:TYR:C	2.56	0.44
2:S:804:LEU:HD13	2:S:823:ILE:HD12	1.98	0.44
1:L:446:ILE:O	1:L:512:VAL:HG13	2.18	0.44
1:L:490:GLU:CB	1:L:491:PRO:CD	2.96	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:847:MET:CE	2:S:867:LEU:HD21	2.47	0.44
1:L:439:GLU:OE1	1:L:439:GLU:N	2.51	0.44
1:L:2:ALA:C	2:S:853:SER:OG	2.56	0.44
1:L:457:ARG:HD2	1:L:457:ARG:O	2.18	0.44
1:L:610:ILE:HD13	1:L:633:GLU:HB2	1.99	0.44
1:L:691:LEU:O	1:L:694:TRP:HB3	2.18	0.44
2:S:950:GLY:C	2:S:952:GLY:H	2.21	0.44
1:L:25:ILE:O	1:L:151:GLU:N	2.49	0.44
1:L:343:LEU:C	1:L:345:PRO:HD2	2.39	0.44
1:L:366:ARG:HA	1:L:366:ARG:HD3	1.72	0.44
1:L:391:LEU:HD12	1:L:482:TYR:HE2	1.83	0.44
2:S:919:ASP:O	2:S:921:SER:N	2.51	0.44
1:L:99:GLN:NE2	1:L:168:VAL:CB	2.81	0.44
1:L:168:VAL:CG1	1:L:179:ALA:HA	2.44	0.44
1:L:242:ILE:O	1:L:243:ASP:C	2.57	0.44
1:L:293:TRP:HZ2	1:L:296:ARG:HB2	1.83	0.44
1:L:424:GLU:O	1:L:426:MET:CE	2.66	0.44
1:L:82:CYS:O	1:L:83:ALA:HB2	2.18	0.44
2:S:822:ASN:O	2:S:823:ILE:C	2.52	0.44
2:S:844:CYS:O	2:S:847:MET:HB2	2.17	0.44
1:L:676:PHE:CE2	2:S:958:ILE:HA	2.53	0.44
1:L:218:LYS:HD3	1:L:335:TYR:HD1	1.83	0.43
1:L:611:TYR:CG	1:L:659:PHE:HD2	2.36	0.43
1:L:19:GLY:O	1:L:149:TRP:HB2	2.17	0.43
1:L:225:PHE:C	1:L:227:ILE:N	2.71	0.43
1:L:600:LEU:O	1:L:603:LYS:N	2.51	0.43
1:L:74:ARG:HB2	1:L:160:THR:OG1	2.18	0.43
1:L:192:TYR:O	1:L:195:LEU:CD1	2.67	0.43
1:L:343:LEU:HG	1:L:346:ASP:OD2	2.19	0.43
1:L:411:LEU:CD1	1:L:486:PRO:HB3	2.48	0.43
1:L:583:MET:CG	1:L:583:MET:O	2.64	0.43
1:L:600:LEU:O	1:L:601:TRP:C	2.56	0.43
1:L:65:PRO:C	1:L:67:SER:N	2.72	0.43
1:L:676:PHE:CE1	1:L:687:ILE:HG23	2.53	0.43
2:S:821:MET:HA	2:S:844:CYS:SG	2.58	0.43
1:L:281:LEU:HD21	1:L:296:ARG:CZ	2.48	0.43
1:L:364:ASN:CB	1:L:366:ARG:HH12	2.23	0.43
1:L:691:LEU:CG	1:L:695:LEU:HD11	2.48	0.43
1:L:186:ALA:O	1:L:191:CYS:N	2.51	0.43
1:L:444:THR:C	1:L:446:ILE:N	2.72	0.43
1:L:624:SER:OG	1:L:655:LEU:O	2.37	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:96:ASP:OD1	1:L:171:ALA:HB3	2.18	0.43
1:L:46:PHE:CD2	1:L:138:ILE:HD12	2.53	0.43
1:L:138:ILE:HD11	1:L:153:VAL:CG1	2.49	0.43
1:L:282:ILE:HG23	1:L:284:ILE:HG13	1.99	0.43
1:L:411:LEU:CD2	1:L:429:ILE:HB	2.48	0.43
1:L:415:HIS:CG	1:L:416:ARG:N	2.87	0.43
1:L:419:GLN:HG2	1:L:425:ASP:CB	2.49	0.43
1:L:102:LEU:HD12	1:L:102:LEU:N	2.34	0.43
1:L:551:PHE:H	1:L:551:PHE:HD1	1.58	0.43
1:L:570:ASP:O	1:L:570:ASP:OD2	2.36	0.43
1:L:611:TYR:OH	1:L:621:THR:HA	2.18	0.43
2:S:848:VAL:O	2:S:852:ASP:HB2	2.19	0.43
2:S:864:PHE:HD2	2:S:865:LYS:N	2.16	0.43
1:L:12:ARG:NH2	2:S:960:GLU:OE2	2.52	0.43
1:L:524:ASP:OD1	1:L:524:ASP:O	2.36	0.43
2:S:912:MET:HE3	2:S:912:MET:HA	2.00	0.43
1:L:241:SER:C	1:L:242:ILE:HG13	2.37	0.43
1:L:328:PHE:C	1:L:330:ASP:N	2.68	0.43
1:L:430:GLY:HA3	1:L:465:PHE:CE1	2.54	0.43
1:L:643:HIS:CD2	1:L:643:HIS:N	2.87	0.43
1:L:644:GLN:O	1:L:645:VAL:C	2.55	0.43
2:S:879:LYS:HB3	2:S:879:LYS:NZ	2.34	0.43
1:L:165:LEU:HB2	1:L:169:HIS:CD2	2.54	0.43
1:L:343:LEU:O	1:L:343:LEU:HD12	2.18	0.43
1:L:372:GLY:O	1:L:491:PRO:HA	2.19	0.43
1:L:611:TYR:CE1	1:L:622:MET:HG2	2.54	0.43
1:L:641:GLN:O	1:L:644:GLN:HB2	2.19	0.43
1:L:7:LYS:O	1:L:7:LYS:HG3	2.19	0.43
2:S:878:TYR:HB2	2:S:929:PHE:HD2	1.79	0.43
2:S:910:TYR:CZ	2:S:914:ILE:HD11	2.54	0.43
1:L:382:TRP:N	1:L:382:TRP:CD1	2.87	0.42
1:L:468:LEU:C	1:L:468:LEU:CD1	2.88	0.42
1:L:490:GLU:HB3	1:L:491:PRO:HD2	2.02	0.42
1:L:367:ARG:HG3	1:L:492:ASN:CB	2.49	0.42
1:L:562:ALA:H	1:L:563:LYS:CD	2.23	0.42
1:L:668:ARG:HG2	1:L:672:LEU:HD23	2.02	0.42
1:L:347:THR:C	1:L:349:THR:H	2.22	0.42
1:L:419:GLN:H	1:L:419:GLN:HG3	1.39	0.42
1:L:468:LEU:HD13	1:L:470:GLU:O	2.19	0.42
1:L:79:THR:C	1:L:81:ILE:N	2.72	0.42
1:L:102:LEU:HD13	1:L:102:LEU:H	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:555:THR:O	1:L:556:ILE:C	2.56	0.42
1:L:658:ASP:OD1	1:L:658:ASP:C	2.58	0.42
1:L:695:LEU:O	1:L:699:VAL:HG12	2.20	0.42
1:L:127:LEU:O	1:L:128:ASN:HB2	2.18	0.42
1:L:202:GLU:O	1:L:204:PHE:N	2.53	0.42
1:L:213:GLU:HB3	1:L:472:LEU:HD21	2.02	0.42
1:L:286:ASN:ND2	1:L:288:TRP:H	2.17	0.42
1:L:37:ASN:ND2	1:L:37:ASN:N	2.68	0.42
1:L:461:ARG:O	1:L:462:SER:C	2.57	0.42
1:L:661:ASN:O	1:L:662:PHE:C	2.57	0.42
1:L:458:ALA:O	1:L:459:ARG:CB	2.62	0.42
1:L:66:TYR:CG	1:L:67:SER:N	2.87	0.42
2:S:877:ILE:CD1	2:S:877:ILE:N	2.68	0.42
1:L:375:ARG:HG2	1:L:376:ASN:H	1.85	0.42
1:L:430:GLY:O	1:L:431:PHE:HB3	2.19	0.42
1:L:499:ILE:CG2	1:L:509:TYR:OH	2.68	0.42
1:L:678:GLN:O	1:L:681:PRO:HG3	2.20	0.42
2:S:882:ASP:OD2	2:S:884:ASP:OD1	2.37	0.42
2:S:919:ASP:O	2:S:920:GLU:C	2.57	0.42
1:L:293:TRP:CZ2	1:L:296:ARG:HB2	2.54	0.42
1:L:341:CYS:HB3	1:L:356:TRP:CE2	2.53	0.42
1:L:352:THR:O	1:L:353:TYR:CB	2.65	0.42
1:L:516:ILE:N	1:L:516:ILE:HD12	2.35	0.42
1:L:563:LYS:CD	1:L:563:LYS:N	2.78	0.42
1:L:366:ARG:CG	1:L:644:GLN:OE1	2.65	0.42
2:S:808:LEU:HD22	2:S:819:GLU:HG2	2.01	0.42
1:L:430:GLY:HA3	1:L:465:PHE:CG	2.54	0.42
2:S:825:ASN:ND2	2:S:839:PHE:HD2	2.18	0.42
1:L:2:ALA:N	3:L:843:HOH:O	2.52	0.42
1:L:559:ARG:HG3	1:L:559:ARG:HH21	1.84	0.42
2:S:863:GLU:OE1	2:S:863:GLU:N	2.53	0.42
1:L:525:ILE:O	1:L:525:ILE:CD1	2.67	0.41
1:L:532:ASP:HA	1:L:535:ARG:CB	2.46	0.41
1:L:548:ILE:HG22	1:L:549:SER:H	1.85	0.41
1:L:604:ILE:O	1:L:605:GLN:C	2.58	0.41
1:L:7:LYS:HB2	2:S:853:SER:O	2.20	0.41
2:S:888:THR:HB	2:S:923:ASN:HB3	2.02	0.41
1:L:574:ILE:O	1:L:575:GLU:C	2.58	0.41
1:L:61:LYS:O	1:L:62:GLU:CB	2.68	0.41
1:L:180:LEU:O	1:L:183:LYS:N	2.53	0.41
1:L:411:LEU:HD23	1:L:429:ILE:CG1	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:562:ALA:C	1:L:563:LYS:HD2	2.39	0.41
1:L:628:ARG:HG3	1:L:643:HIS:HE1	1.85	0.41
1:L:208:THR:O	1:L:343:LEU:HD21	2.20	0.41
1:L:470:GLU:HG3	1:L:471:VAL:H	1.83	0.41
1:L:506:LYS:HB2	1:L:506:LYS:NZ	2.35	0.41
1:L:611:TYR:OH	1:L:621:THR:CA	2.69	0.41
2:S:828:VAL:C	2:S:830:ARG:H	2.23	0.41
2:S:909:LEU:O	2:S:910:TYR:C	2.57	0.41
2:S:850:VAL:HG13	2:S:938:ALA:CB	2.50	0.41
1:L:330:ASP:O	1:L:333:ARG:N	2.47	0.41
1:L:548:ILE:O	1:L:591:LYS:HA	2.21	0.41
1:L:574:ILE:CG2	1:L:575:GLU:N	2.84	0.41
1:L:579:ILE:HG23	1:L:667:VAL:CG1	2.51	0.41
1:L:369:SER:CB	1:L:647:VAL:HG21	2.36	0.41
1:L:88:ILE:O	1:L:88:ILE:HG23	2.21	0.41
2:S:870:ASN:HD22	2:S:870:ASN:HA	1.66	0.41
1:L:411:LEU:HD11	1:L:486:PRO:HB3	2.03	0.41
1:L:435:GLU:O	1:L:437:PRO:HD3	2.21	0.41
1:L:52:PRO:CB	1:L:54:ILE:HD11	2.44	0.41
1:L:558:ARG:C	1:L:560:VAL:N	2.70	0.41
1:L:126:PRO:HD3	1:L:141:PHE:HA	2.02	0.41
1:L:51:PHE:HB2	1:L:187:LYS:HE3	2.02	0.41
1:L:58:LEU:HA	1:L:58:LEU:HD12	1.93	0.41
1:L:638:MET:HA	1:L:639:PRO:HD3	1.78	0.41
1:L:680:ASP:N	1:L:681:PRO:HD3	2.34	0.41
1:L:500:ARG:C	1:L:501:VAL:HG23	2.41	0.41
1:L:579:ILE:O	1:L:580:MET:C	2.58	0.41
1:L:208:THR:OG1	1:L:209:GLY:N	2.53	0.41
1:L:538:PHE:O	1:L:540:GLN:N	2.53	0.41
1:L:691:LEU:HG	1:L:695:LEU:CD1	2.51	0.41
2:S:951:THR:C	2:S:953:GLN:N	2.72	0.41
1:L:17:GLY:O	1:L:18:LEU:C	2.58	0.41
1:L:294:THR:HG23	1:L:294:THR:O	2.21	0.41
1:L:447:HIS:HA	1:L:512:VAL:CG1	2.51	0.41
1:L:386:GLN:OE1	1:L:448:LEU:HB2	2.21	0.41
1:L:542:ALA:HB3	1:L:546:ALA:HA	2.01	0.41
1:L:608:GLN:HA	1:L:659:PHE:HE2	1.86	0.41
2:S:910:TYR:CE1	2:S:914:ILE:HD11	2.55	0.41
2:S:917:TYR:CE2	2:S:932:CYS:HA	2.56	0.41
1:L:694:TRP:CD1	2:S:943:PHE:HD2	2.39	0.41
1:L:180:LEU:C	1:L:182:GLU:N	2.73	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:22:GLU:CD	1:L:22:GLU:N	2.57	0.41
1:L:411:LEU:HD12	1:L:499:ILE:CG1	2.47	0.41
2:S:840:GLY:HA2	3:S:157:HOH:O	2.21	0.41
1:L:160:THR:HA	1:L:164:GLU:O	2.21	0.40
1:L:373:GLY:O	1:L:489:PHE:O	2.38	0.40
1:L:380:THR:HA	1:L:383:MET:CE	2.50	0.40
1:L:499:ILE:HG22	1:L:499:ILE:O	2.21	0.40
1:L:642:LEU:HA	1:L:645:VAL:HG13	2.02	0.40
1:L:168:VAL:HG11	1:L:182:GLU:HB2	2.04	0.40
1:L:227:ILE:HA	1:L:227:ILE:HD13	1.87	0.40
1:L:690:ASP:OD1	1:L:693:SER:OG	2.38	0.40
2:S:821:MET:CB	2:S:844:CYS:SG	3.08	0.40
1:L:161:LYS:HB3	1:L:166:LEU:HD21	2.04	0.40
1:L:185:TYR:O	1:L:188:ILE:HG22	2.21	0.40
1:L:343:LEU:HD13	1:L:345:PRO:CG	2.48	0.40
1:L:365:TRP:CZ2	1:L:487:SER:HA	2.56	0.40
1:L:448:LEU:H	1:L:512:VAL:CG1	2.34	0.40
2:S:929:PHE:O	2:S:933:LEU:CD1	2.69	0.40
1:L:205:GLU:O	1:L:209:GLY:N	2.53	0.40
1:L:499:ILE:HG21	1:L:509:TYR:OH	2.21	0.40
1:L:630:ALA:O	1:L:633:GLU:N	2.55	0.40
1:L:68:SER:O	1:L:69:LYS:C	2.60	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	L	628/699 (90%)	416 (66%)	149 (24%)	63 (10%)	0	3
2	S	174/184 (95%)	132 (76%)	28 (16%)	14 (8%)	1	5
All	All	802/883 (91%)	548 (68%)	177 (22%)	77 (10%)	0	3

All (77) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	34	ALA
1	L	61	LYS
1	L	62	GLU
1	L	82	CYS
1	L	83	ALA
1	L	128	ASN
1	L	198	GLY
1	L	350	SER
1	L	458	ALA
1	L	459	ARG
1	L	464	THR
1	L	470	GLU
1	L	479	PRO
1	L	490	GLU
1	L	544	GLU
1	L	562	ALA
1	L	616	VAL
2	S	826	LYS
2	S	877	ILE
2	S	916	ARG
2	S	927	ASP
1	L	3	GLY
1	L	17	GLY
1	L	18	LEU
1	L	80	GLU
1	L	81	ILE
1	L	92	ALA
1	L	105	CYS
1	L	127	LEU
1	L	174	SER
1	L	178	SER
1	L	196	SER
1	L	373	GLY
1	L	374	CYS
1	L	417	ARG
1	L	489	PHE
1	L	506	LYS
1	L	569	SER
2	S	833	ASP
2	S	905	LEU
2	S	920	GLU
2	S	952	GLY

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Mol	Chain	Res	Type
1	L	46	PHE
1	L	101	ALA
1	L	161	LYS
1	L	226	LYS
1	L	231	ALA
1	L	275	ASN
1	L	327	SER
1	L	418	ARG
1	L	445	ASN
1	L	532	ASP
1	L	539	ALA
2	S	841	ILE
2	S	902	GLY
1	L	72	GLY
1	L	491	PRO
1	L	630	ALA
1	L	655	LEU
1	L	692	ILE
1	L	699	VAL
2	S	813	MET
2	S	950	GLY
1	L	7	LYS
1	L	203	GLY
1	L	462	SER
1	L	589	SER
1	L	600	LEU
1	L	673	PHE
1	L	691	LEU
1	L	698	SER
2	S	951	THR
1	L	146	TYR
1	L	460	GLU
2	S	910	TYR
1	L	65	PRO
1	L	295	GLY

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	L	550/602 (91%)	467 (85%)	83 (15%)	3	13
2	S	155/162 (96%)	142 (92%)	13 (8%)	11	37
All	All	705/764 (92%)	609 (86%)	96 (14%)	3	16

All (96) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	4	ILE
1	L	7	LYS
1	L	10	LYS
1	L	12	ARG
1	L	39	CYS
1	L	44	THR
1	L	48	ASP
1	L	54	ILE
1	L	58	LEU
1	L	66	TYR
1	L	84	ASP
1	L	93	THR
1	L	108	LEU
1	L	117	ASN
1	L	118	GLU
1	L	131	PHE
1	L	134	ASN
1	L	140	HIS
1	L	154	VAL
1	L	156	ASP
1	L	168	VAL
1	L	188	ILE
1	L	191	CYS
1	L	201	THR
1	L	208	THR
1	L	219	LYS
1	L	223	ASN
1	L	240	CYS
1	L	280	LYS
1	L	282	ILE
1	L	285	ARG
1	L	328	PHE
1	L	336	SER
1	L	338	LEU

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Mol	Chain	Res	Type
1	L	355	LYS
1	L	357	LYS
1	L	361	MET
1	L	364	ASN
1	L	374	CYS
1	L	379	ASN
1	L	408	LEU
1	L	412	ILE
1	L	416	ARG
1	L	426	MET
1	L	429	ILE
1	L	433	ILE
1	L	459	ARG
1	L	463	ASP
1	L	466	ILE
1	L	468	LEU
1	L	470	GLU
1	L	472	LEU
1	L	473	ASN
1	L	479	PRO
1	L	484	LEU
1	L	500	ARG
1	L	506	LYS
1	L	520	LEU
1	L	525	ILE
1	L	527	GLU
1	L	540	GLN
1	L	551	PHE
1	L	557	LEU
1	L	563	LYS
1	L	568	LYS
1	L	579	ILE
1	L	595	LYS
1	L	600	LEU
1	L	602	THR
1	L	612	ARG
1	L	617	ASP
1	L	618	ARG
1	L	622	MET
1	L	627	MET
1	L	638	MET
1	L	641	GLN

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Mol	Chain	Res	Type
1	L	645	VAL
1	L	653	ASP
1	L	671	THR
1	L	686	THR
1	L	689	LEU
1	L	693	SER
1	L	699	VAL
2	S	801	PHE
2	S	804	LEU
2	S	808	LEU
2	S	815	VAL
2	S	816	SER
2	S	822	ASN
2	S	833	ASP
2	S	863	GLU
2	S	869	ASN
2	S	872	LYS
2	S	912	MET
2	S	933	LEU
2	S	958	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	30	GLN
1	L	37	ASN
1	L	99	GLN
1	L	134	ASN
1	L	189	ASN
1	L	223	ASN
1	L	229	GLN
1	L	286	ASN
1	L	364	ASN
1	L	379	ASN
1	L	384	ASN
1	L	492	ASN
1	L	519	ASN
1	L	623	ASN
2	S	822	ASN
2	S	825	ASN
2	S	870	ASN
2	S	875	GLN

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Mol	Chain	Res	Type
2	S	880	GLN
2	S	953	GLN
2	S	955	GLN
2	S	959	GLN

5.3.3 RNA [i](#)

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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.