



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 10:45 AM UTC

PDB ID : 1KFU / pdb_00001kfu
Title : Crystal Structure of Human m-Calpain Form II
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 : 2.50 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	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

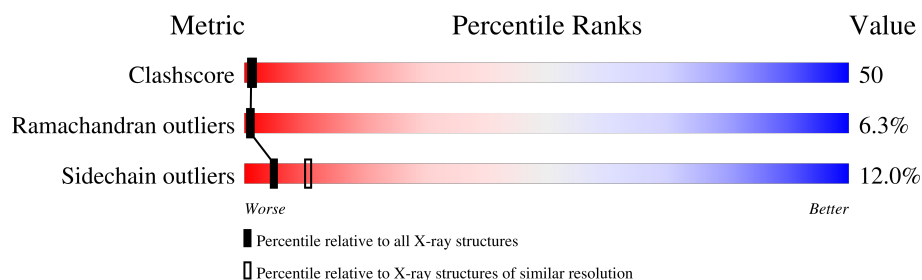
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 Å.

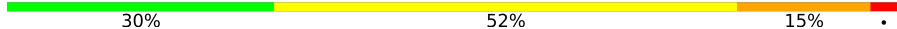
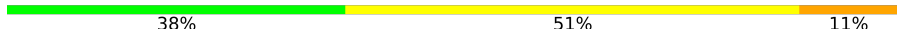
Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)

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 $\leq 5\%$.

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 7530 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 M-CALPAIN LARGE SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	699	Total	C	N	O	S	0	0	0
			5628	3568	955	1079	26			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	S	184	Total	C	N	O	S	10	0	0
			1491	935	255	290	11			

- Molecule 3 is water.

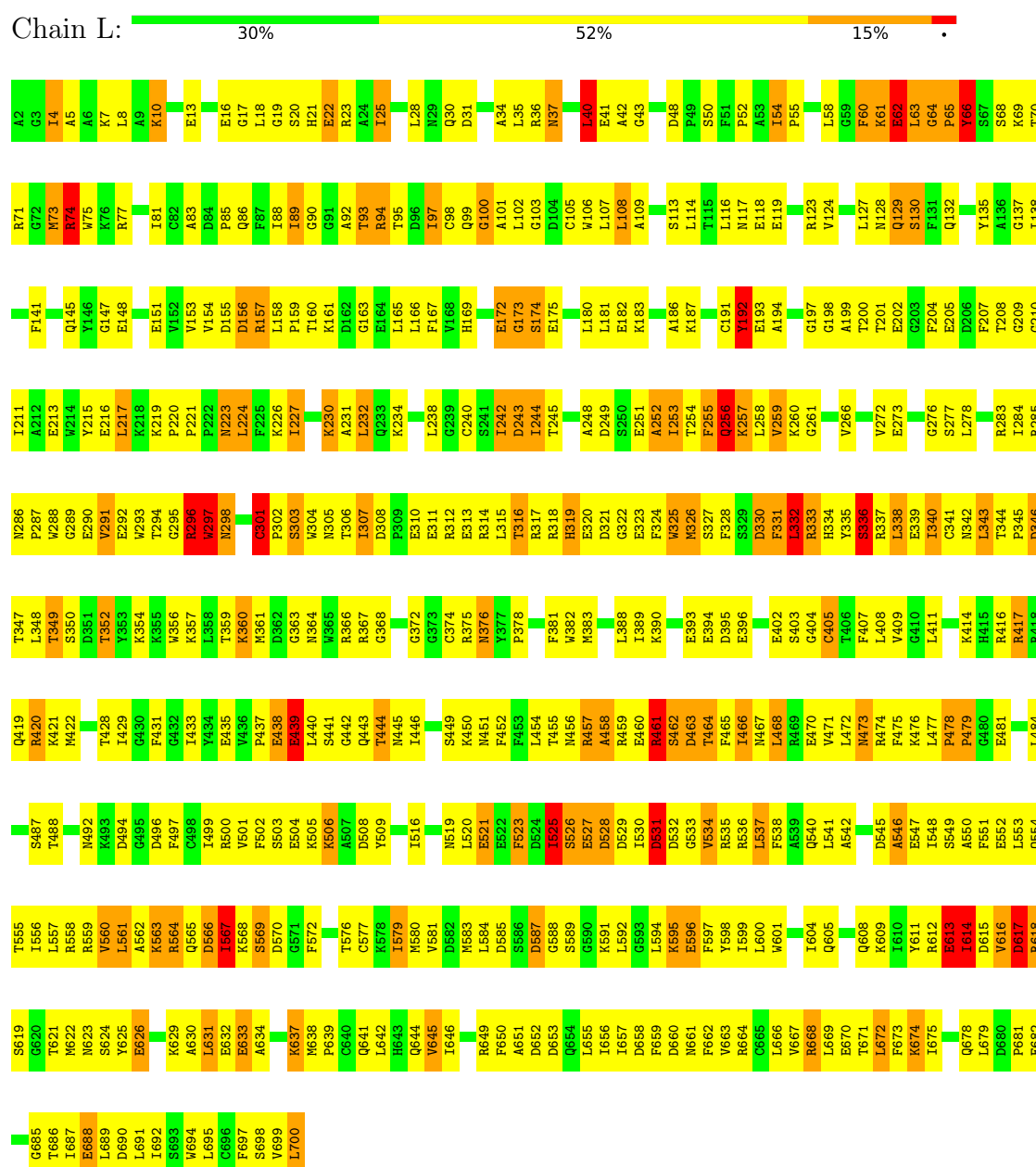
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	L	287	Total	O	0	0
			287	287		
3	S	124	Total	O	0	0
			124	124		

3 Residue-property plots

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.

Note EDS was not executed.

• Molecule 1: M-CALPAIN LARGE SUBUNIT



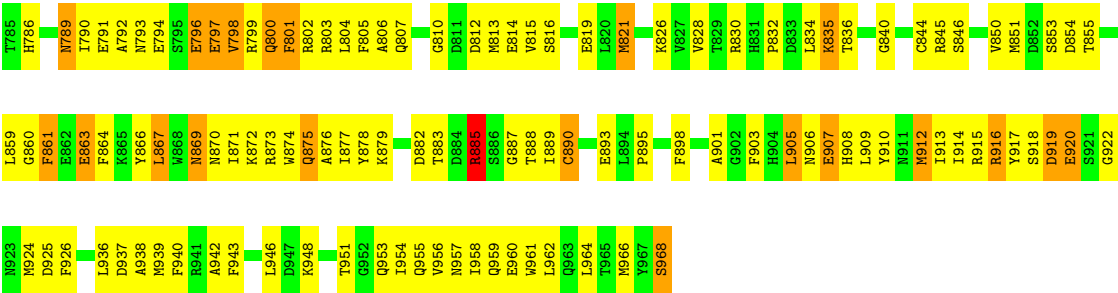
● Molecule 2: M-CALPAIN SMALL SUBUNIT

Chain S:

38%

51%

11%



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	51.88Å 169.84Å 64.44Å 90.00° 95.12° 90.00°	Depositor
Resolution (Å)	30.00 – 2.50	Depositor
% Data completeness (in resolution range)	(Not available) (30.00-2.50)	Depositor
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.221 , 0.276	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7530	wwPDB-VP
Average B, all atoms (Å ²)	17.0	wwPDB-VP

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	L	0.77	12/5752 (0.2%)	1.23	62/7768 (0.8%)
2	S	0.70	2/1520 (0.1%)	1.09	10/2046 (0.5%)
All	All	0.75	14/7272 (0.2%)	1.20	72/9814 (0.7%)

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	462	SER	N-CA	7.98	1.56	1.46
1	L	62	GLU	C-N	-7.73	1.20	1.34
1	L	461	ARG	C-N	7.36	1.44	1.33
1	L	322	GLY	C-N	-6.90	1.23	1.33
1	L	326	MET	N-CA	6.27	1.54	1.45
1	L	325	TRP	N-CA	6.26	1.54	1.46
2	S	968	SER	C-O	5.99	1.35	1.23
1	L	463	ASP	C-N	-5.97	1.25	1.33
1	L	325	TRP	NE1-CE2	-5.88	1.30	1.37
1	L	154	VAL	CA-CB	5.62	1.61	1.55
2	S	968	SER	C-OXT	5.61	1.34	1.23
1	L	66	TYR	N-CA	5.54	1.53	1.46
1	L	325	TRP	CA-C	5.53	1.60	1.52
1	L	463	ASP	N-CA	5.18	1.52	1.46

All (72) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	62	GLU	CA-C-N	11.38	138.47	119.35
1	L	62	GLU	C-N-CA	11.38	138.47	119.35
1	L	375	ARG	N-CA-C	-10.16	100.89	113.18
1	L	396	GLU	N-CA-C	8.44	124.19	113.55
1	L	220	PRO	CA-C-N	8.11	125.50	119.66
1	L	220	PRO	C-N-CA	8.11	125.50	119.66
1	L	197	GLY	N-CA-C	-8.01	104.51	114.92
1	L	63	LEU	O-C-N	7.62	128.94	121.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	336	SER	N-CA-C	7.62	120.45	108.79
1	L	478	PRO	CA-C-N	7.51	129.23	119.84
1	L	478	PRO	C-N-CA	7.51	129.23	119.84
1	L	531	ASP	N-CA-C	7.38	121.59	112.58
1	L	521	GLU	N-CA-C	7.36	121.17	110.28
1	L	440	LEU	N-CA-C	-7.31	104.22	113.72
1	L	372	GLY	N-CA-C	7.13	121.29	112.73
1	L	209	GLY	N-CA-C	-7.00	105.82	114.92
1	L	458	ALA	N-CA-C	-6.87	99.40	109.63
1	L	352	THR	N-CA-C	6.72	118.61	111.28
1	L	296	ARG	N-CA-C	-6.64	96.66	110.80
2	S	908	HIS	N-CA-C	6.62	119.34	111.33
2	S	800	GLN	N-CA-C	-6.48	104.30	111.36
1	L	89	ILE	N-CA-C	6.43	117.36	107.78
1	L	613	GLU	N-CA-C	-6.22	105.54	113.01
1	L	255	PHE	O-C-N	6.22	130.80	122.96
1	L	63	LEU	N-CA-C	-6.21	104.51	113.21
1	L	297	TRP	N-CA-C	-6.18	97.64	110.80
1	L	403	SER	CB-CA-C	-6.14	109.48	116.54
1	L	305	ASN	N-CA-C	-6.13	106.78	114.56
1	L	54	ILE	CA-C-N	6.09	125.71	119.56
1	L	54	ILE	C-N-CA	6.09	125.71	119.56
1	L	598	TYR	N-CA-C	-6.03	104.82	111.82
1	L	64	GLY	CA-C-N	6.02	125.70	119.56
1	L	64	GLY	C-N-CA	6.02	125.70	119.56
1	L	308	ASP	N-CA-C	-5.99	96.58	109.81
1	L	653	ASP	N-CA-C	-5.95	105.99	113.18
2	S	940	PHE	N-CA-C	-5.94	104.19	112.45
1	L	530	ILE	N-CA-C	-5.89	103.41	111.89
1	L	301	CYS	N-CA-C	5.84	122.73	109.81
1	L	256	GLN	O-C-N	5.84	130.36	122.59
1	L	322	GLY	CA-C-N	5.82	131.92	123.13
1	L	322	GLY	C-N-CA	5.82	131.92	123.13
1	L	457	ARG	N-CA-C	-5.80	103.28	110.41
1	L	61	LYS	N-CA-C	5.77	119.35	111.39
1	L	124	VAL	N-CA-C	-5.72	106.89	111.81
1	L	405	CYS	N-CA-C	5.64	118.37	109.96
1	L	40	LEU	N-CA-C	-5.63	105.05	111.07
1	L	48	ASP	CA-C-N	5.61	126.10	120.04
1	L	48	ASP	C-N-CA	5.61	126.10	120.04
1	L	631	LEU	N-CA-C	-5.61	106.39	113.18
2	S	916	ARG	N-CA-C	5.55	117.33	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	S	801	PHE	N-CA-C	-5.51	105.17	111.07
1	L	697	PHE	N-CA-C	5.49	118.44	111.69
2	S	875	GLN	N-CA-C	-5.46	105.42	111.36
2	S	869	ASN	N-CA-C	-5.41	105.28	111.07
1	L	257	LYS	CA-C-N	-5.37	114.23	122.87
1	L	257	LYS	C-N-CA	-5.37	114.23	122.87
1	L	534	VAL	N-CA-C	-5.36	104.35	111.05
1	L	668	ARG	N-CA-C	-5.32	105.38	111.07
2	S	919	ASP	O-C-N	5.30	129.00	123.06
1	L	100	GLY	N-CA-C	-5.29	104.23	112.58
1	L	65	PRO	N-CA-C	5.25	120.66	113.84
1	L	445	ASN	N-CA-C	5.24	118.98	112.59
1	L	332	LEU	N-CA-C	-5.23	99.66	110.80
1	L	74	ARG	N-CA-C	5.23	118.14	109.46
1	L	272	VAL	N-CA-C	5.14	116.13	108.46
2	S	867	LEU	N-CA-C	5.10	116.53	110.97
2	S	861	PHE	N-CA-C	-5.10	104.70	112.04
1	L	129	GLN	N-CA-C	5.08	117.69	109.40
1	L	614	ILE	N-CA-C	-5.08	106.70	111.48
1	L	637	LYS	N-CA-C	-5.03	101.77	109.41
1	L	217	LEU	N-CA-C	5.02	119.25	113.18
1	L	192	TYR	N-CA-C	-5.01	105.94	111.71

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	L	5628	0	5467	587	0
2	S	1491	0	1423	143	0
3	L	287	0	0	21	0
3	S	124	0	0	10	0
All	All	7530	0	6890	699	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 50.

All (699) 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:248:ALA:O	1:L:259:VAL:HG12	1.36	1.21
1:L:525:ILE:HG22	1:L:595:LYS:HD2	1.27	1.17
1:L:61:LYS:H	1:L:64:GLY:HA3	1.05	1.11
2:S:869:ASN:HA	2:S:872:LYS:HE2	1.24	1.10
1:L:74:ARG:H	1:L:74:ARG:HD2	1.10	1.09
2:S:799:ARG:HD3	2:S:802:ARG:HD2	1.36	1.08
1:L:61:LYS:N	1:L:64:GLY:HA3	1.67	1.06
1:L:506:LYS:H	1:L:506:LYS:HD2	1.20	1.05
1:L:248:ALA:O	1:L:259:VAL:CG1	2.07	1.02
1:L:116:LEU:HD22	1:L:285:ARG:HH12	1.18	1.02
1:L:61:LYS:HE3	1:L:66:TYR:HB3	1.41	1.01
1:L:315:LEU:HA	1:L:318:ARG:HH21	1.25	0.98
1:L:516:ILE:HD11	2:S:959:GLN:HG2	1.44	0.97
1:L:450:LYS:HG2	1:L:454:LEU:HD11	1.48	0.95
1:L:204:PHE:HB3	1:L:340:ILE:HG13	1.46	0.95
2:S:905:LEU:HD22	2:S:905:LEU:H	1.28	0.95
1:L:116:LEU:HD22	1:L:285:ARG:NH1	1.81	0.94
1:L:253:ILE:HG22	1:L:254:THR:H	1.29	0.94
1:L:61:LYS:HE3	1:L:66:TYR:CB	1.96	0.94
1:L:576:THR:HG22	1:L:580:MET:HE2	1.47	0.93
1:L:315:LEU:HA	1:L:318:ARG:NH2	1.83	0.93
1:L:631:LEU:HD13	1:L:638:MET:HE1	1.52	0.92
1:L:561:LEU:H	1:L:561:LEU:HD23	1.34	0.91
1:L:525:ILE:CG2	1:L:595:LYS:HD2	1.99	0.91
2:S:957:ASN:HB2	3:S:221:HOH:O	1.70	0.90
1:L:431:PHE:H	1:L:462:SER:HB2	1.36	0.90
1:L:588:GLY:HA2	2:S:915:ARG:HH12	1.36	0.88
1:L:374:CYS:SG	3:L:838:HOH:O	2.31	0.86
1:L:208:THR:HG22	1:L:210:GLY:H	1.41	0.85
1:L:77:ARG:HD3	1:L:156:ASP:OD2	1.77	0.85
1:L:28:LEU:HD13	1:L:50:SER:HB3	1.58	0.84
1:L:74:ARG:HD2	1:L:74:ARG:N	1.91	0.84
1:L:626:GLU:HG3	1:L:629:LYS:HD2	1.55	0.84
1:L:4:ILE:HD11	2:S:964:LEU:HA	1.60	0.84
1:L:74:ARG:H	1:L:74:ARG:CD	1.91	0.84
1:L:296:ARG:HG3	1:L:317:ARG:NH1	1.93	0.83
1:L:668:ARG:O	1:L:672:LEU:HD22	1.78	0.83
1:L:52:PRO:HB2	1:L:54:ILE:HG12	1.59	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:204:PHE:HB3	1:L:340:ILE:CG1	2.09	0.82
1:L:71:ARG:O	1:L:161:LYS:HE2	1.79	0.82
1:L:560:VAL:HB	1:L:561:LEU:HD23	1.62	0.82
1:L:442:GLY:HA2	1:L:446:ILE:HB	1.60	0.81
2:S:799:ARG:NH1	2:S:802:ARG:HD3	1.95	0.81
1:L:506:LYS:H	1:L:506:LYS:CD	1.92	0.81
1:L:506:LYS:HD2	1:L:506:LYS:N	1.96	0.80
1:L:86:GLN:O	1:L:175:GLU:HA	1.82	0.80
1:L:248:ALA:C	1:L:259:VAL:CG1	2.54	0.80
1:L:626:GLU:HA	1:L:629:LYS:NZ	1.97	0.80
2:S:873:ARG:HD2	3:S:268:HOH:O	1.81	0.80
1:L:208:THR:HG21	1:L:340:ILE:HG21	1.63	0.79
2:S:797:GLU:HG3	2:S:798:VAL:H	1.45	0.79
1:L:698:SER:HB2	2:S:939:MET:HG3	1.63	0.79
1:L:13:GLU:OE1	1:L:23:ARG:NH2	2.15	0.78
1:L:617:ASP:O	1:L:619:SER:N	2.15	0.78
1:L:563:LYS:O	1:L:564:ARG:HB2	1.82	0.78
1:L:549:SER:HA	1:L:591:LYS:HA	1.65	0.78
1:L:256:GLN:CD	1:L:256:GLN:H	1.90	0.77
1:L:328:PHE:C	1:L:330:ASP:H	1.92	0.77
1:L:405:CYS:SG	1:L:479:PRO:HG3	2.25	0.77
1:L:428:THR:HG22	1:L:465:PHE:HB3	1.63	0.77
1:L:156:ASP:HA	1:L:180:LEU:HD21	1.66	0.77
1:L:588:GLY:HA2	2:S:915:ARG:NH1	1.99	0.77
1:L:253:ILE:HG13	1:L:332:LEU:HD22	1.66	0.77
2:S:877:ILE:HD13	2:S:901:ALA:HA	1.67	0.77
1:L:258:LEU:HB3	1:L:260:LYS:HD2	1.67	0.76
1:L:663:VAL:O	1:L:667:VAL:HG23	1.84	0.76
1:L:505:LYS:HG3	1:L:506:LYS:NZ	2.01	0.76
1:L:31:ASP:HB3	1:L:34:ALA:HB3	1.66	0.76
1:L:248:ALA:C	1:L:259:VAL:HG11	2.10	0.76
1:L:242:ILE:O	1:L:261:GLY:HA2	1.86	0.76
1:L:361:MET:HG3	1:L:509:TYR:CE2	2.21	0.75
1:L:116:LEU:CD2	1:L:285:ARG:HH12	1.97	0.75
1:L:217:LEU:HD22	1:L:331:PHE:HE2	1.49	0.75
1:L:347:THR:O	1:L:349:THR:N	2.20	0.75
1:L:669:LEU:O	1:L:673:PHE:HD2	1.69	0.74
1:L:699:VAL:HG11	2:S:912:MET:HB3	1.69	0.74
1:L:208:THR:HG21	1:L:340:ILE:CG2	2.17	0.74
1:L:554:GLN:CG	1:L:558:ARG:HH22	2.00	0.74
1:L:256:GLN:HB3	3:L:870:HOH:O	1.87	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:637:LYS:O	1:L:638:MET:HG3	1.88	0.73
1:L:255:PHE:HD2	1:L:333:ARG:HB3	1.53	0.73
1:L:301:CYS:O	1:L:303:SER:N	2.19	0.73
1:L:361:MET:HG3	1:L:509:TYR:HE2	1.54	0.73
1:L:95:THR:HG22	1:L:97:ILE:HG22	1.70	0.73
2:S:910:TYR:O	2:S:914:ILE:HG12	1.89	0.72
1:L:561:LEU:HD23	1:L:561:LEU:N	2.03	0.72
3:L:916:HOH:O	2:S:790:ILE:HD12	1.90	0.72
1:L:450:LYS:HG2	1:L:454:LEU:CD1	2.18	0.72
1:L:259:VAL:CG1	1:L:259:VAL:O	2.38	0.71
1:L:301:CYS:C	1:L:303:SER:H	1.98	0.71
1:L:660:ASP:O	1:L:663:VAL:HG22	1.90	0.71
1:L:296:ARG:HG2	3:L:821:HOH:O	1.91	0.71
1:L:537:LEU:HD23	1:L:537:LEU:H	1.55	0.71
2:S:879:LYS:HB3	2:S:885:ARG:NH2	2.05	0.71
1:L:383:MET:HE1	1:L:625:TYR:HB3	1.72	0.71
1:L:595:LYS:O	1:L:599:ILE:HG12	1.91	0.71
1:L:285:ARG:O	1:L:287:PRO:HD3	1.91	0.71
1:L:414:LYS:HD2	1:L:496:ASP:HB3	1.71	0.71
1:L:433:ILE:HG22	1:L:461:ARG:HA	1.71	0.71
2:S:905:LEU:HD22	2:S:905:LEU:N	2.04	0.70
1:L:211:ILE:HB	1:L:500:ARG:NH2	2.07	0.70
1:L:315:LEU:HD23	1:L:318:ARG:HE	1.56	0.70
1:L:463:ASP:O	1:L:464:THR:OG1	2.06	0.70
1:L:554:GLN:HG2	1:L:558:ARG:HH12	1.56	0.70
1:L:577:CYS:HA	1:L:580:MET:HE3	1.72	0.70
1:L:414:LYS:HD2	1:L:496:ASP:CB	2.21	0.70
1:L:429:ILE:O	1:L:471:VAL:HG21	1.93	0.69
1:L:253:ILE:HG22	1:L:254:THR:N	2.07	0.69
1:L:343:LEU:HD13	1:L:345:PRO:HG2	1.74	0.69
1:L:287:PRO:HB2	1:L:288:TRP:CZ3	2.27	0.69
1:L:333:ARG:HG2	1:L:334:HIS:N	2.06	0.69
1:L:550:ALA:HB2	1:L:581:VAL:HG21	1.75	0.68
2:S:905:LEU:H	2:S:905:LEU:CD2	2.04	0.68
1:L:242:ILE:HB	1:L:260:LYS:O	1.94	0.68
1:L:259:VAL:O	1:L:259:VAL:HG13	1.93	0.68
1:L:255:PHE:CD2	1:L:333:ARG:HB3	2.28	0.67
1:L:408:LEU:HD13	1:L:474:ARG:HB2	1.75	0.67
1:L:700:LEU:HD13	2:S:916:ARG:HE	1.59	0.67
1:L:525:ILE:HG22	1:L:526:SER:H	1.58	0.67
1:L:328:PHE:C	1:L:330:ASP:N	2.52	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:13:GLU:HA	1:L:16:GLU:HG2	1.75	0.67
2:S:879:LYS:HB3	2:S:885:ARG:HH21	1.59	0.67
1:L:516:ILE:HG12	1:L:639:PRO:HD3	1.77	0.66
1:L:441:SER:C	1:L:446:ILE:HD12	2.20	0.66
1:L:238:LEU:HG	1:L:339:GLU:HB3	1.75	0.66
1:L:390:LYS:HG2	1:L:481:GLU:HG2	1.77	0.66
1:L:394:GLU:HB3	1:L:405:CYS:SG	2.36	0.66
1:L:337:ARG:HH21	1:L:339:GLU:CD	2.03	0.66
1:L:553:LEU:HG	1:L:557:LEU:HD12	1.78	0.66
1:L:527:GLU:HG2	1:L:528:ASP:OD1	1.96	0.66
2:S:917:TYR:CB	2:S:924:MET:HE2	2.26	0.65
1:L:77:ARG:O	1:L:81:ILE:HG13	1.95	0.65
1:L:37:ASN:O	1:L:41:GLU:HG3	1.96	0.65
2:S:872:LYS:HD2	3:S:200:HOH:O	1.96	0.65
1:L:13:GLU:O	1:L:16:GLU:HG2	1.96	0.65
1:L:251:GLU:HG3	1:L:252:ALA:N	2.11	0.65
1:L:10:LYS:NZ	1:L:18:LEU:HD23	2.10	0.65
1:L:99:GLN:HB2	1:L:108:LEU:HD11	1.78	0.65
1:L:277:SER:O	1:L:278:LEU:HB2	1.97	0.65
1:L:679:LEU:CD1	1:L:689:LEU:HD21	2.27	0.65
2:S:867:LEU:O	2:S:871:ILE:HG13	1.96	0.65
1:L:243:ASP:HB2	1:L:335:TYR:CG	2.32	0.65
1:L:360:LYS:HA	1:L:500:ARG:HA	1.77	0.65
1:L:516:ILE:HD12	2:S:958:ILE:HG23	1.79	0.65
1:L:542:ALA:HA	1:L:548:ILE:HD11	1.79	0.65
1:L:587:ASP:OD2	1:L:587:ASP:N	2.30	0.65
1:L:273:GLU:OE2	1:L:276:GLY:HA2	1.97	0.65
1:L:208:THR:HG22	1:L:210:GLY:N	2.11	0.64
2:S:885:ARG:H	2:S:885:ARG:HD2	1.62	0.64
1:L:20:SER:OG	1:L:22:GLU:HG3	1.96	0.64
1:L:318:ARG:HG3	1:L:319:HIS:H	1.63	0.64
1:L:86:GLN:HG3	1:L:89:ILE:HD11	1.79	0.64
1:L:216:GLU:CD	1:L:216:GLU:H	2.05	0.64
1:L:287:PRO:HB2	1:L:288:TRP:CE3	2.33	0.64
1:L:626:GLU:HA	1:L:629:LYS:HZ2	1.61	0.64
2:S:877:ILE:CD1	2:S:901:ALA:HA	2.27	0.64
1:L:66:TYR:O	1:L:71:ARG:NH2	2.26	0.63
1:L:114:LEU:HD11	1:L:207:PHE:HD2	1.63	0.63
1:L:505:LYS:HG3	1:L:506:LYS:HZ2	1.63	0.63
1:L:382:TRP:CZ2	1:L:383:MET:HE2	2.32	0.63
1:L:108:LEU:HD12	1:L:108:LEU:H	1.62	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:318:ARG:HG3	1:L:319:HIS:N	2.14	0.63
1:L:420:ARG:HG2	3:S:378:HOH:O	1.98	0.63
2:S:905:LEU:HD12	2:S:909:LEU:CD2	2.29	0.63
1:L:354:LYS:NZ	1:L:504:GLU:OE1	2.31	0.63
1:L:61:LYS:H	1:L:65:PRO:HD2	1.64	0.63
1:L:616:VAL:O	1:L:617:ASP:HB2	1.98	0.63
2:S:885:ARG:HD2	2:S:885:ARG:N	2.13	0.63
1:L:31:ASP:O	1:L:35:LEU:HG	1.99	0.63
1:L:83:ALA:O	1:L:85:PRO:HD3	1.98	0.63
1:L:113:SER:O	1:L:116:LEU:HG	1.99	0.63
1:L:298:ASN:N	1:L:298:ASN:HD22	1.97	0.62
1:L:253:ILE:C	1:L:255:PHE:H	2.05	0.62
1:L:10:LYS:HZ3	1:L:18:LEU:HD23	1.62	0.62
1:L:311:GLU:HA	1:L:314:ARG:NH1	2.13	0.62
1:L:4:ILE:HG13	3:L:701:HOH:O	2.00	0.62
1:L:234:LYS:HG2	1:L:356:TRP:CD1	2.35	0.62
1:L:527:GLU:HG3	3:L:883:HOH:O	1.98	0.62
1:L:600:LEU:O	1:L:604:ILE:HG13	1.99	0.62
1:L:310:GLU:HA	1:L:313:GLU:HB3	1.81	0.62
1:L:389:ILE:HD11	1:L:484:LEU:HD11	1.82	0.62
2:S:806:ALA:HA	2:S:810:GLY:H	1.65	0.62
1:L:217:LEU:HD22	1:L:331:PHE:CE2	2.33	0.62
1:L:291:VAL:HG12	1:L:292:GLU:N	2.14	0.62
1:L:576:THR:O	1:L:579:ILE:HG22	1.98	0.62
2:S:815:VAL:HG13	2:S:819:GLU:HB2	1.81	0.62
1:L:16:GLU:HG3	1:L:23:ARG:HH12	1.64	0.61
1:L:572:PHE:CE1	1:L:663:VAL:HG21	2.35	0.61
1:L:596:GLU:H	1:L:596:GLU:CD	2.08	0.61
2:S:869:ASN:HA	2:S:872:LYS:CE	2.14	0.61
2:S:942:ALA:O	2:S:946:LEU:CD2	2.48	0.61
1:L:307:ILE:HG22	1:L:307:ILE:O	2.00	0.61
2:S:870:ASN:HB3	2:S:874:TRP:CZ3	2.35	0.61
2:S:903:PHE:HZ	2:S:937:ASP:HB2	1.65	0.61
1:L:317:ARG:HB2	3:L:899:HOH:O	2.01	0.61
1:L:417:ARG:NH2	3:L:877:HOH:O	2.33	0.61
1:L:691:LEU:O	1:L:695:LEU:HG	2.01	0.61
1:L:378:PRO:HD2	3:L:839:HOH:O	2.00	0.61
1:L:631:LEU:HD13	1:L:638:MET:CE	2.29	0.61
2:S:869:ASN:CA	2:S:872:LYS:HE2	2.16	0.61
1:L:307:ILE:HD12	1:L:307:ILE:H	1.66	0.60
1:L:560:VAL:HG11	1:L:601:TRP:HH2	1.65	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:534:VAL:O	1:L:538:PHE:HB3	2.01	0.60
2:S:890:CYS:HB3	2:S:893:GLU:HB2	1.82	0.60
1:L:4:ILE:O	1:L:8:LEU:HG	2.02	0.60
1:L:223:ASN:HD22	1:L:223:ASN:H	1.49	0.60
1:L:671:THR:O	1:L:674:LYS:HG3	2.02	0.60
2:S:888:THR:HA	2:S:925:ASP:HA	1.84	0.60
1:L:553:LEU:HD21	1:L:600:LEU:HD21	1.84	0.60
2:S:850:VAL:HG11	2:S:938:ALA:CB	2.31	0.60
1:L:561:LEU:HD11	1:L:572:PHE:CE2	2.36	0.60
1:L:135:TYR:CE1	1:L:137:GLY:HA2	2.37	0.59
1:L:172:GLU:OE1	1:L:173:GLY:N	2.35	0.59
1:L:472:LEU:O	1:L:473:ASN:HB2	2.00	0.59
1:L:532:ASP:HA	1:L:535:ARG:HD2	1.83	0.59
1:L:567:ILE:O	1:L:568:LYS:HB2	2.01	0.59
1:L:484:LEU:HD13	1:L:499:ILE:HD11	1.85	0.59
1:L:363:GLY:HA3	1:L:497:PHE:CZ	2.38	0.59
1:L:256:GLN:CD	1:L:256:GLN:N	2.56	0.59
1:L:193:GLU:O	1:L:421:LYS:NZ	2.34	0.59
1:L:416:ARG:HB2	1:L:416:ARG:HH11	1.68	0.58
2:S:850:VAL:HG11	2:S:938:ALA:HB2	1.84	0.58
2:S:798:VAL:HA	2:S:801:PHE:HD1	1.68	0.58
1:L:60:PHE:N	1:L:60:PHE:CD2	2.71	0.58
1:L:98:CYS:HB2	3:L:761:HOH:O	2.02	0.58
1:L:234:LYS:HG2	1:L:356:TRP:NE1	2.19	0.58
1:L:245:THR:O	1:L:248:ALA:HB2	2.03	0.58
1:L:328:PHE:CZ	1:L:331:PHE:CE1	2.92	0.58
1:L:433:ILE:HG22	1:L:461:ARG:CA	2.33	0.58
2:S:917:TYR:HB3	2:S:924:MET:HE2	1.86	0.58
1:L:382:TRP:CE3	1:L:449:SER:HA	2.38	0.58
1:L:626:GLU:HA	1:L:629:LYS:HZ3	1.67	0.58
1:L:107:LEU:HD21	1:L:182:GLU:HG3	1.86	0.58
1:L:525:ILE:O	1:L:526:SER:HB2	2.03	0.58
2:S:800:GLN:O	2:S:804:LEU:HG	2.02	0.58
1:L:52:PRO:C	1:L:54:ILE:H	2.11	0.58
1:L:326:MET:HE1	1:L:333:ARG:CZ	2.34	0.58
1:L:315:LEU:CA	1:L:318:ARG:HH21	2.09	0.57
1:L:516:ILE:CD1	2:S:959:GLN:HG2	2.28	0.57
1:L:659:PHE:O	1:L:663:VAL:HG13	2.04	0.57
1:L:679:LEU:HD11	1:L:689:LEU:HD21	1.86	0.57
2:S:834:LEU:HD22	2:S:875:GLN:OE1	2.05	0.57
1:L:52:PRO:HB2	1:L:54:ILE:CG1	2.31	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:62:GLU:H	1:L:64:GLY:H	1.50	0.57
1:L:215:TYR:CD1	1:L:337:ARG:NH2	2.72	0.57
1:L:609:LYS:O	1:L:613:GLU:HB2	2.05	0.57
1:L:243:ASP:HB2	1:L:335:TYR:CB	2.33	0.57
1:L:359:THR:HG21	1:L:509:TYR:HB3	1.85	0.57
1:L:438:GLU:HG3	1:L:439:GLU:H	1.68	0.57
2:S:875:GLN:HA	2:S:926:PHE:HE1	1.70	0.57
1:L:614:ILE:HG22	1:L:615:ASP:N	2.19	0.57
2:S:942:ALA:O	2:S:946:LEU:HD22	2.04	0.57
1:L:366:ARG:HA	1:L:494:ASP:OD1	2.05	0.57
1:L:383:MET:SD	1:L:625:TYR:CD2	2.98	0.57
1:L:669:LEU:HG	1:L:673:PHE:HE2	1.70	0.57
1:L:7:LYS:NZ	2:S:854:ASP:OD2	2.38	0.56
1:L:155:ASP:OD2	1:L:157:ARG:HB2	2.04	0.56
1:L:466:ILE:HB	1:L:468:LEU:HD11	1.88	0.56
1:L:632:GLU:C	1:L:634:ALA:H	2.13	0.56
1:L:16:GLU:HG3	1:L:23:ARG:NH1	2.21	0.56
1:L:240:CYS:HA	1:L:336:SER:O	2.05	0.56
1:L:283:ARG:HA	1:L:325:TRP:HA	1.88	0.56
1:L:579:ILE:HG23	1:L:667:VAL:CG1	2.35	0.56
2:S:835:LYS:HE2	2:S:836:THR:N	2.19	0.56
1:L:669:LEU:O	1:L:673:PHE:CD2	2.55	0.56
2:S:919:ASP:O	2:S:920:GLU:C	2.48	0.56
1:L:94:ARG:HD2	1:L:288:TRP:O	2.06	0.56
1:L:109:ALA:HB3	1:L:200:THR:HG21	1.88	0.56
1:L:114:LEU:HD11	1:L:207:PHE:CD2	2.39	0.55
1:L:251:GLU:HB2	1:L:255:PHE:O	2.05	0.55
1:L:383:MET:SD	1:L:625:TYR:HD2	2.29	0.55
1:L:234:LYS:HD3	1:L:354:LYS:HB2	1.88	0.55
1:L:337:ARG:NE	1:L:339:GLU:OE2	2.37	0.55
1:L:429:ILE:HG13	1:L:471:VAL:CG2	2.36	0.55
1:L:566:ASP:C	1:L:566:ASP:OD1	2.49	0.55
1:L:631:LEU:HD11	1:L:646:ILE:HD13	1.87	0.55
1:L:4:ILE:CD1	2:S:964:LEU:HA	2.35	0.55
2:S:875:GLN:HG2	2:S:879:LYS:NZ	2.22	0.55
1:L:388:LEU:O	1:L:509:TYR:HA	2.07	0.55
2:S:855:THR:O	2:S:855:THR:HG22	2.07	0.55
2:S:918:SER:HB3	2:S:922:GLY:HA2	1.87	0.55
1:L:671:THR:O	1:L:675:ILE:HG13	2.07	0.55
1:L:443:GLN:O	1:L:444:THR:OG1	2.20	0.55
2:S:872:LYS:HB2	3:S:292:HOH:O	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:99:GLN:HG3	1:L:103:GLY:HA3	1.88	0.55
1:L:223:ASN:HD22	1:L:223:ASN:N	2.05	0.55
1:L:563:LYS:O	1:L:564:ARG:CB	2.54	0.55
1:L:186:ALA:HB1	1:L:192:TYR:HA	1.89	0.54
2:S:815:VAL:HG13	2:S:819:GLU:CB	2.37	0.54
1:L:99:GLN:HG2	1:L:100:GLY:O	2.07	0.54
1:L:253:ILE:C	1:L:255:PHE:N	2.64	0.54
1:L:651:ALA:HA	1:L:657:ILE:HG12	1.88	0.54
1:L:428:THR:CG2	1:L:465:PHE:HB3	2.34	0.54
1:L:484:LEU:CD1	1:L:499:ILE:HD11	2.38	0.54
1:L:691:LEU:HD13	2:S:943:PHE:CG	2.43	0.54
2:S:798:VAL:O	2:S:801:PHE:HB2	2.08	0.54
2:S:877:ILE:CG1	3:S:290:HOH:O	2.55	0.54
1:L:55:PRO:HD2	3:L:735:HOH:O	2.07	0.54
1:L:88:ILE:HG12	1:L:89:ILE:N	2.23	0.54
1:L:662:PHE:CZ	1:L:666:LEU:HD11	2.43	0.54
1:L:327:SER:O	1:L:330:ASP:HB3	2.08	0.54
1:L:429:ILE:HG13	1:L:471:VAL:HG23	1.90	0.54
1:L:252:ALA:O	1:L:255:PHE:HB2	2.08	0.53
1:L:553:LEU:HG	1:L:557:LEU:CD1	2.38	0.53
1:L:361:MET:HB2	1:L:499:ILE:HG23	1.91	0.53
1:L:527:GLU:C	1:L:535:ARG:HH21	2.15	0.53
1:L:557:LEU:O	1:L:561:LEU:HG	2.08	0.53
2:S:801:PHE:O	2:S:805:PHE:HD1	1.92	0.53
1:L:253:ILE:CG2	1:L:254:THR:H	2.12	0.53
1:L:584:LEU:HB3	1:L:596:GLU:HB2	1.89	0.53
1:L:674:LYS:HD2	1:L:674:LYS:C	2.34	0.53
2:S:869:ASN:O	2:S:872:LYS:HG2	2.09	0.53
1:L:561:LEU:H	1:L:561:LEU:CD2	2.04	0.53
2:S:821:MET:HG3	2:S:844:CYS:SG	2.48	0.53
2:S:840:GLY:HA3	3:S:310:HOH:O	2.09	0.53
1:L:614:ILE:HD12	1:L:630:ALA:HB2	1.90	0.53
2:S:803:ARG:NE	2:S:803:ARG:HA	2.22	0.53
1:L:520:LEU:HG	1:L:521:GLU:N	2.22	0.53
1:L:193:GLU:O	1:L:193:GLU:HG2	2.08	0.53
1:L:527:GLU:HG2	1:L:528:ASP:N	2.24	0.53
1:L:93:THR:HG22	1:L:94:ARG:N	2.23	0.53
1:L:244:ILE:HG23	1:L:244:ILE:O	2.09	0.53
1:L:313:GLU:O	1:L:316:THR:HG23	2.09	0.53
2:S:828:VAL:HG11	2:S:926:PHE:HE2	1.73	0.53
1:L:333:ARG:HG2	1:L:334:HIS:H	1.72	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:350:SER:C	1:L:352:THR:H	2.16	0.52
2:S:905:LEU:HD11	2:S:936:LEU:HD21	1.90	0.52
1:L:301:CYS:C	1:L:303:SER:N	2.62	0.52
1:L:611:TYR:OH	1:L:658:ASP:HA	2.10	0.52
1:L:451:ASN:HA	1:L:454:LEU:HD12	1.92	0.52
1:L:642:LEU:HD21	2:S:962:LEU:HB3	1.91	0.52
2:S:917:TYR:HB2	2:S:924:MET:HE2	1.91	0.52
1:L:642:LEU:HD21	2:S:962:LEU:CB	2.40	0.52
1:L:135:TYR:C	1:L:137:GLY:H	2.18	0.52
1:L:284:ILE:HG22	1:L:285:ARG:N	2.24	0.52
1:L:538:PHE:HE2	1:L:548:ILE:HG13	1.73	0.52
1:L:583:MET:SD	1:L:670:GLU:OE1	2.68	0.52
2:S:828:VAL:O	2:S:834:LEU:HD23	2.09	0.52
1:L:307:ILE:HD12	1:L:307:ILE:N	2.24	0.52
1:L:389:ILE:HD11	1:L:484:LEU:CD1	2.38	0.52
1:L:343:LEU:O	1:L:346:ASP:HB2	2.10	0.52
2:S:835:LYS:O	2:S:887:GLY:HA2	2.10	0.52
2:S:882:ASP:HB2	2:S:889:ILE:HG12	1.91	0.52
1:L:5:ALA:HB1	2:S:946:LEU:HD21	1.92	0.52
1:L:28:LEU:HD13	1:L:50:SER:CB	2.37	0.52
1:L:343:LEU:HD12	1:L:346:ASP:HB2	1.92	0.52
2:S:821:MET:HA	2:S:844:CYS:SG	2.50	0.52
1:L:442:GLY:N	1:L:446:ILE:HD12	2.24	0.51
1:L:343:LEU:HD13	1:L:345:PRO:CG	2.38	0.51
1:L:156:ASP:HA	1:L:180:LEU:CD2	2.40	0.51
1:L:457:ARG:HG3	1:L:458:ALA:O	2.09	0.51
2:S:806:ALA:HA	2:S:810:GLY:N	2.26	0.51
1:L:278:LEU:HD11	3:L:909:HOH:O	2.10	0.51
1:L:328:PHE:CE2	1:L:331:PHE:HE1	2.29	0.51
1:L:538:PHE:O	1:L:541:LEU:N	2.43	0.51
1:L:297:TRP:CD1	1:L:297:TRP:C	2.89	0.51
1:L:328:PHE:CZ	1:L:331:PHE:HE1	2.28	0.51
2:S:914:ILE:O	2:S:918:SER:HB2	2.11	0.51
1:L:405:CYS:O	1:L:476:LYS:HA	2.11	0.51
1:L:560:VAL:HG11	1:L:601:TRP:CH2	2.46	0.51
2:S:791:GLU:C	2:S:793:ASN:H	2.18	0.51
2:S:810:GLY:O	2:S:813:MET:HG2	2.11	0.51
1:L:232:LEU:HD11	1:L:266:VAL:O	2.10	0.51
1:L:560:VAL:CB	1:L:561:LEU:HD23	2.36	0.51
1:L:251:GLU:HG3	1:L:252:ALA:H	1.76	0.51
1:L:414:LYS:HD2	1:L:496:ASP:HB2	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:248:ALA:C	1:L:259:VAL:HG12	2.16	0.51
1:L:629:LYS:O	1:L:632:GLU:HB3	2.10	0.51
2:S:799:ARG:HH11	2:S:802:ARG:HD3	1.74	0.51
1:L:240:CYS:HB3	1:L:337:ARG:HG3	1.94	0.50
1:L:343:LEU:O	1:L:343:LEU:HD12	2.11	0.50
1:L:368:GLY:HA3	1:L:655:LEU:HD22	1.93	0.50
1:L:393:GLU:HG2	1:L:505:LYS:HG2	1.93	0.50
1:L:106:TRP:HB2	1:L:200:THR:HG23	1.92	0.50
1:L:452:PHE:O	1:L:456:ASN:ND2	2.28	0.50
1:L:699:VAL:HG13	2:S:912:MET:HE3	1.93	0.50
2:S:846:SER:HA	2:S:968:SER:O	2.11	0.50
1:L:461:ARG:O	1:L:475:PHE:HZ	1.95	0.50
1:L:519:ASN:CG	1:L:519:ASN:O	2.54	0.50
1:L:61:LYS:CA	1:L:64:GLY:HA3	2.40	0.50
1:L:572:PHE:HE1	1:L:663:VAL:HG11	1.76	0.50
1:L:663:VAL:HG23	1:L:664:ARG:N	2.27	0.50
2:S:919:ASP:O	2:S:922:GLY:N	2.41	0.50
1:L:230:LYS:O	1:L:234:LYS:HB2	2.10	0.50
1:L:528:ASP:O	1:L:529:ASP:HB2	2.12	0.50
2:S:792:ALA:N	2:S:794:GLU:OE2	2.44	0.50
2:S:828:VAL:CG1	2:S:926:PHE:HE2	2.24	0.50
1:L:86:GLN:N	1:L:174:SER:O	2.38	0.49
1:L:601:TRP:NE1	1:L:605:GLN:OE1	2.44	0.49
1:L:566:ASP:O	1:L:567:ILE:HB	2.12	0.49
1:L:650:PHE:HB3	1:L:661:ASN:HB3	1.94	0.49
2:S:951:THR:C	2:S:953:GLN:N	2.68	0.49
1:L:145:GLN:O	1:L:148:GLU:HG2	2.12	0.49
1:L:356:TRP:CE3	1:L:502:PHE:HB3	2.47	0.49
1:L:364:ASN:HB2	1:L:644:GLN:HE22	1.78	0.49
1:L:621:THR:HG23	1:L:621:THR:O	2.13	0.49
1:L:685:GLY:O	2:S:957:ASN:HA	2.12	0.49
2:S:850:VAL:CG1	2:S:938:ALA:CB	2.91	0.49
1:L:194:ALA:O	1:L:422:MET:HG2	2.12	0.49
1:L:433:ILE:HG22	1:L:461:ARG:H	1.76	0.49
1:L:58:LEU:HD13	1:L:70:THR:HB	1.95	0.49
1:L:213:GLU:HA	1:L:472:LEU:HD13	1.95	0.49
1:L:227:ILE:HD13	1:L:474:ARG:NH1	2.27	0.49
1:L:505:LYS:HG3	1:L:506:LYS:HZ3	1.73	0.49
2:S:806:ALA:HA	2:S:810:GLY:HA2	1.94	0.49
1:L:161:LYS:C	1:L:163:GLY:H	2.19	0.49
1:L:438:GLU:O	1:L:439:GLU:C	2.55	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:830:ARG:O	2:S:832:PRO:HD3	2.12	0.49
2:S:878:TYR:CD2	2:S:889:ILE:HD11	2.48	0.49
1:L:83:ALA:C	1:L:85:PRO:HD3	2.37	0.49
1:L:341:CYS:O	1:L:502:PHE:CE2	2.65	0.49
1:L:364:ASN:HB3	1:L:366:ARG:NH1	2.28	0.49
1:L:416:ARG:NH2	1:L:496:ASP:OD2	2.39	0.49
1:L:622:MET:HG2	1:L:623:ASN:O	2.12	0.49
2:S:797:GLU:HG3	2:S:798:VAL:N	2.22	0.49
1:L:211:ILE:O	1:L:211:ILE:HG23	2.12	0.49
1:L:417:ARG:HH12	2:S:860:GLY:HA2	1.78	0.49
1:L:605:GLN:HA	1:L:608:GLN:OE1	2.13	0.49
1:L:652:ASP:HB3	1:L:656:ILE:H	1.78	0.49
1:L:36:ARG:HG2	1:L:40:LEU:HD13	1.95	0.48
1:L:221:PRO:HB3	1:L:223:ASN:ND2	2.28	0.48
1:L:226:LYS:O	1:L:230:LYS:HD2	2.13	0.48
1:L:19:GLY:HA2	1:L:25:ILE:CG1	2.42	0.48
1:L:304:TRP:CZ3	1:L:316:THR:HG21	2.49	0.48
1:L:330:ASP:O	1:L:332:LEU:N	2.47	0.48
1:L:333:ARG:O	1:L:334:HIS:HB2	2.13	0.48
1:L:611:TYR:HE1	1:L:622:MET:HE2	1.78	0.48
1:L:286:ASN:ND2	1:L:290:GLU:O	2.46	0.48
1:L:390:LYS:HB3	1:L:508:ASP:HB3	1.95	0.48
1:L:102:LEU:HD13	1:L:166:LEU:HB3	1.94	0.48
1:L:138:ILE:HD11	1:L:153:VAL:CG1	2.43	0.48
1:L:548:ILE:HG23	1:L:552:GLU:HB3	1.95	0.48
1:L:553:LEU:HD11	1:L:600:LEU:HD23	1.94	0.48
1:L:554:GLN:CD	1:L:558:ARG:HH22	2.22	0.48
2:S:951:THR:C	2:S:953:GLN:H	2.20	0.48
1:L:551:PHE:CD2	2:S:920:GLU:HG3	2.49	0.48
1:L:690:ASP:OD1	1:L:692:ILE:HB	2.14	0.48
1:L:699:VAL:CG1	2:S:912:MET:HB3	2.42	0.48
1:L:516:ILE:HG12	1:L:639:PRO:CD	2.42	0.48
2:S:905:LEU:HD12	2:S:909:LEU:HD23	1.95	0.48
1:L:88:ILE:CG1	1:L:89:ILE:N	2.77	0.48
2:S:806:ALA:HA	2:S:810:GLY:CA	2.43	0.48
1:L:357:LYS:HG3	1:L:505:LYS:C	2.38	0.48
1:L:562:ALA:HB1	1:L:570:ASP:OD1	2.13	0.47
1:L:7:LYS:HG2	2:S:853:SER:HB2	1.97	0.47
1:L:68:SER:O	1:L:69:LYS:C	2.56	0.47
1:L:438:GLU:HG3	1:L:439:GLU:N	2.28	0.47
2:S:791:GLU:OE1	2:S:794:GLU:HA	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:61:LYS:HE3	1:L:66:TYR:HB2	1.87	0.47
1:L:98:CYS:HA	1:L:108:LEU:CD2	2.44	0.47
1:L:132:GLN:CD	1:L:132:GLN:N	2.73	0.47
1:L:310:GLU:O	1:L:314:ARG:HG2	2.14	0.47
1:L:204:PHE:O	1:L:208:THR:HB	2.15	0.47
1:L:583:MET:SD	1:L:667:VAL:HG13	2.54	0.47
1:L:585:ASP:OD2	1:L:589:SER:OG	2.32	0.47
1:L:631:LEU:HD23	1:L:666:LEU:CD2	2.45	0.47
2:S:851:MET:HE2	2:S:863:GLU:O	2.14	0.47
1:L:75:TRP:HD1	3:L:747:HOH:O	1.98	0.47
1:L:310:GLU:C	1:L:312:ARG:H	2.23	0.47
1:L:319:HIS:C	1:L:320:GLU:HG3	2.40	0.47
1:L:328:PHE:O	1:L:330:ASP:N	2.47	0.47
1:L:649:ARG:O	2:S:845:ARG:HD3	2.14	0.47
2:S:946:LEU:HD22	2:S:946:LEU:N	2.29	0.47
1:L:20:SER:O	1:L:21:HIS:C	2.57	0.47
1:L:123:ARG:HG2	3:L:712:HOH:O	2.15	0.47
1:L:295:GLY:O	1:L:296:ARG:NE	2.47	0.47
1:L:307:ILE:N	1:L:307:ILE:CD1	2.78	0.47
1:L:354:LYS:HE2	1:L:354:LYS:HB3	1.69	0.47
1:L:374:CYS:SG	1:L:376:ASN:HB2	2.55	0.47
1:L:546:ALA:HB1	1:L:594:LEU:HB2	1.97	0.47
1:L:612:ARG:HD3	1:L:615:ASP:O	2.15	0.47
1:L:679:LEU:HD13	1:L:689:LEU:HD21	1.97	0.47
1:L:688:GLU:O	1:L:689:LEU:HD23	2.14	0.47
1:L:248:ALA:HB1	1:L:259:VAL:HG11	1.96	0.47
1:L:525:ILE:CG2	1:L:595:LYS:CD	2.84	0.47
1:L:617:ASP:C	1:L:619:SER:N	2.73	0.47
1:L:460:GLU:OE2	1:L:477:LEU:HD21	2.15	0.46
1:L:561:LEU:N	1:L:561:LEU:CD2	2.73	0.46
1:L:641:GLN:O	1:L:644:GLN:HB2	2.15	0.46
1:L:691:LEU:HD13	2:S:943:PHE:CD1	2.50	0.46
1:L:256:GLN:NE2	1:L:294:THR:OG1	2.47	0.46
1:L:306:THR:O	1:L:307:ILE:C	2.58	0.46
1:L:431:PHE:O	1:L:462:SER:CB	2.63	0.46
1:L:466:ILE:HB	1:L:468:LEU:CD1	2.45	0.46
2:S:851:MET:HB2	2:S:859:LEU:CD1	2.46	0.46
1:L:460:GLU:O	1:L:461:ARG:HG3	2.15	0.46
1:L:251:GLU:CG	1:L:252:ALA:N	2.79	0.46
1:L:289:GLY:O	1:L:290:GLU:C	2.58	0.46
2:S:861:PHE:O	2:S:864:PHE:HB3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:224:LEU:HD22	1:L:224:LEU:O	2.15	0.46
1:L:13:GLU:CA	1:L:16:GLU:HG2	2.43	0.46
1:L:52:PRO:HB2	1:L:54:ILE:CD1	2.46	0.46
1:L:198:GLY:CA	1:L:422:MET:HE2	2.45	0.46
1:L:694:TRP:CZ2	2:S:939:MET:SD	3.09	0.46
1:L:408:LEU:CD1	1:L:474:ARG:HB2	2.45	0.46
1:L:73:MET:HE1	1:L:159:PRO:HB3	1.98	0.46
1:L:221:PRO:HB3	1:L:223:ASN:HD21	1.81	0.46
1:L:534:VAL:O	1:L:538:PHE:CB	2.64	0.46
1:L:245:THR:H	1:L:248:ALA:HB3	1.81	0.45
1:L:562:ALA:C	1:L:564:ARG:H	2.23	0.45
1:L:556:ILE:HA	1:L:559:ARG:HH12	1.80	0.45
1:L:577:CYS:O	1:L:581:VAL:HG23	2.16	0.45
1:L:117:ASN:OD1	1:L:119:GLU:HB2	2.16	0.45
1:L:529:ASP:C	1:L:531:ASP:N	2.68	0.45
2:S:873:ARG:O	2:S:876:ALA:HB3	2.15	0.45
1:L:199:ALA:O	1:L:202:GLU:HB2	2.16	0.45
1:L:389:ILE:HG12	1:L:509:TYR:CD1	2.51	0.45
1:L:532:ASP:HA	1:L:535:ARG:HB3	1.99	0.45
1:L:601:TRP:O	1:L:605:GLN:HG3	2.17	0.45
1:L:614:ILE:CD1	1:L:630:ALA:HB2	2.46	0.45
1:L:326:MET:SD	1:L:330:ASP:HB2	2.56	0.45
1:L:359:THR:CG2	1:L:509:TYR:HB3	2.46	0.45
1:L:409:VAL:HG22	1:L:501:VAL:HG22	1.98	0.45
1:L:437:PRO:O	1:L:438:GLU:HB3	2.17	0.45
1:L:520:LEU:CG	1:L:521:GLU:H	2.29	0.45
1:L:525:ILE:O	1:L:526:SER:CB	2.65	0.45
1:L:579:ILE:HG22	1:L:580:MET:N	2.31	0.45
1:L:611:TYR:CE1	1:L:622:MET:HE2	2.52	0.45
2:S:898:PHE:CZ	2:S:913:ILE:HG21	2.51	0.45
1:L:343:LEU:HD12	1:L:343:LEU:C	2.42	0.45
1:L:296:ARG:HB3	1:L:304:TRP:HE1	1.82	0.45
1:L:411:LEU:O	1:L:470:GLU:HG3	2.17	0.45
1:L:433:ILE:HG22	1:L:461:ARG:N	2.30	0.45
1:L:455:THR:O	1:L:455:THR:HG22	2.16	0.45
2:S:850:VAL:HG13	2:S:938:ALA:HB1	1.99	0.45
1:L:205:GLU:HG2	1:L:340:ILE:HD11	1.99	0.45
1:L:394:GLU:HB2	1:L:404:GLY:HA3	1.99	0.45
1:L:529:ASP:C	1:L:531:ASP:H	2.24	0.45
1:L:130:SER:OG	1:L:132:GLN:NE2	2.50	0.45
1:L:699:VAL:HG13	1:L:699:VAL:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:791:GLU:O	2:S:792:ALA:HB3	2.17	0.45
1:L:4:ILE:HG13	1:L:4:ILE:H	1.54	0.45
1:L:16:GLU:CG	1:L:23:ARG:HH12	2.29	0.45
1:L:17:GLY:O	1:L:23:ARG:HB2	2.17	0.45
1:L:61:LYS:O	1:L:61:LYS:HG2	2.17	0.45
1:L:298:ASN:N	1:L:298:ASN:ND2	2.60	0.45
1:L:450:LYS:CG	1:L:454:LEU:HD11	2.34	0.45
1:L:579:ILE:CG2	1:L:667:VAL:HB	2.47	0.45
1:L:662:PHE:CE1	1:L:666:LEU:HD11	2.51	0.45
1:L:687:ILE:O	2:S:955:GLN:HA	2.16	0.45
2:S:799:ARG:NH1	2:S:802:ARG:CD	2.73	0.45
1:L:216:GLU:CD	1:L:216:GLU:N	2.74	0.44
1:L:374:CYS:HB3	1:L:376:ASN:HB2	1.99	0.44
1:L:633:GLU:H	1:L:633:GLU:HG2	1.51	0.44
1:L:330:ASP:C	1:L:332:LEU:N	2.74	0.44
1:L:576:THR:HG23	1:L:663:VAL:HG23	1.99	0.44
1:L:679:LEU:C	1:L:681:PRO:HD3	2.42	0.44
1:L:698:SER:CB	2:S:939:MET:HG3	2.42	0.44
2:S:875:GLN:HA	2:S:926:PHE:CE1	2.51	0.44
1:L:127:LEU:C	1:L:129:GLN:H	2.24	0.44
1:L:566:ASP:O	1:L:567:ILE:CB	2.66	0.44
1:L:165:LEU:HD12	1:L:169:HIS:HB3	1.98	0.44
1:L:347:THR:CG2	1:L:350:SER:HB2	2.47	0.44
1:L:459:ARG:HD2	1:L:477:LEU:HD22	1.98	0.44
1:L:545:ASP:O	1:L:546:ALA:HB2	2.18	0.44
1:L:614:ILE:HD11	1:L:629:LYS:HG3	1.97	0.44
1:L:7:LYS:HA	1:L:7:LYS:HD3	1.77	0.44
1:L:30:GLN:OE1	1:L:187:LYS:NZ	2.48	0.44
1:L:256:GLN:HE22	1:L:294:THR:CB	2.30	0.44
1:L:457:ARG:HH21	1:L:459:ARG:HA	1.82	0.44
2:S:914:ILE:HG23	2:S:918:SER:OG	2.17	0.44
1:L:631:LEU:HD23	1:L:666:LEU:HD21	2.00	0.44
2:S:906:ASN:O	2:S:907:GLU:C	2.60	0.44
2:S:942:ALA:O	2:S:946:LEU:HD23	2.17	0.44
1:L:61:LYS:N	1:L:65:PRO:HD2	2.31	0.44
1:L:337:ARG:NH2	1:L:339:GLU:OE1	2.47	0.44
1:L:562:ALA:HB1	1:L:570:ASP:CG	2.43	0.44
1:L:141:PHE:CE2	1:L:181:LEU:HA	2.53	0.44
1:L:577:CYS:HA	1:L:580:MET:CE	2.46	0.44
1:L:674:LYS:O	1:L:678:GLN:HG2	2.17	0.44
1:L:165:LEU:CD1	1:L:169:HIS:HB3	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:404:GLY:HA2	3:L:844:HOH:O	2.17	0.43
1:L:461:ARG:HE	1:L:461:ARG:HB2	1.63	0.43
1:L:523:PHE:HB2	1:L:599:ILE:HD12	1.99	0.43
1:L:532:ASP:OD2	1:L:535:ARG:HD2	2.18	0.43
1:L:579:ILE:HD11	1:L:668:ARG:HA	2.00	0.43
1:L:36:ARG:O	1:L:40:LEU:HD13	2.18	0.43
1:L:165:LEU:HD12	1:L:169:HIS:CB	2.49	0.43
1:L:198:GLY:HA3	1:L:422:MET:HE2	1.99	0.43
1:L:572:PHE:CE1	1:L:663:VAL:HG11	2.54	0.43
2:S:799:ARG:HH11	2:S:802:ARG:CD	2.30	0.43
1:L:248:ALA:CB	1:L:259:VAL:HG11	2.48	0.43
2:S:960:GLU:HG3	3:S:221:HOH:O	2.17	0.43
1:L:98:CYS:HA	1:L:108:LEU:HD23	2.00	0.43
1:L:101:ALA:C	1:L:102:LEU:HD12	2.43	0.43
1:L:367:ARG:HD2	1:L:492:ASN:O	2.16	0.43
1:L:452:PHE:O	1:L:456:ASN:HB2	2.18	0.43
1:L:549:SER:HB3	1:L:591:LYS:HE3	1.99	0.43
1:L:62:GLU:H	1:L:64:GLY:N	2.16	0.43
1:L:77:ARG:HG2	1:L:157:ARG:HG3	1.99	0.43
1:L:296:ARG:O	1:L:324:PHE:O	2.37	0.43
1:L:461:ARG:NH2	1:L:465:PHE:HE1	2.17	0.43
2:S:796:GLU:HA	3:S:192:HOH:O	2.18	0.43
2:S:797:GLU:O	2:S:798:VAL:C	2.62	0.43
1:L:318:ARG:CG	1:L:319:HIS:H	2.30	0.43
1:L:18:LEU:HB2	1:L:23:ARG:NH2	2.34	0.43
1:L:339:GLU:O	1:L:339:GLU:HG2	2.17	0.43
2:S:815:VAL:HG12	2:S:816:SER:O	2.19	0.43
1:L:106:TRP:CZ2	1:L:198:GLY:HA3	2.54	0.43
1:L:224:LEU:HD12	1:L:331:PHE:HZ	1.84	0.43
2:S:905:LEU:HD12	2:S:909:LEU:HD21	2.01	0.43
1:L:221:PRO:C	1:L:223:ASN:H	2.27	0.43
1:L:416:ARG:O	1:L:417:ARG:C	2.62	0.43
1:L:533:GLY:O	1:L:537:LEU:HD23	2.19	0.43
1:L:10:LYS:HD3	1:L:10:LYS:C	2.44	0.43
1:L:256:GLN:NE2	1:L:294:THR:H	2.17	0.43
1:L:295:GLY:O	1:L:296:ARG:HD2	2.18	0.43
1:L:374:CYS:HG	1:L:376:ASN:HB2	1.84	0.43
1:L:463:ASP:O	1:L:464:THR:CB	2.67	0.43
1:L:478:PRO:HA	1:L:479:PRO:HD3	1.81	0.43
1:L:503:SER:OG	1:L:505:LYS:O	2.33	0.43
1:L:155:ASP:O	1:L:183:LYS:NZ	2.38	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:219:LYS:HD2	1:L:219:LYS:HA	1.77	0.42
1:L:616:VAL:O	1:L:617:ASP:CB	2.67	0.42
1:L:694:TRP:HZ3	2:S:961:TRP:CZ3	2.36	0.42
1:L:532:ASP:HA	1:L:535:ARG:CB	2.49	0.42
1:L:595:LYS:C	1:L:597:PHE:H	2.28	0.42
2:S:890:CYS:O	2:S:893:GLU:HB3	2.19	0.42
1:L:75:TRP:CZ3	1:L:159:PRO:HG3	2.54	0.42
1:L:88:ILE:HD11	3:L:756:HOH:O	2.19	0.42
1:L:435:GLU:HB3	1:L:459:ARG:HH21	1.84	0.42
1:L:520:LEU:CG	1:L:521:GLU:N	2.80	0.42
1:L:626:GLU:CG	1:L:629:LYS:HD2	2.38	0.42
2:S:895:PRO:HG3	2:S:910:TYR:CE1	2.54	0.42
1:L:318:ARG:CG	1:L:319:HIS:N	2.82	0.42
1:L:381:PHE:C	1:L:383:MET:H	2.27	0.42
1:L:526:SER:OG	1:L:527:GLU:N	2.48	0.42
2:S:851:MET:HE3	2:S:863:GLU:HB3	2.01	0.42
1:L:330:ASP:C	1:L:332:LEU:H	2.28	0.42
1:L:295:GLY:O	1:L:296:ARG:CD	2.67	0.42
1:L:311:GLU:HA	1:L:314:ARG:HH12	1.80	0.42
1:L:407:PHE:HZ	1:L:477:LEU:HD12	1.84	0.42
2:S:826:LYS:O	2:S:830:ARG:HB2	2.19	0.42
2:S:828:VAL:CG1	2:S:926:PHE:CE2	3.02	0.42
2:S:905:LEU:HB3	2:S:909:LEU:HB3	2.00	0.42
2:S:871:ILE:C	2:S:873:ARG:N	2.76	0.42
1:L:37:ASN:HB3	3:L:948:HOH:O	2.20	0.42
1:L:238:LEU:HD23	1:L:337:ARG:HD2	2.01	0.42
1:L:61:LYS:HE2	3:L:738:HOH:O	2.20	0.41
1:L:100:GLY:HA3	1:L:166:LEU:O	2.20	0.41
1:L:158:LEU:HA	1:L:159:PRO:HD3	1.95	0.41
1:L:231:ALA:CB	1:L:238:LEU:HD11	2.50	0.41
1:L:328:PHE:CZ	1:L:331:PHE:CZ	3.08	0.41
1:L:41:GLU:C	1:L:43:GLY:H	2.28	0.41
1:L:58:LEU:HA	1:L:192:TYR:HB2	2.03	0.41
1:L:319:HIS:HB3	1:L:320:GLU:H	1.57	0.41
1:L:472:LEU:O	1:L:473:ASN:CB	2.68	0.41
1:L:227:ILE:HD13	1:L:474:ARG:CZ	2.50	0.41
1:L:516:ILE:CD1	2:S:959:GLN:HA	2.51	0.41
1:L:594:LEU:C	1:L:594:LEU:HD23	2.45	0.41
1:L:698:SER:HB2	2:S:939:MET:CG	2.41	0.41
1:L:54:ILE:HB	1:L:55:PRO:CD	2.50	0.41
1:L:106:TRP:O	1:L:200:THR:HG22	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:419:GLN:OE1	3:L:931:HOH:O	2.22	0.41
1:L:700:LEU:CD1	2:S:916:ARG:HE	2.30	0.41
2:S:866:TYR:O	2:S:869:ASN:HB3	2.21	0.41
1:L:19:GLY:HA2	1:L:25:ILE:HG12	2.02	0.41
1:L:61:LYS:CD	1:L:66:TYR:HB2	2.50	0.41
1:L:429:ILE:HG22	1:L:488:THR:HG22	2.03	0.41
1:L:438:GLU:CG	1:L:439:GLU:H	2.33	0.41
1:L:565:GLN:O	1:L:570:ASP:OD1	2.38	0.41
1:L:612:ARG:HH21	1:L:618:ARG:HA	1.85	0.41
2:S:812:ASP:HB3	2:S:814:GLU:HG2	2.01	0.41
1:L:547:GLU:HA	1:L:592:LEU:O	2.19	0.41
2:S:799:ARG:HD3	2:S:802:ARG:CD	2.27	0.41
1:L:22:GLU:HG3	1:L:23:ARG:N	2.35	0.41
1:L:63:LEU:HB3	1:L:193:GLU:HB2	2.03	0.41
1:L:548:ILE:HA	1:L:552:GLU:OE1	2.21	0.41
1:L:487:SER:HB2	3:L:833:HOH:O	2.21	0.41
1:L:75:TRP:HA	1:L:158:LEU:O	2.21	0.41
1:L:161:LYS:C	1:L:163:GLY:N	2.79	0.41
1:L:201:THR:HG23	1:L:338:LEU:HD22	2.02	0.41
1:L:293:TRP:CD1	1:L:333:ARG:HH12	2.39	0.41
1:L:350:SER:C	1:L:352:THR:N	2.79	0.41
1:L:538:PHE:C	1:L:540:GLN:N	2.77	0.41
1:L:566:ASP:HA	1:L:570:ASP:HB2	2.03	0.41
1:L:655:LEU:HD23	1:L:655:LEU:HA	1.77	0.41
2:S:850:VAL:CG1	2:S:938:ALA:HB1	2.51	0.41
2:S:867:LEU:HG	2:S:871:ILE:HD11	2.03	0.41
2:S:962:LEU:O	2:S:966:MET:HB2	2.21	0.41
1:L:155:ASP:OD2	1:L:157:ARG:HD3	2.21	0.41
1:L:205:GLU:HG2	1:L:210:GLY:O	2.20	0.41
1:L:645:VAL:CG2	1:L:646:ILE:N	2.84	0.41
1:L:99:GLN:H	1:L:108:LEU:HD21	1.86	0.40
1:L:686:THR:HG22	2:S:957:ASN:ND2	2.36	0.40
1:L:41:GLU:O	1:L:43:GLY:N	2.54	0.40
1:L:94:ARG:CD	1:L:289:GLY:HA3	2.51	0.40
1:L:592:LEU:HD13	1:L:596:GLU:O	2.21	0.40
2:S:948:LYS:HG2	3:S:227:HOH:O	2.21	0.40
1:L:167:PHE:HB3	1:L:182:GLU:OE1	2.21	0.40
1:L:284:ILE:CG2	1:L:285:ARG:N	2.85	0.40
1:L:288:TRP:HB2	3:L:869:HOH:O	2.21	0.40
1:L:337:ARG:HB3	1:L:337:ARG:CZ	2.52	0.40
1:L:466:ILE:HG22	1:L:467:ASN:H	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:25:ILE:O	1:L:151:GLU:N	2.43	0.40
1:L:147:GLY:O	1:L:360:LYS:HE2	2.21	0.40
1:L:224:LEU:HD21	1:L:337:ARG:HH12	1.87	0.40
1:L:253:ILE:HG13	1:L:332:LEU:CD2	2.43	0.40
2:S:953:GLN:HG2	2:S:954:ILE:N	2.36	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	697/699 (100%)	546 (78%)	103 (15%)	48 (7%)	1	1
2	S	182/184 (99%)	157 (86%)	18 (10%)	7 (4%)	2	3
All	All	879/883 (100%)	703 (80%)	121 (14%)	55 (6%)	1	1

All (55) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	253	ILE
1	L	256	GLN
1	L	296	ARG
1	L	298	ASN
1	L	301	CYS
1	L	319	HIS
1	L	348	LEU
1	L	402	GLU
1	L	417	ARG
1	L	438	GLU
1	L	444	THR
1	L	464	THR
1	L	473	ASN

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Mol	Chain	Res	Type
1	L	523	PHE
1	L	525	ILE
1	L	526	SER
1	L	546	ALA
1	L	567	ILE
1	L	617	ASP
1	L	618	ARG
2	S	920	GLU
1	L	42	ALA
1	L	90	GLY
1	L	93	THR
1	L	173	GLY
1	L	291	VAL
1	L	331	PHE
1	L	395	ASP
1	L	439	GLU
1	L	564	ARG
1	L	569	SER
2	S	797	GLU
2	S	885	ARG
1	L	92	ALA
1	L	128	ASN
1	L	172	GLU
1	L	257	LYS
1	L	342	ASN
1	L	349	THR
2	S	789	ASN
1	L	94	ARG
1	L	332	LEU
1	L	479	PRO
1	L	536	ARG
1	L	563	LYS
2	S	798	VAL
2	S	907	GLU
1	L	62	GLU
1	L	156	ASP
1	L	302	PRO
1	L	321	ASP
1	L	560	VAL
1	L	252	ALA
2	S	796	GLU
1	L	307	ILE

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	602/602 (100%)	522 (87%)	80 (13%)	4	8
2	S	162/162 (100%)	150 (93%)	12 (7%)	13	27
All	All	764/764 (100%)	672 (88%)	92 (12%)	5	10

All (92) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	4	ILE
1	L	10	LYS
1	L	22	GLU
1	L	25	ILE
1	L	37	ASN
1	L	40	LEU
1	L	60	PHE
1	L	66	TYR
1	L	73	MET
1	L	74	ARG
1	L	97	ILE
1	L	105	CYS
1	L	108	LEU
1	L	118	GLU
1	L	130	SER
1	L	157	ARG
1	L	160	THR
1	L	174	SER
1	L	191	CYS
1	L	192	TYR
1	L	223	ASN
1	L	224	LEU
1	L	227	ILE
1	L	230	LYS
1	L	232	LEU
1	L	242	ILE
1	L	243	ASP

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Mol	Chain	Res	Type
1	L	244	ILE
1	L	249	ASP
1	L	256	GLN
1	L	259	VAL
1	L	296	ARG
1	L	297	TRP
1	L	301	CYS
1	L	303	SER
1	L	316	THR
1	L	323	GLU
1	L	330	ASP
1	L	333	ARG
1	L	336	SER
1	L	338	LEU
1	L	340	ILE
1	L	343	LEU
1	L	344	THR
1	L	346	ASP
1	L	360	LYS
1	L	376	ASN
1	L	420	ARG
1	L	439	GLU
1	L	461	ARG
1	L	466	ILE
1	L	468	LEU
1	L	506	LYS
1	L	525	ILE
1	L	527	GLU
1	L	528	ASP
1	L	531	ASP
1	L	537	LEU
1	L	555	THR
1	L	561	LEU
1	L	566	ASP
1	L	567	ILE
1	L	569	SER
1	L	579	ILE
1	L	587	ASP
1	L	595	LYS
1	L	596	GLU
1	L	613	GLU
1	L	614	ILE

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Mol	Chain	Res	Type
1	L	616	VAL
1	L	617	ASP
1	L	624	SER
1	L	626	GLU
1	L	633	GLU
1	L	645	VAL
1	L	672	LEU
1	L	674	LYS
1	L	682	GLU
1	L	688	GLU
1	L	700	LEU
2	S	786	HIS
2	S	789	ASN
2	S	807	GLN
2	S	821	MET
2	S	835	LYS
2	S	863	GLU
2	S	883	THR
2	S	885	ARG
2	S	890	CYS
2	S	905	LEU
2	S	912	MET
2	S	956	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	47	GLN
1	L	99	GLN
1	L	128	ASN
1	L	132	GLN
1	L	142	GLN
1	L	223	ASN
1	L	256	GLN
1	L	298	ASN
1	L	334	HIS
1	L	364	ASN
1	L	384	ASN
1	L	415	HIS
1	L	419	GLN
1	L	447	HIS
1	L	492	ASN

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Mol	Chain	Res	Type
1	L	519	ASN
1	L	641	GLN
1	L	643	HIS
1	L	644	GLN
1	L	654	GLN
2	S	793	ASN
2	S	870	ASN
2	S	880	GLN
2	S	911	ASN
2	S	957	ASN

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 oligosaccharides 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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	L	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	L	62:GLU	C	63:LEU	N	1.20

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.