



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 12, 2024 – 06:57 AM EDT

PDB ID : 1Z0G
Title : Crystal Structure of A. fulgidus Lon proteolytic domain
Authors : Botos, I.; Melnikov, E.E.; Cherry, S.; Kozlov, S.; Makhovskaya, O.V.; Tropea, J.E.; Gustchina, A.; Rotanova, T.V.; Wlodawer, A.
Deposited on : 2005-03-01
Resolution : 2.27 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.20.1
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

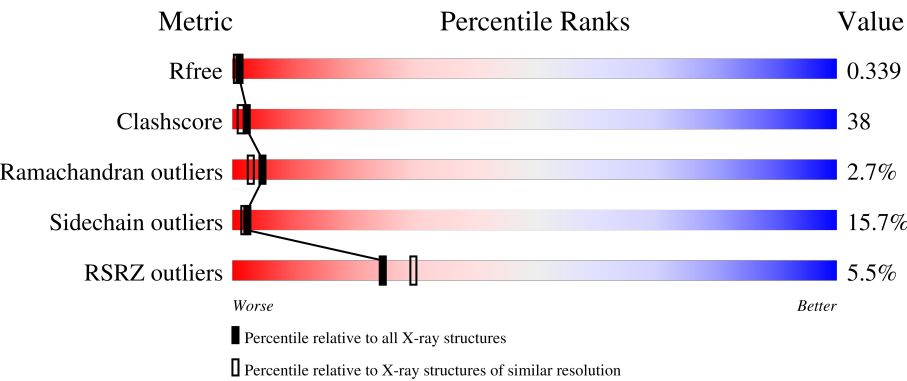
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.27 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	130704	6980 (2.30-2.26)
Clashscore	141614	7711 (2.30-2.26)
Ramachandran outliers	138981	7597 (2.30-2.26)
Sidechain outliers	138945	7598 (2.30-2.26)
RSRZ outliers	127900	6849 (2.30-2.26)

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

Mol	Chain	Length	Quality of chain
1	A	205	<div><div>%</div><div><div></div><div></div><div></div><div></div><div></div></div><div>50%30%11%•5%</div></div>
1	B	205	<div><div>9%</div><div><div></div><div></div><div></div><div></div><div></div></div><div>39%37%16%••</div></div>
1	C	205	<div><div>3%</div><div><div></div><div></div><div></div><div></div><div></div></div><div>36%39%15%5%•</div></div>
1	D	205	<div><div>%</div><div><div></div><div></div><div></div><div></div><div></div></div><div>46%32%15%••</div></div>
1	E	205	<div><div>13%</div><div><div></div><div></div><div></div><div></div><div></div></div><div>40%39%13%•5%</div></div>

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Mol	Chain	Length	Quality of chain
1	F	205	<div><div></div><div>3%</div><div>45%</div><div>30%</div><div>15%</div><div>6%</div><div></div></div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9873 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 Putative protease La homolog type.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	195	Total	C	N	O	S	0	0	0
			1457	921	247	284	5			
1	B	196	Total	C	N	O	S	0	0	0
			1466	926	248	287	5			
1	C	196	Total	C	N	O	S	0	0	0
			1466	926	248	287	5			
1	D	196	Total	C	N	O	S	0	0	0
			1466	926	248	287	5			
1	E	195	Total	C	N	O	S	0	0	0
			1457	921	247	284	5			
1	F	196	Total	C	N	O	S	0	0	0
			1466	926	248	287	5			

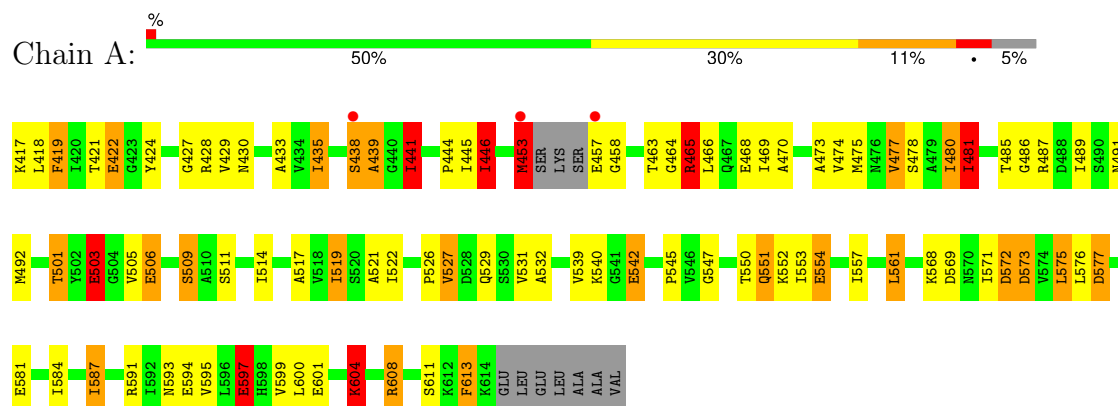
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	163	Total	O	0	0
			163	163		
2	B	165	Total	O	0	0
			165	165		
2	C	198	Total	O	0	0
			198	198		
2	D	197	Total	O	0	0
			197	197		
2	E	147	Total	O	0	0
			147	147		
2	F	225	Total	O	0	0
			225	225		

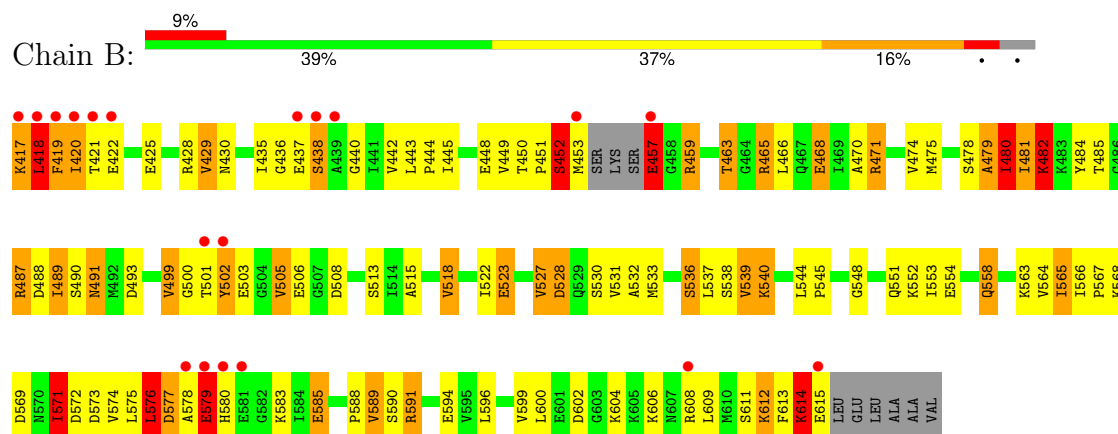
3 Residue-property plots

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 and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

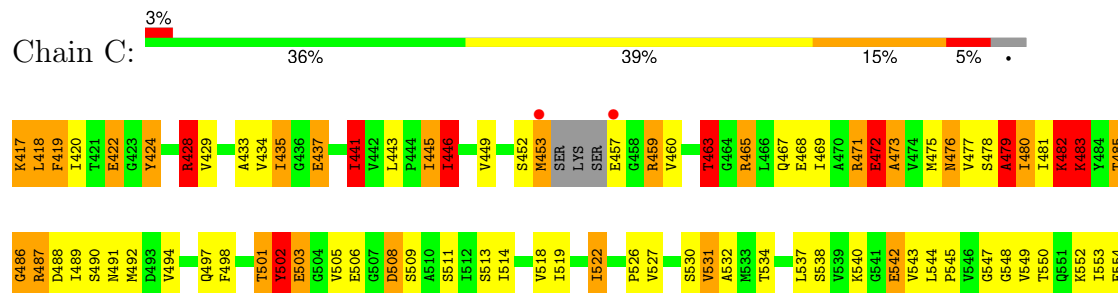
• Molecule 1: Putative protease La homolog type

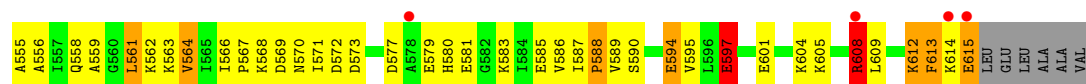


• Molecule 1: Putative protease La homolog type

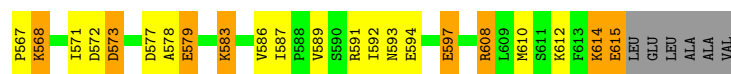
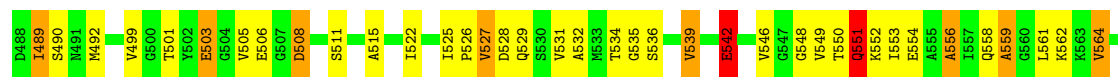
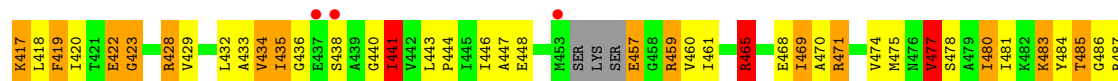


• Molecule 1: Putative protease La homolog type

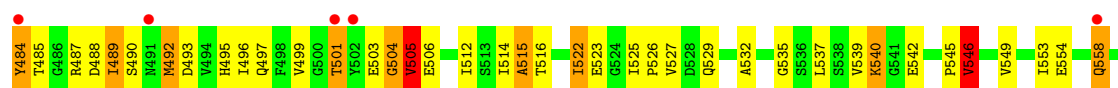
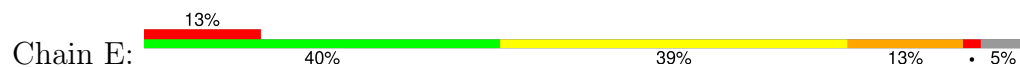




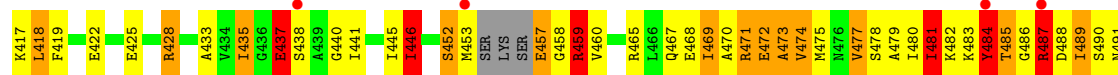
• Molecule 1: Putative protease La homolog type



• Molecule 1: Putative protease La homolog type



• Molecule 1: Putative protease La homolog type



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	85.65Å 88.69Å 147.24Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.27 14.97 – 2.27	Depositor EDS
% Data completeness (in resolution range)	100.0 (15.00-2.27) 96.2 (14.97-2.27)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.42 (at 2.27Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.195 , 0.329 0.212 , 0.339	Depositor DCC
R_{free} test set	1038 reflections (2.06%)	wwPDB-VP
Wilson B-factor (Å ²)	24.8	Xtriage
Anisotropy	0.582	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 64.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.57$, $\langle L^2 \rangle = 0.42$	Xtriage
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9873	wwPDB-VP
Average B, all atoms (Å ²)	14.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 57.46 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.3605e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	2.00	35/1470 (2.4%)	1.51	19/1983 (1.0%)
1	B	2.11	26/1479 (1.8%)	1.54	24/1995 (1.2%)
1	C	2.23	44/1479 (3.0%)	1.69	30/1995 (1.5%)
1	D	2.13	45/1479 (3.0%)	1.65	25/1995 (1.3%)
1	E	1.83	21/1470 (1.4%)	1.54	17/1983 (0.9%)
1	F	2.08	45/1479 (3.0%)	1.70	26/1995 (1.3%)
All	All	2.07	216/8856 (2.4%)	1.61	141/11946 (1.2%)

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
1	B	0	1
1	C	0	2
1	D	1	1
1	E	0	3
1	F	1	3
All	All	2	10

All (216) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	579	GLU	CD-OE1	26.73	1.55	1.25
1	B	579	GLU	CD-OE2	20.38	1.48	1.25
1	D	597	GLU	CD-OE1	17.72	1.45	1.25
1	C	597	GLU	CG-CD	16.45	1.76	1.51
1	A	597	GLU	CG-CD	15.68	1.75	1.51
1	B	579	GLU	CG-CD	14.21	1.73	1.51
1	C	479	ALA	CA-CB	13.61	1.81	1.52
1	C	597	GLU	CD-OE2	12.64	1.39	1.25
1	C	502	TYR	CE1-CZ	12.32	1.54	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	594	GLU	CD-OE1	-11.93	1.12	1.25
1	D	539	VAL	CB-CG1	11.20	1.76	1.52
1	F	474	VAL	CB-CG1	11.12	1.76	1.52
1	C	472	GLU	CG-CD	10.40	1.67	1.51
1	D	506	GLU	CB-CG	-10.23	1.32	1.52
1	C	473	ALA	CA-CB	-10.17	1.31	1.52
1	C	503	GLU	CB-CG	10.16	1.71	1.52
1	D	597	GLU	CG-CD	10.05	1.67	1.51
1	D	556	ALA	CA-CB	10.02	1.73	1.52
1	E	471	ARG	CZ-NH1	9.64	1.45	1.33
1	D	468	GLU	CD-OE1	9.56	1.36	1.25
1	C	503	GLU	CG-CD	9.53	1.66	1.51
1	F	473	ALA	CA-CB	-9.43	1.32	1.52
1	F	594	GLU	CB-CG	9.41	1.70	1.52
1	F	612	LYS	CD-CE	9.20	1.74	1.51
1	B	429	VAL	CB-CG2	-9.17	1.33	1.52
1	C	597	GLU	CB-CG	9.07	1.69	1.52
1	A	542	GLU	CG-CD	9.03	1.65	1.51
1	F	597	GLU	CG-CD	9.03	1.65	1.51
1	E	477	VAL	CB-CG1	8.94	1.71	1.52
1	A	542	GLU	CD-OE2	8.94	1.35	1.25
1	F	597	GLU	CD-OE2	8.90	1.35	1.25
1	E	527	VAL	CB-CG1	8.77	1.71	1.52
1	F	597	GLU	CD-OE1	8.68	1.35	1.25
1	D	527	VAL	CB-CG2	-8.52	1.34	1.52
1	F	472	GLU	CB-CG	8.49	1.68	1.52
1	C	527	VAL	CA-CB	8.49	1.72	1.54
1	E	515	ALA	CA-CB	8.41	1.70	1.52
1	B	564	VAL	CB-CG2	8.40	1.70	1.52
1	A	506	GLU	CB-CG	-8.38	1.36	1.52
1	B	527	VAL	CB-CG1	8.33	1.70	1.52
1	C	449	VAL	CB-CG1	8.31	1.70	1.52
1	F	502	TYR	CB-CG	8.20	1.64	1.51
1	C	472	GLU	CB-CG	8.12	1.67	1.52
1	F	578	ALA	C-O	8.11	1.38	1.23
1	A	506	GLU	CG-CD	-8.10	1.39	1.51
1	C	518	VAL	CB-CG2	8.04	1.69	1.52
1	C	424	TYR	CD1-CE1	-8.03	1.27	1.39
1	D	499	VAL	CB-CG2	7.90	1.69	1.52
1	C	601	GLU	CD-OE2	-7.88	1.17	1.25
1	E	424	TYR	CE2-CZ	7.75	1.48	1.38
1	B	574	VAL	CB-CG2	7.65	1.69	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	527	VAL	CA-CB	7.60	1.70	1.54
1	D	506	GLU	CG-CD	-7.57	1.40	1.51
1	C	589	VAL	CB-CG2	7.50	1.68	1.52
1	D	422	GLU	CB-CG	7.37	1.66	1.52
1	D	447	ALA	CA-CB	-7.24	1.37	1.52
1	C	428	ARG	CB-CG	7.19	1.72	1.52
1	D	539	VAL	CB-CG2	-7.17	1.37	1.52
1	D	480	ILE	CA-CB	7.06	1.71	1.54
1	B	523	GLU	CG-CD	7.06	1.62	1.51
1	F	579	GLU	CD-OE2	7.05	1.33	1.25
1	C	597	GLU	CD-OE1	7.03	1.33	1.25
1	F	484	TYR	CB-CG	6.97	1.62	1.51
1	A	424	TYR	CD1-CE1	6.93	1.49	1.39
1	E	542	GLU	CG-CD	6.92	1.62	1.51
1	B	518	VAL	CB-CG2	6.91	1.67	1.52
1	E	522	ILE	CB-CG2	6.89	1.74	1.52
1	D	571	ILE	CB-CG2	6.87	1.74	1.52
1	D	549	VAL	CB-CG2	6.81	1.67	1.52
1	D	535	GLY	N-CA	6.81	1.56	1.46
1	C	522	ILE	CB-CG2	6.73	1.73	1.52
1	A	531	VAL	CB-CG1	6.61	1.66	1.52
1	C	502	TYR	CZ-OH	6.57	1.49	1.37
1	D	587	ILE	CB-CG2	6.54	1.73	1.52
1	A	521	ALA	CA-CB	6.54	1.66	1.52
1	F	568	LYS	CD-CE	6.54	1.67	1.51
1	B	457	GLU	CG-CD	6.52	1.61	1.51
1	D	468	GLU	CD-OE2	6.51	1.32	1.25
1	C	542	GLU	C-O	-6.47	1.11	1.23
1	B	515	ALA	CA-CB	6.45	1.66	1.52
1	A	577	ASP	N-CA	6.39	1.59	1.46
1	A	480	ILE	CA-CB	6.39	1.69	1.54
1	D	579	GLU	CD-OE2	6.34	1.32	1.25
1	D	423	GLY	C-O	-6.33	1.13	1.23
1	B	482	LYS	CG-CD	6.32	1.74	1.52
1	D	615	GLU	CB-CG	6.32	1.64	1.52
1	A	531	VAL	CA-CB	-6.29	1.41	1.54
1	F	589	VAL	CB-CG2	6.26	1.66	1.52
1	F	554	GLU	CD-OE2	6.26	1.32	1.25
1	A	542	GLU	CB-CG	6.25	1.64	1.52
1	A	527	VAL	N-CA	6.23	1.58	1.46
1	D	552	LYS	CE-NZ	6.23	1.64	1.49
1	B	480	ILE	CA-CB	6.22	1.69	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	601	GLU	CD-OE2	-6.21	1.18	1.25
1	E	558	GLN	CG-CD	6.20	1.65	1.51
1	A	481	ILE	CA-CB	6.20	1.69	1.54
1	B	479	ALA	CA-CB	6.14	1.65	1.52
1	B	499	VAL	CB-CG2	6.09	1.65	1.52
1	D	428	ARG	CB-CG	6.06	1.69	1.52
1	A	506	GLU	CD-OE1	6.04	1.32	1.25
1	F	422	GLU	CD-OE2	6.03	1.32	1.25
1	A	593	ASN	CB-CG	6.01	1.64	1.51
1	C	608	ARG	CG-CD	5.97	1.66	1.51
1	B	482	LYS	CB-CG	5.97	1.68	1.52
1	A	597	GLU	CD-OE2	5.96	1.32	1.25
1	D	551	GLN	CD-OE1	5.96	1.37	1.24
1	E	554	GLU	CB-CG	5.94	1.63	1.52
1	E	445	ILE	CB-CG2	5.92	1.71	1.52
1	F	542	GLU	CB-CG	5.89	1.63	1.52
1	C	564	VAL	CA-CB	5.88	1.67	1.54
1	D	592	ILE	CA-CB	5.88	1.68	1.54
1	B	536	SER	CB-OG	5.88	1.49	1.42
1	C	489	ILE	CA-CB	5.88	1.68	1.54
1	A	473	ALA	CA-CB	-5.87	1.40	1.52
1	B	585	GLU	CG-CD	5.85	1.60	1.51
1	F	595	VAL	CB-CG2	5.85	1.65	1.52
1	F	579	GLU	CB-CG	5.84	1.63	1.52
1	F	579	GLU	CG-CD	5.82	1.60	1.51
1	C	503	GLU	CD-OE1	5.81	1.32	1.25
1	E	535	GLY	N-CA	5.81	1.54	1.46
1	A	547	GLY	N-CA	-5.80	1.37	1.46
1	F	522	ILE	CB-CG2	5.78	1.70	1.52
1	E	424	TYR	CG-CD2	5.77	1.46	1.39
1	A	554	GLU	CG-CD	5.76	1.60	1.51
1	C	555	ALA	CA-CB	5.75	1.64	1.52
1	A	441	ILE	CA-CB	5.75	1.68	1.54
1	F	425	GLU	CB-CG	5.75	1.63	1.52
1	F	567	PRO	C-O	5.73	1.34	1.23
1	F	472	GLU	CG-CD	5.72	1.60	1.51
1	F	532	ALA	CA-CB	5.71	1.64	1.52
1	D	419	PHE	C-O	5.71	1.34	1.23
1	F	499	VAL	CB-CG1	-5.68	1.41	1.52
1	C	498	PHE	CD2-CE2	5.67	1.50	1.39
1	B	513	SER	C-O	-5.64	1.12	1.23
1	F	536	SER	CA-CB	5.63	1.61	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	508	ASP	CB-CG	5.60	1.63	1.51
1	D	471	ARG	CD-NE	5.57	1.55	1.46
1	F	612	LYS	CE-NZ	5.57	1.62	1.49
1	F	457	GLU	CD-OE2	5.56	1.31	1.25
1	A	594	GLU	CG-CD	5.55	1.60	1.51
1	F	459	ARG	CZ-NH1	5.54	1.40	1.33
1	C	531	VAL	CB-CG2	5.52	1.64	1.52
1	F	468	GLU	CB-CG	-5.50	1.41	1.52
1	F	605	LYS	CB-CG	5.50	1.67	1.52
1	C	459	ARG	C-O	5.49	1.33	1.23
1	D	578	ALA	C-O	5.49	1.33	1.23
1	A	464	GLY	N-CA	5.47	1.54	1.46
1	A	503	GLU	CB-CG	5.45	1.62	1.52
1	D	506	GLU	CD-OE2	5.45	1.31	1.25
1	D	417	LYS	CD-CE	5.45	1.64	1.51
1	D	440	GLY	C-O	-5.42	1.15	1.23
1	E	565	ILE	CA-CB	-5.42	1.42	1.54
1	B	482	LYS	CD-CE	5.41	1.64	1.51
1	F	590	SER	CB-OG	-5.41	1.35	1.42
1	C	612	LYS	CE-NZ	5.40	1.62	1.49
1	C	530	SER	CB-OG	5.40	1.49	1.42
1	C	595	VAL	N-CA	-5.38	1.35	1.46
1	E	568	LYS	CD-CE	5.38	1.64	1.51
1	D	503	GLU	CB-CG	5.37	1.62	1.52
1	A	517	ALA	CA-CB	5.35	1.63	1.52
1	B	589	VAL	CB-CG2	5.34	1.64	1.52
1	D	586	VAL	CB-CG2	5.34	1.64	1.52
1	A	551	GLN	CG-CD	5.33	1.63	1.51
1	C	585	GLU	CG-CD	-5.33	1.44	1.51
1	E	433	ALA	CA-CB	5.33	1.63	1.52
1	D	536	SER	N-CA	-5.30	1.35	1.46
1	E	419	PHE	CD2-CE2	5.30	1.49	1.39
1	C	419	PHE	CG-CD1	-5.29	1.30	1.38
1	C	453	MET	CB-CG	5.28	1.68	1.51
1	D	468	GLU	CG-CD	5.27	1.59	1.51
1	D	506	GLU	C-O	5.27	1.33	1.23
1	D	577	ASP	CG-OD2	5.26	1.37	1.25
1	F	568	LYS	CE-NZ	5.26	1.62	1.49
1	C	589	VAL	CB-CG1	5.26	1.63	1.52
1	D	531	VAL	C-O	5.25	1.33	1.23
1	F	471	ARG	CZ-NH1	5.25	1.39	1.33
1	D	594	GLU	CD-OE1	5.25	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	599	VAL	CB-CG1	5.22	1.63	1.52
1	D	583	LYS	CE-NZ	5.21	1.62	1.49
1	F	504	GLY	C-O	-5.20	1.15	1.23
1	C	542	GLU	CA-C	-5.19	1.39	1.52
1	A	519	ILE	CA-CB	5.18	1.66	1.54
1	A	611	SER	C-O	-5.17	1.13	1.23
1	A	446	ILE	CB-CG2	5.17	1.68	1.52
1	A	604	LYS	CD-CE	5.17	1.64	1.51
1	C	558	GLN	CB-CG	-5.17	1.38	1.52
1	F	419	PHE	CB-CG	5.17	1.60	1.51
1	E	516	THR	C-O	5.15	1.33	1.23
1	A	542	GLU	CD-OE1	5.14	1.31	1.25
1	C	554	GLU	CD-OE2	5.14	1.31	1.25
1	F	437	GLU	CB-CG	5.13	1.61	1.52
1	D	559	ALA	CA-CB	5.13	1.63	1.52
1	D	564	VAL	CA-CB	5.12	1.65	1.54
1	C	483	LYS	N-CA	5.12	1.56	1.46
1	F	542	GLU	CD-OE1	5.11	1.31	1.25
1	C	494	VAL	CB-CG1	-5.10	1.42	1.52
1	A	419	PHE	CE1-CZ	5.10	1.47	1.37
1	B	448	GLU	CB-CG	-5.10	1.42	1.52
1	E	542	GLU	CB-CG	5.10	1.61	1.52
1	E	572	ASP	CB-CG	5.09	1.62	1.51
1	C	587	ILE	CA-CB	5.09	1.66	1.54
1	F	518	VAL	CB-CG1	5.08	1.63	1.52
1	F	422	GLU	CD-OE1	5.08	1.31	1.25
1	D	477	VAL	C-O	5.08	1.32	1.23
1	F	566	ILE	CA-CB	5.08	1.66	1.54
1	B	571	ILE	CB-CG2	5.07	1.68	1.52
1	D	529	GLN	CD-OE1	-5.06	1.12	1.24
1	A	581	GLU	CG-CD	5.06	1.59	1.51
1	D	460	VAL	CB-CG1	5.05	1.63	1.52
1	A	427	GLY	N-CA	-5.04	1.38	1.46
1	B	527	VAL	CB-CG2	-5.04	1.42	1.52
1	C	613	PHE	CE2-CZ	5.03	1.47	1.37
1	C	566	ILE	CA-CB	5.02	1.66	1.54
1	B	513	SER	CB-OG	-5.02	1.35	1.42
1	B	468	GLU	CD-OE2	5.02	1.31	1.25
1	E	565	ILE	CB-CG2	-5.00	1.37	1.52

All (141) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	471	ARG	NE-CZ-NH2	-14.75	112.92	120.30
1	F	471	ARG	NE-CZ-NH2	-12.66	113.97	120.30
1	F	594	GLU	OE1-CD-OE2	-11.58	109.41	123.30
1	A	600	LEU	CB-CG-CD1	-10.88	92.51	111.00
1	D	577	ASP	CB-CG-OD1	-10.53	108.83	118.30
1	C	502	TYR	CB-CG-CD2	-10.07	114.96	121.00
1	C	428	ARG	NE-CZ-NH1	9.66	125.13	120.30
1	C	428	ARG	NE-CZ-NH2	-9.11	115.74	120.30
1	C	471	ARG	NE-CZ-NH2	-9.06	115.77	120.30
1	B	471	ARG	NE-CZ-NH2	-8.94	115.83	120.30
1	F	549	VAL	CG1-CB-CG2	-8.78	96.84	110.90
1	A	506	GLU	OE1-CD-OE2	8.49	133.49	123.30
1	D	459	ARG	NE-CZ-NH2	-8.29	116.16	120.30
1	B	418	LEU	CA-CB-CG	8.26	134.30	115.30
1	D	528	ASP	CB-CG-OD1	8.17	125.65	118.30
1	F	459	ARG	NE-CZ-NH1	8.15	124.38	120.30
1	E	572	ASP	CB-CG-OD1	8.11	125.59	118.30
1	F	612	LYS	CD-CE-NZ	7.97	130.03	111.70
1	D	591	ARG	NE-CZ-NH1	7.83	124.22	120.30
1	C	502	TYR	CB-CG-CD1	7.83	125.70	121.00
1	F	591	ARG	NE-CZ-NH2	-7.72	116.44	120.30
1	F	428	ARG	NE-CZ-NH2	7.66	124.13	120.30
1	F	459	ARG	NE-CZ-NH2	-7.66	116.47	120.30
1	F	572	ASP	CB-CG-OD1	7.60	125.14	118.30
1	D	573	ASP	CB-CG-OD2	7.51	125.06	118.30
1	B	528	ASP	CB-CG-OD1	7.46	125.02	118.30
1	C	463	THR	CA-CB-CG2	7.40	122.76	112.40
1	D	597	GLU	CG-CD-OE2	-7.34	103.62	118.30
1	D	583	LYS	CD-CE-NZ	7.27	128.43	111.70
1	C	418	LEU	CB-CG-CD1	-7.26	98.66	111.00
1	D	597	GLU	OE1-CD-OE2	7.11	131.83	123.30
1	B	442	VAL	CG1-CB-CG2	-7.10	99.53	110.90
1	A	446	ILE	CB-CA-C	-7.08	97.44	111.60
1	F	608	ARG	NE-CZ-NH1	7.01	123.80	120.30
1	D	528	ASP	CB-CG-OD2	-6.93	112.06	118.30
1	F	487	ARG	NE-CZ-NH1	6.76	123.68	120.30
1	F	572	ASP	CB-CG-OD2	-6.72	112.25	118.30
1	B	459	ARG	NE-CZ-NH1	6.67	123.63	120.30
1	B	481	ILE	CG1-CB-CG2	-6.66	96.74	111.40
1	D	428	ARG	CG-CD-NE	6.63	125.73	111.80
1	D	589	VAL	CG1-CB-CG2	6.62	121.50	110.90
1	F	474	VAL	CG1-CB-CG2	6.55	121.38	110.90
1	F	540	LYS	CD-CE-NZ	-6.51	96.72	111.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	615	GLU	N-CA-C	6.42	128.34	111.00
1	C	441	ILE	CB-CA-C	-6.41	98.78	111.60
1	B	579	GLU	OE1-CD-OE2	6.38	130.96	123.30
1	E	471	ARG	NE-CZ-NH1	6.37	123.48	120.30
1	C	609	LEU	CB-CG-CD1	-6.36	100.18	111.00
1	D	448	GLU	CA-CB-CG	-6.36	99.42	113.40
1	B	565	ILE	CB-CA-C	-6.32	98.95	111.60
1	F	471	ARG	NE-CZ-NH1	6.30	123.45	120.30
1	C	561	LEU	CB-CG-CD1	-6.29	100.30	111.00
1	C	487	ARG	NE-CZ-NH2	-6.28	117.16	120.30
1	B	596	LEU	CB-CG-CD1	6.28	121.67	111.00
1	E	596	LEU	CB-CG-CD2	6.28	121.67	111.00
1	A	539	VAL	CG1-CB-CG2	6.26	120.92	110.90
1	B	572	ASP	CB-CG-OD1	6.25	123.93	118.30
1	A	446	ILE	CA-CB-CG2	6.22	123.35	110.90
1	C	471	ARG	CG-CD-NE	-6.22	98.74	111.80
1	C	502	TYR	CA-CB-CG	-6.18	101.65	113.40
1	E	546	VAL	CG1-CB-CG2	-6.16	101.05	110.90
1	F	481	ILE	CG1-CB-CG2	-6.14	97.89	111.40
1	F	498	PHE	N-CA-C	-6.12	94.47	111.00
1	E	445	ILE	CB-CA-C	-6.08	99.44	111.60
1	B	539	VAL	CG1-CB-CG2	6.07	120.61	110.90
1	E	436	GLY	N-CA-C	-6.04	98.00	113.10
1	A	552	LYS	CD-CE-NZ	-6.02	97.85	111.70
1	C	605	LYS	CD-CE-NZ	-6.00	97.90	111.70
1	D	487	ARG	NE-CZ-NH1	5.93	123.27	120.30
1	B	445	ILE	CB-CA-C	-5.92	99.75	111.60
1	F	509	SER	N-CA-C	-5.92	95.03	111.00
1	E	568	LYS	CD-CE-NZ	5.91	125.29	111.70
1	A	453	MET	CG-SD-CE	5.90	109.65	100.20
1	A	465	ARG	CB-CG-CD	5.86	126.84	111.60
1	B	573	ASP	CB-CG-OD2	5.85	123.56	118.30
1	D	428	ARG	NE-CZ-NH1	5.82	123.21	120.30
1	F	574	VAL	N-CA-C	-5.81	95.30	111.00
1	C	487	ARG	CG-CD-NE	-5.80	99.62	111.80
1	B	576	LEU	CA-CB-CG	-5.79	101.98	115.30
1	B	614	LYS	N-CA-C	-5.76	95.44	111.00
1	A	573	ASP	CB-CG-OD2	5.74	123.46	118.30
1	F	602	ASP	CB-CG-OD1	5.73	123.46	118.30
1	B	471	ARG	NE-CZ-NH1	5.73	123.16	120.30
1	B	480	ILE	CA-CB-CG2	5.69	122.28	110.90
1	C	589	VAL	CG1-CB-CG2	5.68	119.99	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	506	GLU	CG-CD-OE2	-5.67	106.95	118.30
1	E	527	VAL	CA-CB-CG1	5.67	119.41	110.90
1	D	441	ILE	CB-CA-C	-5.66	100.27	111.60
1	C	543	VAL	CG1-CB-CG2	5.65	119.94	110.90
1	E	566	ILE	CG1-CB-CG2	5.62	123.76	111.40
1	C	445	ILE	CB-CA-C	-5.60	100.40	111.60
1	A	572	ASP	CB-CG-OD1	-5.56	113.29	118.30
1	E	418	LEU	CA-CB-CG	5.55	128.07	115.30
1	D	468	GLU	OE1-CD-OE2	5.54	129.94	123.30
1	F	600	LEU	CB-CG-CD1	-5.51	101.63	111.00
1	A	575	LEU	CB-CG-CD1	5.50	120.35	111.00
1	F	608	ARG	NE-CZ-NH2	-5.49	117.56	120.30
1	E	595	VAL	CG1-CB-CG2	-5.48	102.13	110.90
1	D	568	LYS	CB-CG-CD	5.48	125.84	111.60
1	C	446	ILE	CB-CG1-CD1	-5.47	98.58	113.90
1	A	587	ILE	CG1-CB-CG2	-5.46	99.39	111.40
1	F	487	ARG	NE-CZ-NH2	-5.45	117.58	120.30
1	C	429	VAL	CG1-CB-CG2	-5.43	102.20	110.90
1	C	572	ASP	CB-CG-OD2	5.43	123.19	118.30
1	C	502	TYR	CB-CA-C	5.42	121.25	110.40
1	C	483	LYS	N-CA-C	5.37	125.51	111.00
1	D	542	GLU	OE1-CD-OE2	5.34	129.70	123.30
1	F	446	ILE	CA-CB-CG2	5.33	121.55	110.90
1	F	577	ASP	CB-CA-C	5.29	120.98	110.40
1	C	446	ILE	N-CA-C	-5.29	96.72	111.00
1	D	508	ASP	CB-CG-OD1	5.28	123.05	118.30
1	B	418	LEU	CB-CG-CD1	5.26	119.94	111.00
1	E	466	LEU	CB-CG-CD1	-5.26	102.06	111.00
1	C	508	ASP	N-CA-CB	5.25	120.06	110.60
1	A	465	ARG	CA-CB-CG	5.25	124.94	113.40
1	A	561	LEU	CB-CG-CD1	5.23	119.88	111.00
1	A	613	PHE	CB-CA-C	-5.22	99.97	110.40
1	B	499	VAL	CG1-CB-CG2	5.20	119.22	110.90
1	C	594	GLU	N-CA-CB	-5.19	101.26	110.60
1	D	465	ARG	NE-CZ-NH2	-5.18	117.71	120.30
1	A	481	ILE	CA-CB-CG2	5.16	121.23	110.90
1	E	443	LEU	CA-CB-CG	5.16	127.17	115.30
1	D	461	ILE	CG1-CB-CG2	-5.16	100.06	111.40
1	F	502	TYR	N-CA-C	5.14	124.89	111.00
1	B	576	LEU	CB-CG-CD1	5.14	119.74	111.00
1	D	562	LYS	CD-CE-NZ	-5.11	99.95	111.70
1	A	591	ARG	NE-CZ-NH2	-5.11	117.75	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	489	ILE	CB-CA-C	5.11	121.81	111.60
1	C	446	ILE	CB-CA-C	-5.10	101.40	111.60
1	E	445	ILE	CB-CG1-CD1	5.09	128.15	113.90
1	C	446	ILE	CA-CB-CG2	5.08	121.06	110.90
1	B	602	ASP	CB-CG-OD1	-5.08	113.73	118.30
1	B	459	ARG	NE-CZ-NH2	-5.07	117.76	120.30
1	D	434	VAL	CB-CA-C	-5.07	101.76	111.40
1	B	591	ARG	NE-CZ-NH2	-5.05	117.77	120.30
1	D	589	VAL	CA-CB-CG2	-5.05	103.32	110.90
1	A	465	ARG	NE-CZ-NH1	5.05	122.83	120.30
1	E	443	LEU	CB-CG-CD1	5.05	119.58	111.00
1	C	478	SER	C-N-CA	5.02	134.26	121.70
1	C	486	GLY	N-CA-C	5.01	125.63	113.10
1	B	585	GLU	OE1-CD-OE2	-5.01	117.29	123.30

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	D	615	GLU	CA
1	F	502	TYR	CA

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	435	ILE	Peptide
1	C	562	LYS	Mainchain
1	C	613	PHE	Peptide
1	D	614	LYS	Peptide
1	E	435	ILE	Peptide
1	E	438	SER	Peptide
1	E	504	GLY	Peptide
1	F	484	TYR	Peptide
1	F	576	LEU	Peptide
1	F	578	ALA	Peptide

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1457	0	1523	95	0
1	B	1466	0	1529	136	0
1	C	1466	0	1529	158	0
1	D	1466	0	1529	84	0
1	E	1457	0	1523	113	0
1	F	1466	0	1529	141	0
2	A	163	0	0	21	0
2	B	165	0	0	41	0
2	C	198	0	0	70	2
2	D	197	0	0	34	2
2	E	147	0	0	38	0
2	F	225	0	0	50	0
All	All	9873	0	9162	686	2

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 38.

All (686) 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:E:461:ILE:CD1	1:E:461:ILE:CG1	1.75	1.60
1:E:445:ILE:CG1	1:E:445:ILE:CD1	1.76	1.60
1:E:512:ILE:CD1	1:E:512:ILE:CG1	1.74	1.59
1:C:479:ALA:CB	1:C:479:ALA:CA	1.81	1.59
1:F:474:VAL:CG1	1:F:474:VAL:CB	1.76	1.55
1:D:539:VAL:CB	1:D:539:VAL:CG1	1.76	1.54
1:C:597:GLU:CD	1:C:597:GLU:CG	1.76	1.51
1:A:597:GLU:CD	1:A:597:GLU:CG	1.75	1.50
1:D:428:ARG:HG2	2:D:818:HOH:O	1.25	1.29
1:C:420:ILE:HG13	2:C:768:HOH:O	1.38	1.24
1:E:497:GLN:HG2	2:E:727:HOH:O	1.35	1.22
1:F:445:ILE:HD11	2:F:811:HOH:O	1.37	1.19
1:D:608:ARG:HE	1:D:612:LYS:HE3	1.11	1.15
1:E:419:PHE:HB2	2:E:763:HOH:O	1.49	1.13
1:C:614:LYS:HA	1:C:615:GLU:C	1.69	1.12
1:B:418:LEU:HD11	2:C:800:HOH:O	1.48	1.12
1:F:554:GLU:HG2	2:F:837:HOH:O	1.46	1.12
1:C:465:ARG:HB2	1:C:503:GLU:OE1	1.49	1.10
1:E:425:GLU:HG2	2:F:828:HOH:O	1.50	1.08
1:F:477:VAL:HG22	1:F:481:ILE:HD12	1.10	1.08
1:C:550:THR:HG23	2:C:807:HOH:O	1.54	1.06
1:B:576:LEU:HD22	1:B:580:HIS:HB3	1.28	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:472:GLU:OE1	1:F:509:SER:HA	1.58	1.02
1:B:420:ILE:HG21	2:B:701:HOH:O	1.60	1.01
1:D:428:ARG:NE	2:D:818:HOH:O	1.93	1.00
1:F:578:ALA:HB1	2:F:803:HOH:O	1.61	1.00
1:D:608:ARG:HH11	1:D:608:ARG:HG2	1.25	1.00
1:D:428:ARG:CD	2:D:818:HOH:O	2.05	0.99
1:B:419:PHE:HA	1:B:428:ARG:HH22	1.24	0.99
1:A:466:LEU:HB3	2:A:781:HOH:O	1.62	0.98
1:D:542:GLU:HG3	2:D:650:HOH:O	1.62	0.98
1:C:446:ILE:HD11	1:C:497:GLN:HB2	1.43	0.97
1:B:482:LYS:HG2	2:B:753:HOH:O	1.62	0.97
1:F:614:LYS:HA	2:F:835:HOH:O	1.65	0.97
1:F:472:GLU:HG3	2:F:665:HOH:O	1.61	0.97
1:B:419:PHE:HA	1:B:428:ARG:NH2	1.79	0.96
1:C:428:ARG:HD2	2:C:666:HOH:O	1.65	0.96
2:A:758:HOH:O	1:B:540:LYS:HE2	1.64	0.96
1:C:577:ASP:OD1	1:C:579:GLU:HB2	1.66	0.95
1:C:482:LYS:HG2	1:C:483:LYS:H	1.32	0.95
1:F:502:TYR:HB2	2:F:734:HOH:O	1.64	0.95
1:F:477:VAL:CG2	1:F:481:ILE:HD12	1.95	0.94
1:D:583:LYS:HG3	2:D:790:HOH:O	1.67	0.94
1:C:463:THR:HG23	2:C:771:HOH:O	1.68	0.94
2:E:746:HOH:O	1:F:539:VAL:HG11	1.67	0.93
1:C:445:ILE:HD11	2:C:782:HOH:O	1.69	0.92
1:B:444:PRO:HB2	1:B:499:VAL:HB	1.52	0.92
1:B:614:LYS:HD2	2:B:710:HOH:O	1.70	0.91
1:B:489:ILE:O	1:B:489:ILE:HG22	1.68	0.91
1:B:478:SER:O	1:B:482:LYS:HD3	1.69	0.91
1:C:506:GLU:HG3	2:C:798:HOH:O	1.69	0.90
1:A:445:ILE:HD11	2:A:767:HOH:O	1.70	0.90
1:B:482:LYS:HB3	2:B:753:HOH:O	1.72	0.89
1:C:465:ARG:CB	1:C:503:GLU:OE1	2.20	0.89
1:D:539:VAL:CG1	1:D:539:VAL:CG2	2.50	0.89
1:A:446:ILE:CD1	1:B:544:LEU:HD13	2.02	0.89
1:F:477:VAL:HB	2:F:658:HOH:O	1.71	0.89
1:C:571:ILE:HG12	2:C:711:HOH:O	1.72	0.89
1:B:419:PHE:HB3	2:B:771:HOH:O	1.71	0.89
1:C:550:THR:HA	2:C:807:HOH:O	1.73	0.89
1:F:469:ILE:O	1:F:472:GLU:HG2	1.73	0.88
1:D:612:LYS:NZ	2:D:744:HOH:O	2.07	0.87
1:C:502:TYR:CE1	2:C:626:HOH:O	2.28	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:487:ARG:HD3	2:B:762:HOH:O	1.75	0.86
1:E:418:LEU:HD21	2:F:810:HOH:O	1.75	0.86
1:C:482:LYS:HG2	1:C:483:LYS:N	1.88	0.86
1:D:465:ARG:HE	1:D:503:GLU:HB2	1.39	0.85
1:A:463:THR:HG22	1:B:468:GLU:HG3	1.57	0.85
1:C:502:TYR:CD2	1:C:505:VAL:HG21	2.12	0.84
1:D:417:LYS:HD2	2:D:777:HOH:O	1.76	0.84
1:F:435:ILE:HG12	1:F:441:ILE:HG23	1.57	0.84
1:C:608:ARG:CB	2:C:713:HOH:O	2.25	0.84
1:D:608:ARG:NE	1:D:612:LYS:HE3	1.92	0.84
1:F:428:ARG:NH2	2:F:686:HOH:O	2.10	0.84
1:F:477:VAL:HG22	1:F:481:ILE:CD1	2.04	0.83
1:B:501:THR:HB	2:B:660:HOH:O	1.78	0.83
1:E:613:PHE:HB3	2:E:747:HOH:O	1.78	0.83
1:F:605:LYS:HE3	2:F:705:HOH:O	1.76	0.83
1:E:418:LEU:CD2	2:F:810:HOH:O	2.26	0.83
1:C:441:ILE:HG21	1:C:502:TYR:OH	1.79	0.83
1:C:446:ILE:CD1	1:C:497:GLN:HB2	2.08	0.82
1:F:502:TYR:CE1	2:F:709:HOH:O	2.31	0.82
1:B:465:ARG:HG2	2:B:746:HOH:O	1.80	0.82
1:C:476:ASN:HB2	2:C:681:HOH:O	1.79	0.82
1:A:477:VAL:HG22	1:A:519:ILE:HD11	1.59	0.82
1:E:424:TYR:HE2	2:E:668:HOH:O	1.62	0.82
1:E:465:ARG:HD3	2:E:745:HOH:O	1.79	0.82
1:B:609:LEU:O	1:B:612:LYS:HB2	1.80	0.82
2:E:746:HOH:O	1:F:539:VAL:HG21	1.79	0.81
1:C:457:GLU:HA	2:C:715:HOH:O	1.78	0.81
1:C:502:TYR:HD1	2:C:699:HOH:O	1.63	0.81
1:B:437:GLU:HB3	2:B:763:HOH:O	1.81	0.81
1:A:481:ILE:CD1	1:A:485:THR:HG21	2.10	0.81
1:D:435:ILE:HG23	1:D:505:VAL:HG22	1.62	0.81
1:D:469:ILE:HD12	2:D:788:HOH:O	1.81	0.81
1:F:502:TYR:HB3	1:F:505:VAL:HG21	1.64	0.80
1:C:608:ARG:HG2	2:C:713:HOH:O	1.81	0.80
1:A:429:VAL:HG22	1:A:527:VAL:HG11	1.64	0.80
1:A:419:PHE:HB3	1:A:444:PRO:HG3	1.64	0.79
2:A:758:HOH:O	1:B:540:LYS:CE	2.27	0.79
1:B:482:LYS:HD2	2:B:785:HOH:O	1.80	0.79
1:C:502:TYR:CD1	2:C:699:HOH:O	2.36	0.79
1:D:615:GLU:HB3	2:D:811:HOH:O	1.81	0.79
1:C:614:LYS:N	2:C:710:HOH:O	2.14	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:459:ARG:HD2	2:C:814:HOH:O	1.82	0.79
1:E:512:ILE:CD1	1:E:512:ILE:CB	2.61	0.79
1:F:577:ASP:O	1:F:578:ALA:O	2.00	0.79
1:A:540:LYS:HG2	1:A:540:LYS:O	1.82	0.78
1:C:437:GLU:OE2	1:C:437:GLU:N	2.14	0.78
1:A:481:ILE:HD11	1:A:485:THR:HG21	1.63	0.78
1:F:579:GLU:N	2:F:803:HOH:O	2.15	0.78
1:F:597:GLU:HG2	2:F:815:HOH:O	1.84	0.78
1:C:459:ARG:HB3	2:C:814:HOH:O	1.83	0.78
1:D:433:ALA:HA	2:D:808:HOH:O	1.83	0.77
1:F:445:ILE:CG2	2:F:701:HOH:O	2.33	0.77
1:B:482:LYS:CB	2:B:753:HOH:O	2.31	0.77
1:E:435:ILE:HD11	1:E:441:ILE:CG2	2.15	0.77
1:B:548:GLY:HA2	1:B:551:GLN:NE2	2.00	0.77
1:A:446:ILE:HD11	1:B:544:LEU:HD13	1.67	0.77
1:E:609:LEU:O	1:E:612:LYS:HB2	1.85	0.76
1:F:479:ALA:HB3	2:F:805:HOH:O	1.84	0.76
1:F:508:ASP:O	2:F:839:HOH:O	2.03	0.76
1:E:437:GLU:HB2	2:E:736:HOH:O	1.84	0.76
1:F:472:GLU:CA	2:F:697:HOH:O	2.33	0.76
1:D:428:ARG:CG	2:D:818:HOH:O	1.90	0.76
1:E:492:MET:HE1	1:E:522:ILE:HG12	1.68	0.75
1:C:457:GLU:N	2:C:817:HOH:O	2.18	0.75
1:F:578:ALA:C	1:F:580:HIS:H	1.90	0.75
1:C:545:PRO:HG3	1:C:569:ASP:HB2	1.69	0.75
1:E:419:PHE:HD2	2:E:733:HOH:O	1.70	0.75
1:B:480:ILE:HG13	1:B:481:ILE:N	2.00	0.74
1:A:466:LEU:HD22	2:A:781:HOH:O	1.87	0.74
1:E:485:THR:HG22	1:E:487:ARG:H	1.53	0.74
1:A:446:ILE:CD1	1:B:544:LEU:CD1	2.65	0.74
1:E:568:LYS:HE2	2:E:744:HOH:O	1.85	0.74
1:B:482:LYS:CG	2:B:753:HOH:O	2.26	0.74
1:F:441:ILE:HG21	2:F:715:HOH:O	1.86	0.74
1:F:472:GLU:CB	2:F:697:HOH:O	2.34	0.74
1:C:480:ILE:HD13	1:C:537:LEU:HD21	1.68	0.74
1:B:508:ASP:OD2	2:B:769:HOH:O	2.06	0.73
1:B:576:LEU:CD2	1:B:580:HIS:HB3	2.12	0.73
1:A:481:ILE:HD12	1:A:485:THR:HB	1.70	0.73
1:D:429:VAL:HG22	1:D:527:VAL:HG11	1.69	0.73
1:A:475:MET:HE1	1:F:459:ARG:NH2	2.03	0.73
1:C:422:GLU:HG2	2:C:818:HOH:O	1.87	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:579:GLU:OE1	2:D:784:HOH:O	2.07	0.73
1:C:475:MET:HG3	2:C:788:HOH:O	1.87	0.73
1:E:576:LEU:HD22	1:E:580:HIS:HB3	1.71	0.72
1:C:608:ARG:CG	2:C:713:HOH:O	2.35	0.72
1:D:608:ARG:HH11	1:D:608:ARG:CG	2.02	0.72
1:D:489:ILE:HA	1:D:492:MET:CE	2.20	0.72
1:E:497:GLN:HE22	1:F:538:SER:HA	1.53	0.72
1:B:505:VAL:HG23	1:B:505:VAL:O	1.89	0.72
1:C:614:LYS:CA	1:C:615:GLU:C	2.54	0.72
1:F:473:ALA:O	1:F:477:VAL:HG12	1.90	0.72
1:A:608:ARG:HG2	2:A:687:HOH:O	1.89	0.71
1:C:435:ILE:HG22	2:C:813:HOH:O	1.90	0.71
1:E:613:PHE:CB	2:E:747:HOH:O	2.34	0.71
1:C:465:ARG:CG	1:C:503:GLU:OE1	2.38	0.71
1:A:463:THR:CG2	1:B:468:GLU:HG3	2.20	0.71
1:A:478:SER:HB2	2:A:707:HOH:O	1.90	0.71
1:E:492:MET:CE	1:E:522:ILE:HG12	2.21	0.71
1:B:465:ARG:CG	2:B:746:HOH:O	2.35	0.70
1:E:448:GLU:HG3	2:E:732:HOH:O	1.90	0.70
1:B:608:ARG:HG3	2:B:639:HOH:O	1.91	0.70
1:E:489:ILE:O	1:E:492:MET:HG2	1.91	0.70
1:B:482:LYS:CD	2:B:785:HOH:O	2.39	0.69
1:F:435:ILE:HG12	1:F:441:ILE:CG2	2.22	0.69
1:C:594:GLU:CD	2:C:785:HOH:O	2.30	0.69
1:F:502:TYR:HD2	1:F:503:GLU:N	1.89	0.69
1:C:547:GLY:O	1:C:552:LYS:NZ	2.17	0.69
1:B:505:VAL:HG22	2:B:745:HOH:O	1.92	0.69
1:F:549:VAL:O	1:F:553:ILE:HG13	1.93	0.69
1:C:492:MET:HE1	1:C:522:ILE:HD11	1.75	0.69
1:F:435:ILE:CG1	1:F:441:ILE:HG23	2.23	0.69
1:B:553:ILE:HG21	1:B:576:LEU:HD11	1.76	0.69
1:F:485:THR:HG23	1:F:523:GLU:OE2	1.93	0.69
1:B:418:LEU:HA	1:C:545:PRO:HG2	1.74	0.68
1:A:435:ILE:CG2	1:A:505:VAL:HG22	2.22	0.68
1:C:435:ILE:HB	2:C:813:HOH:O	1.93	0.68
1:A:475:MET:HG3	2:A:754:HOH:O	1.91	0.68
1:C:548:GLY:O	1:C:552:LYS:HG3	1.94	0.68
1:A:435:ILE:HG12	1:A:441:ILE:HG23	1.75	0.68
1:A:509:SER:HB3	1:F:497:GLN:OE1	1.93	0.68
1:C:550:THR:CG2	2:C:807:HOH:O	2.24	0.68
1:C:463:THR:CG2	2:C:771:HOH:O	2.31	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:597:GLU:HG2	2:C:769:HOH:O	1.92	0.68
1:D:428:ARG:CZ	2:D:818:HOH:O	2.36	0.68
1:A:492:MET:CE	1:A:522:ILE:HD13	2.24	0.67
1:F:613:PHE:HB3	2:F:802:HOH:O	1.94	0.67
1:C:472:GLU:HB2	2:C:757:HOH:O	1.94	0.67
1:A:481:ILE:HD11	1:A:485:THR:CG2	2.24	0.67
1:E:439:ALA:HB2	2:E:736:HOH:O	1.93	0.67
1:C:434:VAL:HB	2:C:806:HOH:O	1.95	0.67
1:C:435:ILE:CB	2:C:813:HOH:O	2.42	0.67
1:C:550:THR:CA	2:C:807:HOH:O	2.33	0.67
1:F:472:GLU:CG	1:F:473:ALA:N	2.58	0.67
1:A:481:ILE:CD1	1:A:485:THR:CG2	2.73	0.66
1:D:422:GLU:HG2	1:D:423:GLY:H	1.61	0.66
1:A:453:MET:HG2	2:A:711:HOH:O	1.94	0.66
1:E:504:GLY:N	1:E:505:VAL:HG22	2.10	0.66
1:F:474:VAL:CG1	1:F:474:VAL:CA	2.70	0.66
1:E:501:THR:HG23	1:E:501:THR:O	1.95	0.66
1:C:550:THR:CB	2:C:807:HOH:O	2.42	0.66
1:F:502:TYR:CA	2:F:829:HOH:O	2.43	0.66
1:C:522:ILE:HG22	1:C:522:ILE:O	1.96	0.66
1:D:612:LYS:HE2	2:D:812:HOH:O	1.94	0.66
1:F:502:TYR:HE1	2:F:709:HOH:O	1.73	0.66
1:D:484:TYR:HB2	2:D:780:HOH:O	1.94	0.65
1:F:445:ILE:HG22	2:F:701:HOH:O	1.95	0.65
1:A:604:LYS:HD2	2:A:779:HOH:O	1.97	0.65
1:C:452:SER:O	1:C:453:MET:HG2	1.96	0.65
1:D:501:THR:HB	2:E:753:HOH:O	1.96	0.65
1:F:477:VAL:CG2	1:F:477:VAL:O	2.44	0.65
1:C:501:THR:HG21	2:D:678:HOH:O	1.95	0.65
1:A:470:ALA:O	1:A:474:VAL:HG23	1.96	0.65
1:B:489:ILE:O	1:B:489:ILE:CG2	2.38	0.65
1:C:522:ILE:O	1:C:522:ILE:CG2	2.44	0.65
1:B:450:THR:HG21	1:C:483:LYS:HB2	1.79	0.65
1:B:471:ARG:NE	2:B:760:HOH:O	2.29	0.65
1:E:417:LYS:HD2	1:E:419:PHE:O	1.97	0.65
1:B:419:PHE:CA	1:B:428:ARG:NH2	2.60	0.64
1:B:465:ARG:HD2	2:B:673:HOH:O	1.96	0.64
1:C:445:ILE:CG2	2:C:645:HOH:O	2.44	0.64
1:C:497:GLN:HB2	2:C:815:HOH:O	1.96	0.64
1:E:419:PHE:CD2	2:E:733:HOH:O	2.47	0.64
1:F:485:THR:HB	1:F:487:ARG:H	1.61	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:422:GLU:HG3	2:A:752:HOH:O	1.97	0.64
1:E:492:MET:HE1	1:E:522:ILE:CD1	2.28	0.64
1:F:441:ILE:CG2	2:F:715:HOH:O	2.43	0.64
1:A:428:ARG:NH2	2:A:776:HOH:O	2.13	0.64
1:C:479:ALA:CB	1:C:479:ALA:N	2.56	0.64
1:A:438:SER:O	1:A:439:ALA:O	2.15	0.64
1:B:575:LEU:O	1:B:576:LEU:HB2	1.98	0.64
1:D:489:ILE:HA	1:D:492:MET:HE3	1.79	0.64
1:D:422:GLU:HG2	1:D:423:GLY:N	2.12	0.64
1:D:608:ARG:HG2	1:D:608:ARG:NH1	2.05	0.64
1:D:532:ALA:HB2	1:D:561:LEU:HD13	1.79	0.63
1:F:588:PRO:HG2	1:F:588:PRO:O	1.98	0.63
1:E:590:SER:N	1:E:594:GLU:OE1	2.29	0.63
1:F:509:SER:HB3	2:F:717:HOH:O	1.99	0.63
1:A:435:ILE:HG23	1:A:505:VAL:HG22	1.80	0.63
1:A:597:GLU:CD	1:A:597:GLU:CB	2.65	0.63
1:D:539:VAL:CG1	1:D:539:VAL:CA	2.71	0.63
1:C:446:ILE:HD11	2:C:815:HOH:O	1.99	0.63
1:F:578:ALA:C	1:F:580:HIS:N	2.52	0.63
1:F:474:VAL:CG1	1:F:474:VAL:HB	2.15	0.62
1:C:476:ASN:HD22	1:C:476:ASN:C	2.01	0.62
1:A:481:ILE:HD11	1:A:487:ARG:HB2	1.82	0.62
1:C:502:TYR:CD1	2:C:626:HOH:O	2.50	0.62
1:D:435:ILE:CG2	1:D:505:VAL:HG22	2.28	0.62
1:F:472:GLU:HB3	2:F:697:HOH:O	1.96	0.62
2:A:775:HOH:O	1:F:417:LYS:HE2	1.98	0.62
1:C:441:ILE:CG2	1:C:502:TYR:OH	2.47	0.62
1:E:435:ILE:HD11	1:E:441:ILE:HG21	1.81	0.62
1:F:435:ILE:HG23	1:F:505:VAL:HG22	1.81	0.62
1:A:492:MET:HE3	1:A:522:ILE:HD13	1.82	0.61
1:A:503:GLU:HG3	1:B:506:GLU:OE1	2.00	0.61
1:C:497:GLN:CB	2:C:815:HOH:O	2.47	0.61
1:C:615:GLU:HB3	2:C:809:HOH:O	1.98	0.61
1:C:501:THR:HB	2:D:775:HOH:O	1.99	0.61
1:C:445:ILE:CD1	1:C:513:SER:HB2	2.30	0.61
1:C:540:LYS:HD3	2:C:764:HOH:O	2.00	0.61
1:E:564:VAL:HG13	1:E:564:VAL:O	2.01	0.61
1:C:477:VAL:O	1:C:477:VAL:HG22	1.99	0.60
1:F:502:TYR:HB3	1:F:505:VAL:CG2	2.30	0.60
1:B:531:VAL:HG22	1:B:563:LYS:HB2	1.82	0.60
1:F:472:GLU:HG3	1:F:473:ALA:N	2.16	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:438:SER:HA	1:B:551:GLN:HG2	1.84	0.60
1:E:418:LEU:HD12	2:E:677:HOH:O	2.01	0.60
1:E:549:VAL:O	1:E:553:ILE:HG13	2.02	0.60
1:F:598:HIS:HE1	2:F:664:HOH:O	1.82	0.60
1:B:501:THR:HG22	2:C:794:HOH:O	2.01	0.60
1:C:511:SER:HB3	1:C:514:ILE:HD12	1.81	0.60
1:F:488:ASP:HB3	1:F:491:ASN:ND2	2.17	0.60
1:F:502:TYR:CD2	1:F:503:GLU:O	2.55	0.59
1:C:428:ARG:NH2	2:C:714:HOH:O	2.25	0.59
1:C:435:ILE:CG2	2:C:813:HOH:O	2.48	0.59
1:C:476:ASN:C	1:C:476:ASN:ND2	2.54	0.59
1:E:484:TYR:HB3	1:E:613:PHE:HD1	1.68	0.58
1:D:438:SER:O	1:D:551:GLN:HG2	2.02	0.58
1:A:501:THR:HG21	2:B:663:HOH:O	2.04	0.58
1:B:480:ILE:HD12	1:B:484:TYR:HD2	1.67	0.58
1:F:477:VAL:CB	2:F:658:HOH:O	2.39	0.58
1:A:428:ARG:CD	1:A:446:ILE:HG23	2.34	0.58
1:C:445:ILE:CG1	2:C:782:HOH:O	2.50	0.58
1:B:501:THR:CA	2:B:660:HOH:O	2.50	0.58
1:D:608:ARG:HE	1:D:612:LYS:CE	2.01	0.58
1:B:480:ILE:HD12	1:B:484:TYR:CD2	2.38	0.58
1:C:597:GLU:HB3	2:C:769:HOH:O	2.04	0.58
1:F:435:ILE:HG21	1:F:502:TYR:CE1	2.39	0.58
1:C:477:VAL:O	1:C:477:VAL:CG2	2.52	0.58
1:D:428:ARG:HD2	2:D:772:HOH:O	2.04	0.58
1:E:497:GLN:C	2:E:727:HOH:O	2.41	0.58
1:A:428:ARG:HD3	1:A:446:ILE:HG23	1.84	0.57
1:D:478:SER:HB2	1:D:489:ILE:HB	1.85	0.57
1:E:477:VAL:CG2	1:E:515:ALA:HB1	2.34	0.57
1:B:501:THR:CG2	2:C:794:HOH:O	2.51	0.57
1:D:489:ILE:HA	1:D:492:MET:HE2	1.86	0.57
1:E:561:LEU:HA	2:E:759:HOH:O	2.04	0.57
1:B:588:PRO:HG3	2:B:696:HOH:O	2.03	0.57
1:B:576:LEU:HD22	1:B:580:HIS:CB	2.20	0.57
1:C:545:PRO:HG3	1:C:569:ASP:CB	2.35	0.57
1:C:452:SER:O	1:C:453:MET:CG	2.53	0.57
1:C:472:GLU:HG2	2:C:635:HOH:O	2.05	0.57
1:A:477:VAL:CG2	1:A:519:ILE:HD11	2.31	0.56
1:C:433:ALA:HB3	1:C:441:ILE:HD11	1.87	0.56
1:E:470:ALA:O	1:E:474:VAL:HG23	2.05	0.56
1:F:554:GLU:OE1	1:F:580:HIS:CD2	2.58	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:418:LEU:N	1:C:418:LEU:HD12	2.20	0.56
1:C:418:LEU:N	1:C:418:LEU:CD1	2.69	0.56
1:E:492:MET:HE1	1:E:522:ILE:CG1	2.33	0.56
1:A:481:ILE:HD12	1:A:485:THR:CB	2.36	0.56
1:C:476:ASN:HD22	1:C:477:VAL:N	2.04	0.56
1:B:579:GLU:OE1	1:B:579:GLU:HA	2.04	0.56
1:E:497:GLN:HE22	1:F:539:VAL:H	1.52	0.56
1:F:428:ARG:HD2	1:F:446:ILE:HG23	1.88	0.55
1:F:482:LYS:O	1:F:486:GLY:HA2	2.06	0.55
1:C:446:ILE:CD1	2:C:815:HOH:O	2.52	0.55
1:E:470:ALA:HA	1:E:514:ILE:HD13	1.88	0.55
1:B:449:VAL:HG21	1:B:522:ILE:HD13	1.88	0.55
1:B:502:TYR:HB2	1:B:505:VAL:HG12	1.87	0.55
1:B:523:GLU:HG3	1:B:609:LEU:HD22	1.89	0.55
1:C:483:LYS:HG3	1:C:483:LYS:O	2.06	0.55
1:E:549:VAL:HB	2:E:735:HOH:O	2.06	0.55
1:F:502:TYR:N	2:F:829:HOH:O	2.38	0.55
1:A:435:ILE:HG22	1:A:505:VAL:HG22	1.88	0.55
1:B:548:GLY:HA2	1:B:551:GLN:HE21	1.70	0.55
1:C:445:ILE:HD11	1:C:513:SER:HB2	1.88	0.55
1:F:477:VAL:HG22	1:F:477:VAL:O	2.06	0.55
1:C:457:GLU:CA	2:C:715:HOH:O	2.45	0.54
1:C:502:TYR:HE1	2:C:626:HOH:O	1.81	0.54
1:E:484:TYR:CB	1:E:613:PHE:HD1	2.20	0.54
1:A:604:LYS:O	1:A:608:ARG:HB3	2.07	0.54
1:C:614:LYS:CA	2:C:710:HOH:O	2.55	0.54
1:C:597:GLU:CG	2:C:769:HOH:O	2.52	0.54
1:F:485:THR:HG21	1:F:487:ARG:HD2	1.88	0.54
1:C:465:ARG:HG2	1:C:503:GLU:OE1	2.07	0.54
1:C:480:ILE:HD13	1:C:537:LEU:CD2	2.37	0.54
1:F:485:THR:CG2	1:F:487:ARG:HD2	2.38	0.54
1:B:457:GLU:HG2	2:B:689:HOH:O	2.08	0.54
1:A:553:ILE:CG2	1:A:576:LEU:HD21	2.37	0.54
1:F:484:TYR:HB3	1:F:613:PHE:CE2	2.43	0.54
1:C:480:ILE:HD11	1:C:519:ILE:HD11	1.88	0.54
1:E:506:GLU:OE2	1:E:506:GLU:HA	2.08	0.54
1:A:446:ILE:HD11	1:B:544:LEU:CD1	2.34	0.53
1:B:503:GLU:HB2	2:B:783:HOH:O	2.07	0.53
1:B:590:SER:N	1:B:594:GLU:OE1	2.32	0.53
1:F:472:GLU:CG	1:F:473:ALA:H	2.21	0.53
1:A:492:MET:HE1	1:A:522:ILE:HD13	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:482:LYS:HG3	1:B:488:ASP:HA	1.91	0.53
1:D:550:THR:O	1:D:554:GLU:HG3	2.09	0.53
1:E:418:LEU:HG	2:F:671:HOH:O	2.08	0.53
1:C:445:ILE:HG22	2:C:645:HOH:O	2.04	0.53
1:C:615:GLU:CB	2:C:809:HOH:O	2.54	0.53
1:D:477:VAL:CG2	1:D:515:ALA:HB1	2.38	0.53
1:E:497:GLN:NE2	1:F:539:VAL:H	2.06	0.53
1:F:554:GLU:OE1	1:F:580:HIS:HD2	1.92	0.53
1:B:478:SER:HB3	1:B:482:LYS:HE3	1.91	0.53
1:E:613:PHE:O	1:E:614:LYS:O	2.27	0.53
1:F:479:ALA:O	2:F:831:HOH:O	2.19	0.53
2:E:746:HOH:O	1:F:539:VAL:CG1	2.39	0.52
1:C:503:GLU:CB	2:C:754:HOH:O	2.57	0.52
1:F:457:GLU:HG3	1:F:490:SER:O	2.08	0.52
1:B:553:ILE:CG2	1:B:576:LEU:HD11	2.38	0.52
1:D:432:LEU:HD21	1:D:556:ALA:HB2	1.90	0.52
1:E:434:VAL:O	1:E:505:VAL:HA	2.09	0.52
1:F:590:SER:HB2	2:F:781:HOH:O	2.09	0.52
1:A:492:MET:CE	1:A:522:ILE:CD1	2.87	0.52
1:C:424:TYR:HB3	1:C:526:PRO:HB2	1.90	0.52
1:E:448:GLU:CG	2:E:732:HOH:O	2.51	0.52
1:D:483:LYS:HB2	2:D:804:HOH:O	2.08	0.52
1:F:548:GLY:O	1:F:552:LYS:HG3	2.09	0.52
1:C:531:VAL:HG22	1:C:563:LYS:HB2	1.91	0.52
1:E:453:MET:C	2:E:700:HOH:O	2.48	0.52
1:E:484:TYR:HB3	1:E:613:PHE:CD1	2.44	0.52
1:E:539:VAL:HG12	1:E:539:VAL:O	2.10	0.52
1:E:539:VAL:O	1:E:539:VAL:CG1	2.56	0.52
1:A:475:MET:CE	1:F:459:ARG:HH22	2.22	0.52
1:F:502:TYR:HD2	1:F:503:GLU:H	1.54	0.52
1:F:502:TYR:CB	2:F:829:HOH:O	2.57	0.52
1:F:597:GLU:HG2	2:F:795:HOH:O	2.08	0.52
1:C:433:ALA:HB3	1:C:441:ILE:CD1	2.40	0.52
1:C:482:LYS:CG	1:C:483:LYS:N	2.67	0.52
1:D:489:ILE:HG12	1:D:492:MET:CE	2.40	0.52
1:E:461:ILE:CG2	1:F:475:MET:HG2	2.39	0.52
1:E:609:LEU:HA	1:E:612:LYS:HG2	1.93	0.51
1:F:445:ILE:HG21	2:F:701:HOH:O	2.01	0.51
1:C:492:MET:HE1	1:C:522:ILE:CD1	2.39	0.51
1:A:526:PRO:HG2	1:A:601:GLU:OE1	2.10	0.51
1:B:528:ASP:OD1	1:B:530:SER:OG	2.21	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:480:ILE:HD12	1:F:537:LEU:HD21	1.92	0.51
1:C:485:THR:OG1	1:C:486:GLY:N	2.43	0.51
1:C:534:THR:O	1:C:567:PRO:HD3	2.10	0.51
1:B:505:VAL:O	1:B:505:VAL:CG2	2.59	0.51
1:F:588:PRO:O	1:F:588:PRO:CG	2.58	0.51
1:B:578:ALA:C	1:B:580:HIS:H	2.14	0.51
1:E:477:VAL:HG21	1:E:515:ALA:HB1	1.91	0.51
1:F:536:SER:OG	2:F:846:HOH:O	2.05	0.51
1:A:475:MET:O	2:A:707:HOH:O	2.18	0.51
1:A:568:LYS:HE2	2:A:766:HOH:O	2.10	0.51
1:E:470:ALA:HA	1:E:514:ILE:HG21	1.93	0.51
1:A:568:LYS:HG3	2:A:730:HOH:O	2.10	0.50
1:A:608:ARG:HG3	1:A:608:ARG:HH11	1.75	0.50
1:B:437:GLU:HG3	2:B:674:HOH:O	2.11	0.50
1:B:480:ILE:HD11	1:B:613:PHE:CE2	2.45	0.50
1:A:435:ILE:HG23	1:A:441:ILE:HD12	1.94	0.50
1:B:585:GLU:HB3	2:B:653:HOH:O	2.12	0.50
1:A:573:ASP:OD2	1:F:417:LYS:N	2.45	0.50
1:C:428:ARG:CD	2:C:666:HOH:O	2.39	0.50
1:F:435:ILE:HG23	1:F:505:VAL:CG2	2.42	0.50
1:B:453:MET:HG2	1:C:482:LYS:NZ	2.27	0.50
1:B:577:ASP:OD1	1:B:580:HIS:ND1	2.36	0.50
1:C:428:ARG:HH11	1:C:428:ARG:HG3	1.76	0.50
1:D:608:ARG:CG	1:D:608:ARG:NH1	2.66	0.50
1:A:475:MET:CE	1:F:459:ARG:NH2	2.73	0.50
1:A:487:ARG:NH1	1:A:487:ARG:HG2	2.27	0.50
1:B:417:LYS:HB2	1:B:419:PHE:CE1	2.46	0.50
1:C:420:ILE:CD1	2:D:722:HOH:O	2.60	0.50
1:C:502:TYR:CE2	1:C:505:VAL:HG21	2.47	0.50
1:D:419:PHE:CE1	1:D:559:ALA:HB1	2.47	0.50
1:D:471:ARG:NH2	2:D:710:HOH:O	2.45	0.50
1:D:485:THR:OG1	1:D:486:GLY:N	2.41	0.50
1:B:457:GLU:HG3	1:B:490:SER:O	2.12	0.49
1:B:479:ALA:HB2	2:B:770:HOH:O	2.12	0.49
1:D:534:THR:O	1:D:567:PRO:HD3	2.12	0.49
1:D:459:ARG:HB3	2:D:724:HOH:O	2.12	0.49
1:C:417:LYS:N	1:D:573:ASP:OD2	2.45	0.49
1:E:430:ASN:O	1:E:532:ALA:HA	2.13	0.49
1:F:485:THR:HG21	1:F:487:ARG:CD	2.43	0.49
1:A:475:MET:CG	2:A:754:HOH:O	2.56	0.49
1:E:598:HIS:HE1	2:E:720:HOH:O	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:501:THR:O	1:E:501:THR:CG2	2.61	0.49
1:E:562:LYS:N	2:E:759:HOH:O	2.46	0.49
1:F:502:TYR:CE2	1:F:503:GLU:O	2.65	0.49
1:D:477:VAL:HG13	1:D:481:ILE:HD12	1.94	0.49
1:F:470:ALA:O	1:F:474:VAL:HG23	2.12	0.49
1:C:488:ASP:O	1:C:491:ASN:HB2	2.13	0.49
1:A:557:ILE:HG12	1:A:584:ILE:HB	1.95	0.48
1:C:468:GLU:O	1:C:472:GLU:HB3	2.13	0.48
1:D:597:GLU:HG3	1:D:610:MET:HE1	1.95	0.48
1:F:472:GLU:HG2	1:F:473:ALA:H	1.78	0.48
1:B:451:PRO:C	1:B:453:MET:H	2.16	0.48
1:C:586:VAL:HB	2:C:793:HOH:O	2.13	0.48
1:C:469:ILE:HD11	2:C:772:HOH:O	2.12	0.48
1:D:492:MET:HG2	2:D:647:HOH:O	2.13	0.48
1:E:577:ASP:O	1:E:581:GLU:HG2	2.12	0.48
1:F:417:LYS:HB3	2:F:780:HOH:O	2.12	0.48
1:B:548:GLY:O	1:B:552:LYS:HG3	2.14	0.48
2:B:774:HOH:O	1:C:545:PRO:HG2	2.12	0.48
1:F:576:LEU:N	2:F:719:HOH:O	2.36	0.48
1:D:548:GLY:HA2	1:D:551:GLN:HE22	1.78	0.48
1:B:450:THR:HG21	1:C:483:LYS:CB	2.43	0.48
1:C:608:ARG:HB3	2:C:713:HOH:O	2.01	0.48
1:E:453:MET:HE2	2:E:687:HOH:O	2.14	0.48
1:B:420:ILE:HD12	1:B:425:GLU:OE2	2.13	0.48
1:C:503:GLU:HB3	2:C:754:HOH:O	2.12	0.48
1:E:418:LEU:HD23	1:F:545:PRO:HG2	1.95	0.48
1:E:600:LEU:HB2	1:E:606:LYS:HE3	1.95	0.48
1:E:546:VAL:HG23	2:E:735:HOH:O	2.14	0.47
1:D:483:LYS:NZ	2:D:766:HOH:O	2.47	0.47
1:B:591:ARG:O	1:B:594:GLU:HB2	2.14	0.47
1:E:496:ILE:O	2:E:626:HOH:O	2.20	0.47
1:E:523:GLU:OE2	1:E:609:LEU:HD13	2.14	0.47
1:E:606:LYS:O	1:E:610:MET:HG2	2.15	0.47
1:B:418:LEU:HB3	2:B:771:HOH:O	2.15	0.47
1:B:429:VAL:HG22	1:B:527:VAL:HG11	1.97	0.47
1:B:612:LYS:O	1:B:615:GLU:HG3	2.13	0.47
2:B:773:HOH:O	1:C:482:LYS:HE2	2.13	0.47
1:F:571:ILE:HD13	1:F:571:ILE:HA	1.64	0.47
1:A:481:ILE:HD12	1:A:485:THR:CG2	2.45	0.47
1:B:545:PRO:HA	1:B:567:PRO:HG2	1.96	0.47
1:F:484:TYR:HB3	1:F:613:PHE:CZ	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:502:TYR:HB2	1:B:505:VAL:CG1	2.45	0.47
2:E:746:HOH:O	1:F:539:VAL:CG2	2.49	0.47
1:D:508:ASP:HB2	2:D:753:HOH:O	2.15	0.47
1:A:568:LYS:O	1:A:571:ILE:HD12	2.15	0.47
1:A:475:MET:HE1	1:F:459:ARG:HH22	1.76	0.46
1:A:475:MET:HE2	1:A:475:MET:HB2	1.84	0.46
1:A:470:ALA:HA	1:A:514:ILE:HD13	1.96	0.46
1:F:472:GLU:N	2:F:697:HOH:O	2.46	0.46
1:D:418:LEU:HD23	1:E:545:PRO:HB2	1.96	0.46
1:E:449:VAL:HA	1:E:493:ASP:O	2.16	0.46
1:B:481:ILE:HG21	1:B:481:ILE:HD13	1.46	0.46
1:D:443:LEU:HD23	2:D:679:HOH:O	2.15	0.46
1:F:467:GLN:OE1	1:F:471:ARG:NH2	2.38	0.46
1:C:532:ALA:HB2	1:C:561:LEU:HD13	1.97	0.46
1:F:550:THR:O	1:F:554:GLU:HB2	2.15	0.46
1:C:460:VAL:HG11	1:C:471:ARG:HA	1.97	0.46
1:D:457:GLU:HG3	1:D:490:SER:HB3	1.96	0.46
1:D:612:LYS:CE	2:D:812:HOH:O	2.59	0.46
1:E:613:PHE:HB2	2:E:747:HOH:O	2.09	0.46
1:B:537:LEU:HG	1:B:538:SER:O	2.16	0.46
1:F:566:ILE:O	1:F:588:PRO:HA	2.16	0.46
1:A:446:ILE:HD13	1:B:544:LEU:HD13	1.93	0.46
1:A:604:LYS:CD	2:A:779:HOH:O	2.60	0.46
1:E:480:ILE:HG23	1:E:484:TYR:HD2	1.79	0.46
1:A:608:ARG:HG3	1:A:608:ARG:NH1	2.31	0.45
1:B:470:ALA:O	1:B:474:VAL:HG23	2.16	0.45
1:D:593:ASN:O	1:D:597:GLU:HG3	2.16	0.45
1:D:593:ASN:O	1:D:610:MET:HE1	2.15	0.45
1:F:478:SER:HA	1:F:481:ILE:HB	1.97	0.45
1:D:435:ILE:O	1:D:436:GLY:C	2.53	0.45
1:E:591:ARG:O	1:E:594:GLU:HB2	2.17	0.45
1:A:466:LEU:O	1:A:469:ILE:HB	2.16	0.45
1:B:588:PRO:CG	2:B:696:HOH:O	2.63	0.45
1:B:418:LEU:CD1	2:C:800:HOH:O	2.30	0.45
1:C:467:GLN:HB2	1:C:471:ARG:NH2	2.30	0.45
1:D:558:GLN:NE2	2:D:795:HOH:O	2.48	0.45
1:B:417:LYS:HE3	2:B:779:HOH:O	2.16	0.45
1:B:554:GLU:O	1:B:558:GLN:HB2	2.16	0.45
1:B:599:VAL:HG23	1:B:600:LEU:HD23	1.97	0.45
1:F:472:GLU:CG	2:F:665:HOH:O	2.38	0.45
1:F:577:ASP:C	1:F:578:ALA:O	2.55	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:485:THR:HG22	1:A:487:ARG:H	1.82	0.45
1:B:451:PRO:O	1:B:453:MET:N	2.47	0.45
1:B:500:GLY:HA2	2:B:659:HOH:O	2.17	0.45
1:B:548:GLY:HA2	1:B:551:GLN:HE22	1.76	0.45
1:C:419:PHE:CE1	1:C:559:ALA:HB1	2.51	0.45
1:E:568:LYS:CE	2:E:744:HOH:O	2.54	0.45
1:B:453:MET:CE	2:C:819:HOH:O	2.65	0.45
1:C:475:MET:CE	2:C:705:HOH:O	2.64	0.45
2:C:779:HOH:O	1:D:475:MET:CG	2.64	0.45
1:F:489:ILE:HD12	1:F:489:ILE:HA	1.48	0.45
1:C:501:THR:HG22	2:D:652:HOH:O	2.17	0.44
1:E:497:GLN:CG	2:E:727:HOH:O	2.18	0.44
1:B:463:THR:HG21	1:C:472:GLU:CG	2.47	0.44
1:B:478:SER:HB3	1:B:482:LYS:CE	2.47	0.44
1:D:548:GLY:HA2	1:D:551:GLN:NE2	2.32	0.44
1:D:553:ILE:HG12	1:D:564:VAL:HG11	1.98	0.44
1:D:419:PHE:HB3	1:D:444:PRO:HG3	1.99	0.44
1:E:480:ILE:HG23	1:E:484:TYR:CD2	2.52	0.44
1:E:484:TYR:CB	1:E:613:PHE:CD1	3.01	0.44
1:E:480:ILE:CD1	1:E:537:LEU:HD21	2.47	0.44
1:F:597:GLU:CG	2:F:815:HOH:O	2.54	0.44
1:A:492:MET:HE3	1:A:522:ILE:CD1	2.44	0.44
1:A:568:LYS:HE3	1:A:568:LYS:HB3	1.77	0.44
1:B:418:LEU:HD13	1:C:545:PRO:HD2	1.99	0.44
1:B:420:ILE:HD12	2:B:701:HOH:O	2.17	0.44
1:C:553:ILE:HG23	1:C:564:VAL:HG11	2.00	0.44
1:E:461:ILE:HG22	1:F:475:MET:HG2	1.99	0.44
1:F:477:VAL:CG2	1:F:481:ILE:CD1	2.82	0.44
1:C:597:GLU:CB	2:C:769:HOH:O	2.62	0.44
1:E:481:ILE:HD13	1:E:481:ILE:HG21	1.68	0.44
1:B:452:SER:OG	1:B:491:ASN:O	2.32	0.44
1:D:465:ARG:NE	1:D:503:GLU:HB2	2.19	0.44
1:F:597:GLU:HB3	2:F:815:HOH:O	2.17	0.44
1:C:420:ILE:HD12	1:C:420:ILE:HG23	1.61	0.44
1:A:487:ARG:HG2	1:A:487:ARG:HH11	1.82	0.44
1:C:556:ALA:HA	1:C:561:LEU:HD12	1.99	0.44
1:A:433:ALA:HB2	2:A:756:HOH:O	2.17	0.43
1:D:465:ARG:HE	1:D:503:GLU:CB	2.20	0.43
1:E:475:MET:SD	2:E:697:HOH:O	2.62	0.43
1:D:489:ILE:HG12	1:D:492:MET:HE3	1.98	0.43
1:E:418:LEU:HA	1:F:545:PRO:HG2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:553:ILE:HG21	1:A:576:LEU:HD21	2.00	0.43
1:B:430:ASN:O	1:B:532:ALA:HA	2.18	0.43
1:A:430:ASN:ND2	1:A:529:GLN:O	2.51	0.43
1:A:550:THR:O	1:A:554:GLU:HG3	2.19	0.43
1:C:446:ILE:CG1	2:C:815:HOH:O	2.66	0.43
1:C:571:ILE:HD11	1:C:588:PRO:HG3	2.01	0.43
1:A:465:ARG:HD3	1:A:503:GLU:HG2	1.99	0.43
1:B:579:GLU:HB2	2:B:647:HOH:O	2.18	0.43
1:C:502:TYR:CD2	1:C:505:VAL:CG2	2.96	0.43
1:D:441:ILE:HG21	1:D:441:ILE:HD13	1.66	0.43
1:D:470:ALA:O	1:D:474:VAL:HG23	2.18	0.43
1:E:421:THR:HG23	1:E:561:LEU:HD23	2.01	0.43
1:E:540:LYS:HB2	1:E:540:LYS:HE2	1.86	0.43
1:B:449:VAL:HG21	1:B:522:ILE:CD1	2.47	0.43
1:B:568:LYS:O	1:B:571:ILE:HB	2.19	0.43
1:E:526:PRO:HG2	2:E:730:HOH:O	2.18	0.43
1:F:446:ILE:HD12	1:F:497:GLN:H	1.83	0.43
1:F:479:ALA:HB3	2:F:628:HOH:O	2.17	0.43
1:B:417:LYS:HD2	1:B:419:PHE:CE1	2.53	0.43
1:C:457:GLU:OE2	1:C:490:SER:HB2	2.19	0.43
1:E:444:PRO:HG2	1:E:499:VAL:HB	2.01	0.43
1:E:532:ALA:HB2	1:E:561:LEU:HD12	2.00	0.43
1:A:421:THR:HG22	1:A:561:LEU:CD2	2.49	0.43
1:B:450:THR:HG22	1:C:483:LYS:NZ	2.33	0.43
1:B:487:ARG:NH2	2:B:709:HOH:O	2.50	0.43
1:D:446:ILE:HB	2:D:818:HOH:O	2.18	0.43
1:E:419:PHE:HA	1:E:428:ARG:HH22	1.83	0.43
1:E:581:GLU:OE2	1:E:581:GLU:HA	2.18	0.43
1:C:501:THR:CG2	2:D:678:HOH:O	2.59	0.43
2:A:626:HOH:O	1:F:501:THR:HG22	2.17	0.42
1:D:532:ALA:HB2	1:D:561:LEU:CD1	2.49	0.42
1:D:583:LYS:HE2	2:D:717:HOH:O	2.18	0.42
1:E:452:SER:HA	2:E:754:HOH:O	2.19	0.42
1:E:495:HIS:HB3	1:F:539:VAL:HG11	2.01	0.42
1:A:446:ILE:HD12	1:B:544:LEU:HD11	2.02	0.42
1:A:457:GLU:HG2	1:A:458:GLY:H	1.84	0.42
1:C:497:GLN:C	2:C:815:HOH:O	2.57	0.42
1:C:568:LYS:HA	1:C:588:PRO:HB2	2.00	0.42
1:C:577:ASP:O	1:C:581:GLU:HG3	2.18	0.42
1:E:480:ILE:HD13	1:E:537:LEU:HD21	2.02	0.42
1:F:549:VAL:HG11	1:F:573:ASP:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:485:THR:HG22	1:B:612:LYS:HB3	2.01	0.42
1:B:531:VAL:HG11	1:B:599:VAL:HG12	2.00	0.42
1:C:435:ILE:HG23	1:C:505:VAL:HG22	2.02	0.42
1:C:437:GLU:N	1:C:437:GLU:CD	2.73	0.42
1:C:480:ILE:HG12	1:C:481:ILE:N	2.34	0.42
1:F:477:VAL:HB	1:F:537:LEU:HD23	2.01	0.42
1:F:568:LYS:HA	1:F:588:PRO:HB2	2.01	0.42
1:F:502:TYR:CD2	1:F:503:GLU:N	2.79	0.42
1:A:468:GLU:CD	1:F:467:GLN:HE22	2.21	0.42
1:F:483:LYS:HB2	2:F:804:HOH:O	2.20	0.42
1:B:614:LYS:N	2:B:698:HOH:O	2.52	0.42
1:E:604:LYS:HD3	2:E:645:HOH:O	2.20	0.42
1:F:474:VAL:CG1	1:F:474:VAL:C	2.88	0.42
1:B:518:VAL:O	1:B:522:ILE:HG12	2.20	0.42
1:C:446:ILE:HG13	2:C:815:HOH:O	2.20	0.42
1:D:525:ILE:HA	1:D:526:PRO:HD3	1.76	0.42
1:E:417:LYS:HE2	2:E:738:HOH:O	2.18	0.42
1:A:545:PRO:HB2	1:F:418:LEU:HD12	2.01	0.42
1:A:573:ASP:C	1:A:575:LEU:HD22	2.40	0.42
1:B:533:MET:HA	1:B:565:ILE:O	2.20	0.42
1:B:576:LEU:HA	1:B:576:LEU:HD23	1.56	0.42
1:E:576:LEU:CD2	1:E:580:HIS:HB3	2.45	0.42
1:A:421:THR:HG22	1:A:561:LEU:HD23	2.02	0.42
1:A:553:ILE:HG22	1:A:576:LEU:HD21	2.00	0.42
1:B:418:LEU:HD22	1:C:545:PRO:O	2.20	0.42
1:C:580:HIS:HA	1:C:583:LYS:HD2	2.01	0.42
1:E:472:GLU:O	1:E:473:ALA:C	2.58	0.42
1:B:487:ARG:NH1	2:B:762:HOH:O	2.50	0.41
1:C:612:LYS:HZ3	1:C:612:LYS:HG3	1.49	0.41
1:E:562:LYS:HD2	1:E:562:LYS:HA	1.73	0.41
1:F:510:ALA:O	1:F:537:LEU:N	2.51	0.41
1:B:418:LEU:CD2	1:C:545:PRO:O	2.68	0.41
1:B:452:SER:O	1:B:453:MET:HB2	2.21	0.41
1:E:503:GLU:C	1:E:505:VAL:HG22	2.40	0.41
1:E:605:LYS:HG3	2:E:696:HOH:O	2.19	0.41
1:D:434:VAL:O	1:D:434:VAL:HG23	2.19	0.41
1:E:525:ILE:HA	1:E:526:PRO:HD3	1.88	0.41
1:D:572:ASP:HB3	2:D:696:HOH:O	2.20	0.41
1:E:579:GLU:O	1:E:580:HIS:ND1	2.53	0.41
1:A:441:ILE:HD13	1:A:441:ILE:H	1.86	0.41
1:E:430:ASN:ND2	1:E:529:GLN:O	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:457:GLU:HB3	1:E:458:GLY:H	1.77	0.41
1:D:597:GLU:CG	1:D:610:MET:HE1	2.51	0.41
1:F:428:ARG:HH11	1:F:428:ARG:HD3	1.73	0.41
1:A:446:ILE:HD12	1:B:544:LEU:CD1	2.48	0.41
1:B:536:SER:HB2	1:B:544:LEU:HB2	2.02	0.41
1:B:614:LYS:O	1:B:615:GLU:HB2	2.21	0.41
1:C:544:LEU:HB3	1:C:545:PRO:HD2	2.02	0.41
1:F:437:GLU:N	1:F:437:GLU:OE2	2.53	0.41
1:F:472:GLU:O	1:F:473:ALA:C	2.59	0.41
1:A:453:MET:HB3	2:A:718:HOH:O	2.19	0.41
1:B:566:ILE:O	1:B:589:VAL:HG22	2.21	0.41
1:B:612:LYS:O	1:B:615:GLU:CG	2.68	0.41
1:B:614:LYS:HA	2:B:698:HOH:O	2.21	0.41
1:C:570:ASN:HA	1:C:573:ASP:OD2	2.21	0.41
1:D:435:ILE:HG23	1:D:505:VAL:CG2	2.44	0.41
1:E:492:MET:CE	1:E:522:ILE:CD1	2.99	0.41
1:E:564:VAL:O	1:E:564:VAL:CG1	2.69	0.41
1:E:589:VAL:O	1:E:589:VAL:HG23	2.21	0.41
1:F:433:ALA:O	1:F:440:GLY:HA2	2.21	0.41
1:F:460:VAL:HG21	2:F:706:HOH:O	2.21	0.41
1:F:490:SER:HB2	2:F:773:HOH:O	2.20	0.41
1:F:509:SER:CB	2:F:796:HOH:O	2.69	0.41
1:B:449:VAL:HA	1:B:493:ASP:O	2.21	0.41
1:B:600:LEU:HB2	1:B:606:LYS:HE3	2.02	0.41
1:C:443:LEU:HD12	1:C:443:LEU:HA	1.87	0.41
1:E:514:ILE:HD13	1:E:514:ILE:HG21	1.68	0.41
1:A:532:ALA:HB2	1:A:561:LEU:HD13	2.03	0.40
1:B:437:GLU:CB	2:B:763:HOH:O	2.56	0.40
1:B:614:LYS:CA	2:B:698:HOH:O	2.69	0.40
1:D:428:ARG:NE	2:D:772:HOH:O	2.53	0.40
1:D:534:THR:OG1	1:D:546:VAL:HG21	2.21	0.40
1:E:417:LYS:HG2	2:E:659:HOH:O	2.21	0.40
1:F:452:SER:HB3	1:F:458:GLY:HA2	2.03	0.40
1:A:417:LYS:N	1:B:569:ASP:O	2.54	0.40
1:A:475:MET:HE1	1:F:459:ARG:HH21	1.83	0.40
1:A:492:MET:HE1	1:A:522:ILE:HG23	2.02	0.40
1:A:569:ASP:O	1:F:417:LYS:N	2.55	0.40
1:B:463:THR:HG21	1:C:472:GLU:HG3	2.03	0.40
1:C:445:ILE:HD12	1:C:513:SER:HB2	2.03	0.40
1:C:473:ALA:HB2	2:C:716:HOH:O	2.21	0.40
1:D:481:ILE:HD13	1:D:522:ILE:HD12	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:469:ILE:HD13	1:E:469:ILE:HG21	1.80	0.40
1:F:502:TYR:CB	1:F:505:VAL:HG21	2.41	0.40
1:F:565:ILE:HA	1:F:587:ILE:O	2.20	0.40
1:A:587:ILE:HD13	1:A:587:ILE:HG21	1.41	0.40
1:B:576:LEU:CD2	1:B:580:HIS:CB	2.93	0.40
1:C:481:ILE:HD13	1:C:481:ILE:HG21	1.90	0.40
1:C:571:ILE:HD13	1:C:571:ILE:HG21	1.77	0.40
1:F:509:SER:HB3	2:F:796:HOH:O	2.20	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:625:HOH:O	2:D:802:HOH:O[4_465]	1.89	0.31
2:C:803:HOH:O	2:D:716:HOH:O[4_465]	2.10	0.10

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	191/205 (93%)	176 (92%)	10 (5%)	5 (3%)	5	3
1	B	192/205 (94%)	166 (86%)	15 (8%)	11 (6%)	1	0
1	C	192/205 (94%)	181 (94%)	8 (4%)	3 (2%)	9	8
1	D	192/205 (94%)	177 (92%)	14 (7%)	1 (0%)	29	34
1	E	191/205 (93%)	167 (87%)	16 (8%)	8 (4%)	3	1
1	F	192/205 (94%)	175 (91%)	14 (7%)	3 (2%)	9	8
All	All	1150/1230 (94%)	1042 (91%)	77 (7%)	31 (3%)	5	3

All (31) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	438	SER
1	A	439	ALA
1	B	438	SER
1	B	505	VAL
1	B	577	ASP
1	B	614	LYS
1	D	614	LYS
1	E	439	ALA
1	E	484	TYR
1	F	578	ALA
1	F	579	GLU
1	B	440	GLY
1	B	612	LYS
1	E	418	LEU
1	E	419	PHE
1	E	421	THR
1	E	505	VAL
1	E	580	HIS
1	A	613	PHE
1	C	479	ALA
1	E	437	GLU
1	F	469	ILE
1	B	452	SER
1	B	482	LYS
1	B	576	LEU
1	C	482	LYS
1	C	483	LYS
1	A	595	VAL
1	A	486	GLY
1	B	436	GLY
1	B	489	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	A	160/168 (95%)	136 (85%)	24 (15%)	3 2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	161/168 (96%)	134 (83%)	27 (17%)	2	1
1	C	161/168 (96%)	132 (82%)	29 (18%)	1	1
1	D	161/168 (96%)	145 (90%)	16 (10%)	8	8
1	E	160/168 (95%)	133 (83%)	27 (17%)	2	1
1	F	161/168 (96%)	133 (83%)	28 (17%)	2	1
All	All	964/1008 (96%)	813 (84%)	151 (16%)	2	2

All (151) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	418	LEU
1	A	422	GLU
1	A	435	ILE
1	A	441	ILE
1	A	446	ILE
1	A	453	MET
1	A	465	ARG
1	A	477	VAL
1	A	480	ILE
1	A	481	ILE
1	A	489	ILE
1	A	491	ASN
1	A	501	THR
1	A	503	GLU
1	A	506	GLU
1	A	509	SER
1	A	511	SER
1	A	542	GLU
1	A	551	GLN
1	A	572	ASP
1	A	577	ASP
1	A	597	GLU
1	A	604	LYS
1	A	608	ARG
1	B	417	LYS
1	B	418	LEU
1	B	419	PHE
1	B	420	ILE
1	B	421	THR
1	B	422	GLU

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Mol	Chain	Res	Type
1	B	443	LEU
1	B	452	SER
1	B	457	GLU
1	B	459	ARG
1	B	463	THR
1	B	465	ARG
1	B	466	LEU
1	B	475	MET
1	B	480	ILE
1	B	482	LYS
1	B	487	ARG
1	B	491	ASN
1	B	502	TYR
1	B	539	VAL
1	B	540	LYS
1	B	558	GLN
1	B	571	ILE
1	B	579	GLU
1	B	583	LYS
1	B	604	LYS
1	B	611	SER
1	C	417	LYS
1	C	422	GLU
1	C	428	ARG
1	C	435	ILE
1	C	437	GLU
1	C	441	ILE
1	C	446	ILE
1	C	463	THR
1	C	465	ARG
1	C	472	GLU
1	C	476	ASN
1	C	480	ILE
1	C	482	LYS
1	C	483	LYS
1	C	485	THR
1	C	487	ARG
1	C	501	THR
1	C	502	TYR
1	C	508	ASP
1	C	509	SER
1	C	538	SER

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Mol	Chain	Res	Type
1	C	542	GLU
1	C	549	VAL
1	C	588	PRO
1	C	590	SER
1	C	597	GLU
1	C	604	LYS
1	C	608	ARG
1	C	615	GLU
1	D	420	ILE
1	D	435	ILE
1	D	441	ILE
1	D	457	GLU
1	D	465	ARG
1	D	469	ILE
1	D	477	VAL
1	D	480	ILE
1	D	483	LYS
1	D	485	THR
1	D	489	ILE
1	D	511	SER
1	D	542	GLU
1	D	551	GLN
1	D	568	LYS
1	D	608	ARG
1	E	417	LYS
1	E	418	LEU
1	E	420	ILE
1	E	422	GLU
1	E	425	GLU
1	E	434	VAL
1	E	443	LEU
1	E	450	THR
1	E	453	MET
1	E	459	ARG
1	E	465	ARG
1	E	475	MET
1	E	477	VAL
1	E	482	LYS
1	E	488	ASP
1	E	490	SER
1	E	492	MET
1	E	501	THR

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Mol	Chain	Res	Type
1	E	505	VAL
1	E	540	LYS
1	E	546	VAL
1	E	558	GLN
1	E	562	LYS
1	E	566	ILE
1	E	597	GLU
1	E	605	LYS
1	E	611	SER
1	F	418	LEU
1	F	435	ILE
1	F	437	GLU
1	F	438	SER
1	F	446	ILE
1	F	452	SER
1	F	453	MET
1	F	459	ARG
1	F	465	ARG
1	F	477	VAL
1	F	481	ILE
1	F	485	THR
1	F	487	ARG
1	F	489	ILE
1	F	492	MET
1	F	501	THR
1	F	502	TYR
1	F	508	ASP
1	F	536	SER
1	F	538	SER
1	F	554	GLU
1	F	571	ILE
1	F	572	ASP
1	F	579	GLU
1	F	588	PRO
1	F	591	ARG
1	F	608	ARG
1	F	614	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	551	GLN

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Mol	Chain	Res	Type
1	A	580	HIS
1	B	491	ASN
1	B	551	GLN
1	B	558	GLN
1	C	476	ASN
1	D	558	GLN
1	D	580	HIS
1	E	497	GLN
1	E	598	HIS
1	F	476	ASN
1	F	580	HIS
1	F	598	HIS

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 monosaccharides 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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	195/205 (95%)	-0.29	3 (1%) 73 78	2, 7, 27, 38	0
1	B	196/205 (95%)	0.41	19 (9%) 7 10	3, 13, 35, 54	0
1	C	196/205 (95%)	-0.18	6 (3%) 49 54	2, 6, 27, 41	0
1	D	196/205 (95%)	-0.26	3 (1%) 73 78	2, 7, 25, 40	0
1	E	195/205 (95%)	0.37	26 (13%) 3 4	3, 14, 34, 49	0
1	F	196/205 (95%)	-0.21	7 (3%) 42 48	2, 7, 30, 52	0
All	All	1174/1230 (95%)	-0.03	64 (5%) 25 30	2, 10, 32, 54	0

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	418	LEU	7.6
1	B	578	ALA	6.2
1	B	453	MET	5.8
1	E	418	LEU	5.3
1	E	453	MET	5.2
1	F	453	MET	5.1
1	A	453	MET	5.0
1	C	453	MET	4.7
1	B	502	TYR	4.6
1	B	419	PHE	4.6
1	E	501	THR	4.4
1	B	417	LYS	4.3
1	B	501	THR	4.3
1	E	578	ALA	4.2
1	B	420	ILE	4.1
1	B	437	GLU	4.1
1	E	579	GLU	4.0
1	D	437	GLU	4.0
1	B	615	GLU	3.9

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Mol	Chain	Res	Type	RSRZ
1	B	579	GLU	3.8
1	F	484	TYR	3.6
1	B	421	THR	3.5
1	E	421	THR	3.4
1	E	502	TYR	3.4
1	B	438	SER	3.4
1	E	437	GLU	3.4
1	B	439	ALA	3.3
1	E	575	LEU	3.3
1	D	453	MET	3.2
1	F	615	GLU	3.0
1	E	582	GLY	3.0
1	B	457	GLU	2.9
1	E	435	ILE	2.8
1	F	438	SER	2.7
1	B	422	GLU	2.7
1	D	438	SER	2.6
1	E	583	LYS	2.6
1	E	604	LYS	2.6
1	F	487	ARG	2.6
1	E	420	ILE	2.5
1	E	457	GLU	2.5
1	E	483	LYS	2.5
1	C	578	ALA	2.5
1	A	438	SER	2.5
1	E	608	ARG	2.4
1	E	419	PHE	2.4
1	E	491	ASN	2.4
1	B	581	GLU	2.4
1	C	457	GLU	2.4
1	B	608	ARG	2.3
1	E	576	LEU	2.3
1	E	438	SER	2.3
1	A	457	GLU	2.3
1	E	580	HIS	2.3
1	E	581	GLU	2.3
1	F	579	GLU	2.2
1	B	580	HIS	2.1
1	C	614	LYS	2.1
1	E	558	GLN	2.1
1	E	484	TYR	2.1
1	F	502	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	615	GLU	2.1
1	C	608	ARG	2.0
1	E	572	ASP	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.