Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2020 – 04:19 am BST

PDB ID	:	1Z0V
Title	:	Crystal Structure of A. fulgidus Lon proteolytic domain
Authors	:	Dauter, Z.; Botos, I.; LaRonde-LeBlanc, N.; Wlodawer, A.
Deposited on	:	2005-03-02
Resolution	:	3.00 Å(reported)

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

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

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

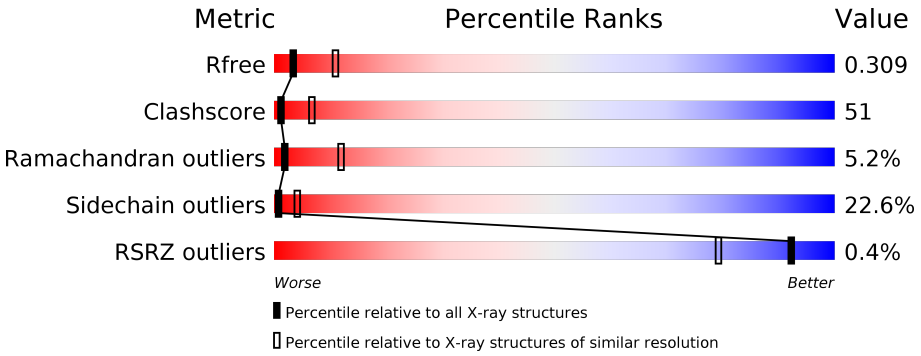
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 3.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	28% 42% 20% • 5%
1	B	205	2% 19% 44% 27% 5% 5%
1	C	205	42% 35% 14% • 5%
1	D	205	38% 37% 15% 6% 5%
1	E	205	30% 46% 14% 5% 5%
1	F	205	28% 48% 13% 5% 5%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9236 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	195	Total	C	N	O	S	0	0	0
			1457	921	247	284	5			
1	C	194	Total	C	N	O	S	0	0	0
			1448	915	245	283	5			
1	D	195	Total	C	N	O	S	0	0	0
			1457	921	247	284	5			
1	E	195	Total	C	N	O	S	0	0	0
			1457	921	247	284	5			
1	F	195	Total	C	N	O	S	0	0	0
			1457	921	247	284	5			

- Molecule 2 is water.

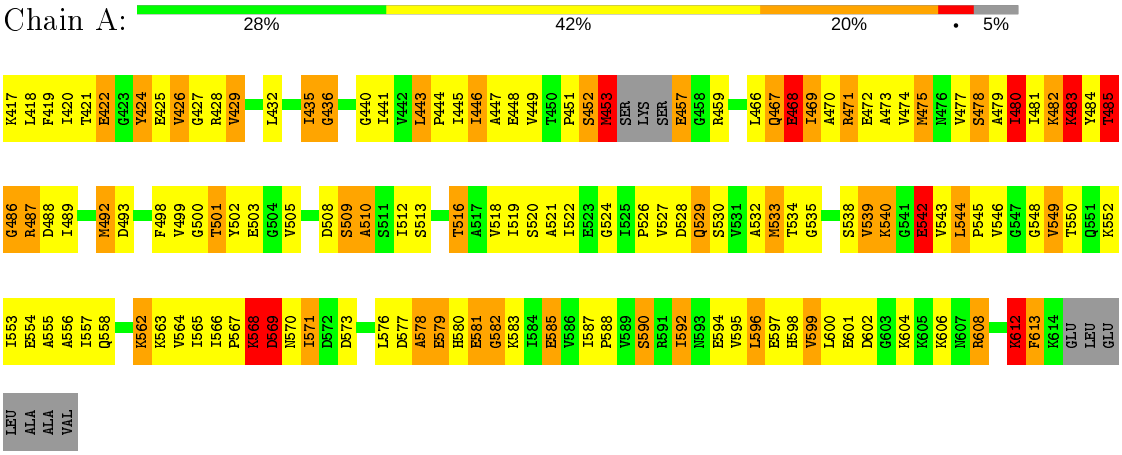
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	78	Total	O	0	0
			78	78		
2	B	74	Total	O	0	0
			74	74		
2	C	104	Total	O	0	0
			104	104		
2	D	99	Total	O	0	0
			99	99		
2	E	69	Total	O	0	0
			69	69		
2	F	79	Total	O	0	0
			79	79		

3 Residue-property plots (i)

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

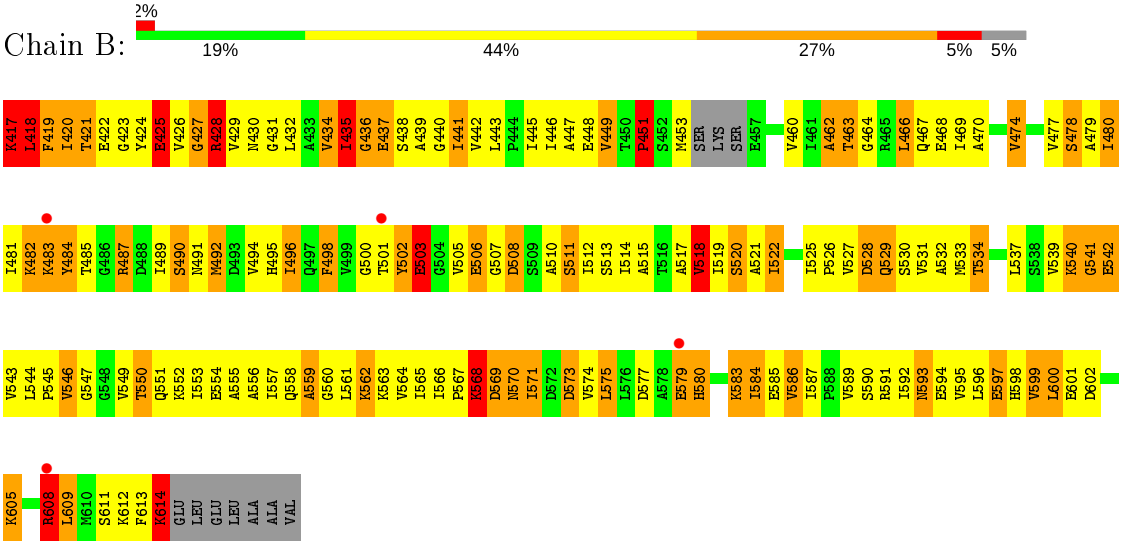
- Molecule 1: Putative protease La homolog type

Chain A:



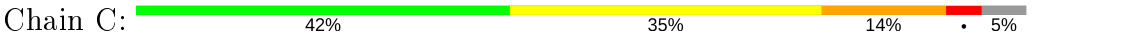
- Molecule 1: Putative protease La homolog type

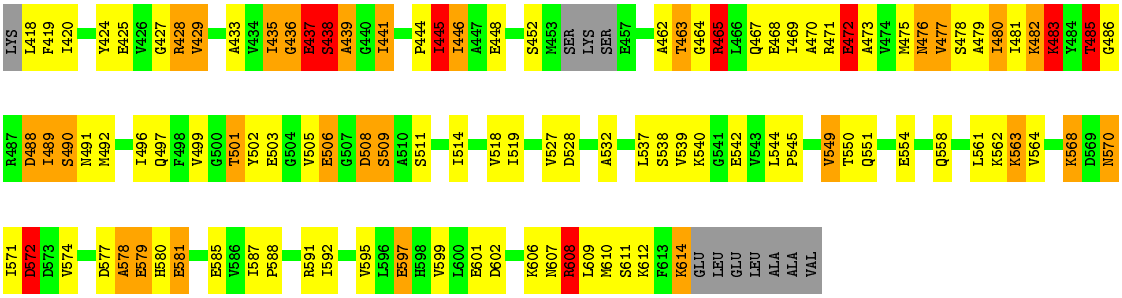
Chain B:



- Molecule 1: Putative protease La homolog type

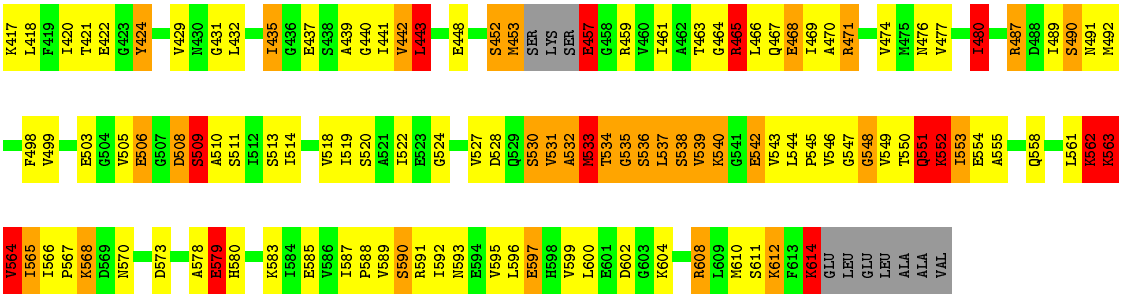
Chain C:





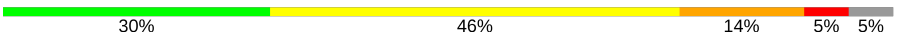
• Molecule 1: Putative protease La homolog type

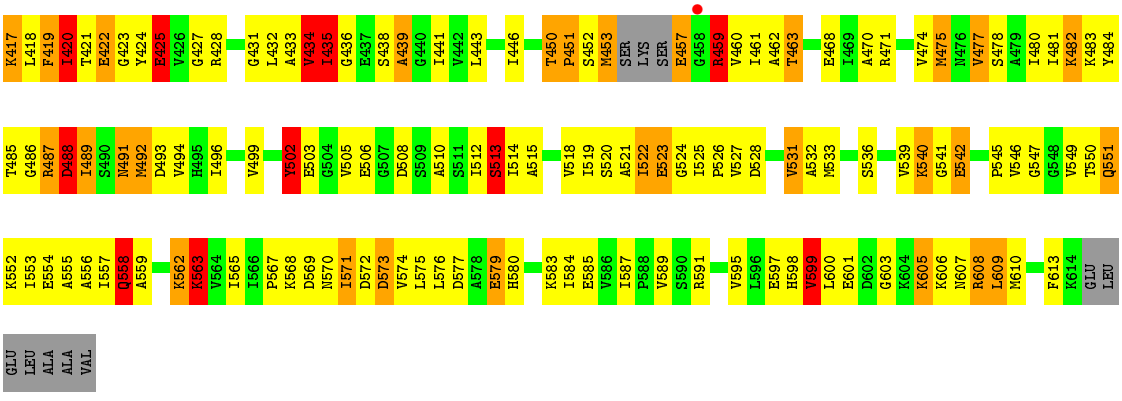
Chain D:



• Molecule 1: Putative protease La homolog type

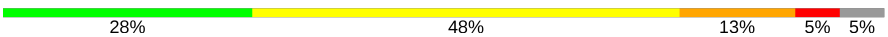
Chain E:

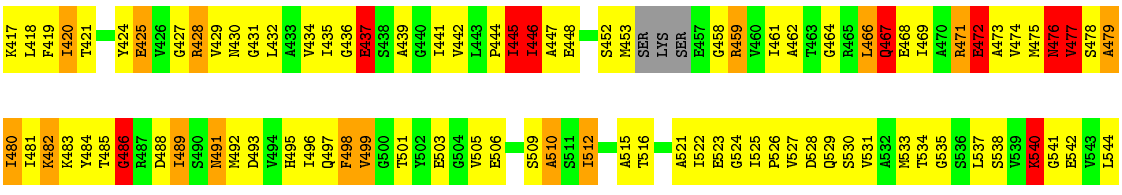




• Molecule 1: Putative protease La homolog type

Chain F:






P545
V546
G547
G548
V549
T550
Q551
K552
I553
E554
A555
A556
I557
Q558
L561
K562
K563
V564
I565
I566
P567
K568
D569
N570
I571
D572
L575
L576
D577
A578
E579
H580
E581
V586
I587
P588
V589
S590
R591
I592
N593
E594
V595
L596
E597
H598
V599
K604
K605
R608
L609
M610
S611
K612
F613
K614
GLU
LEU
GLU
LEU
ALA
ALA
VAL

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	48.45Å 86.28Å 137.97Å 90.00° 92.30° 90.00°	Depositor
Resolution (Å)	15.00 – 3.00 14.99 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.1 (15.00-3.00) 99.1 (14.99-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.90 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.215 , 0.310 0.215 , 0.309	Depositor DCC
R_{free} test set	1148 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å^2)	43.6	Xtriage
Anisotropy	0.171	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 60.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	0.046 for h,-k,-l	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	9236	wwPDB-VP
Average B, all atoms (Å^2)	17.0	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 22.69 % 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 5.4102e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	1.67	19/1470 (1.3%)	1.46	9/1983 (0.5%)
1	B	1.85	23/1470 (1.6%)	1.47	13/1983 (0.7%)
1	C	1.71	17/1461 (1.2%)	1.50	17/1972 (0.9%)
1	D	2.37	58/1470 (3.9%)	2.11	61/1983 (3.1%)
1	E	1.71	16/1470 (1.1%)	1.45	14/1983 (0.7%)
1	F	1.54	16/1470 (1.1%)	1.45	17/1983 (0.9%)
All	All	1.83	149/8811 (1.7%)	1.59	131/11887 (1.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	5
1	C	0	1
1	D	0	5
1	E	0	3
1	F	0	3
All	All	0	18

All (149) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	552	LYS	CE-NZ	23.76	2.08	1.49
1	D	563	LYS	CE-NZ	21.05	2.01	1.49
1	D	534	THR	C-O	19.61	1.60	1.23
1	D	531	VAL	C-N	14.71	1.67	1.34
1	D	508	ASP	CB-CG	-14.54	1.21	1.51
1	D	532	ALA	C-N	14.11	1.66	1.34
1	D	532	ALA	C-O	13.70	1.49	1.23
1	D	563	LYS	N-CA	12.51	1.71	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	468	GLU	CD-OE2	11.87	1.38	1.25
1	D	531	VAL	N-CA	11.13	1.68	1.46
1	C	468	GLU	CG-CD	10.48	1.67	1.51
1	D	568	LYS	CE-NZ	10.10	1.74	1.49
1	A	453	MET	C-O	10.05	1.42	1.23
1	D	535	GLY	CA-C	-10.04	1.35	1.51
1	D	532	ALA	N-CA	9.72	1.65	1.46
1	D	537	LEU	CA-C	-9.72	1.27	1.52
1	D	468	GLU	CG-CD	9.44	1.66	1.51
1	D	564	VAL	CA-CB	-9.32	1.35	1.54
1	D	535	GLY	C-O	9.22	1.38	1.23
1	D	562	LYS	CA-C	9.21	1.76	1.52
1	A	604	LYS	CD-CE	9.17	1.74	1.51
1	D	562	LYS	CE-NZ	9.14	1.71	1.49
1	D	536	SER	CB-OG	9.09	1.54	1.42
1	D	597	GLU	CG-CD	9.04	1.65	1.51
1	D	531	VAL	CA-CB	-9.03	1.35	1.54
1	E	542	GLU	CB-CG	9.00	1.69	1.52
1	A	483	LYS	CE-NZ	8.45	1.70	1.49
1	C	597	GLU	CD-OE1	8.35	1.34	1.25
1	D	547	GLY	C-O	8.34	1.36	1.23
1	F	509	SER	CB-OG	8.25	1.52	1.42
1	B	462	ALA	CA-CB	8.19	1.69	1.52
1	C	483	LYS	CB-CG	8.16	1.74	1.52
1	B	542	GLU	CB-CG	8.07	1.67	1.52
1	A	579	GLU	CB-CG	8.05	1.67	1.52
1	A	568	LYS	CE-NZ	7.86	1.68	1.49
1	D	563	LYS	C-O	7.78	1.38	1.23
1	E	425	GLU	CD-OE2	7.75	1.34	1.25
1	D	534	THR	CA-CB	7.67	1.73	1.53
1	B	542	GLU	CG-CD	7.58	1.63	1.51
1	D	537	LEU	C-O	7.52	1.37	1.23
1	D	532	ALA	CA-CB	-7.42	1.36	1.52
1	B	435	ILE	CA-CB	7.41	1.72	1.54
1	C	562	LYS	CD-CE	7.36	1.69	1.51
1	B	511	SER	CB-OG	7.36	1.51	1.42
1	E	542	GLU	CG-CD	7.36	1.62	1.51
1	D	437	GLU	CB-CG	7.32	1.66	1.52
1	C	597	GLU	CD-OE2	7.27	1.33	1.25
1	D	422	GLU	CG-CD	7.18	1.62	1.51
1	D	536	SER	C-N	7.14	1.50	1.34
1	D	552	LYS	CD-CE	-7.04	1.33	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	531	VAL	CB-CG2	7.03	1.67	1.52
1	D	533	MET	CG-SD	6.97	1.99	1.81
1	A	597	GLU	CD-OE1	6.97	1.33	1.25
1	E	562	LYS	CD-CE	6.95	1.68	1.51
1	A	579	GLU	CG-CD	6.86	1.62	1.51
1	F	477	VAL	CB-CG2	6.82	1.67	1.52
1	A	604	LYS	CE-NZ	6.75	1.66	1.49
1	D	468	GLU	CD-OE1	6.69	1.33	1.25
1	B	605	LYS	CB-CG	6.63	1.70	1.52
1	B	608	ARG	CG-CD	6.62	1.68	1.51
1	E	513	SER	CB-OG	6.58	1.50	1.42
1	D	508	ASP	CG-OD1	-6.54	1.10	1.25
1	F	506	GLU	CG-CD	6.54	1.61	1.51
1	B	591	ARG	CG-CD	6.53	1.68	1.51
1	F	472	GLU	CG-CD	6.51	1.61	1.51
1	B	419	PHE	N-CA	6.44	1.59	1.46
1	D	437	GLU	CG-CD	6.42	1.61	1.51
1	E	608	ARG	CG-CD	6.37	1.67	1.51
1	D	480	ILE	CB-CG2	6.32	1.72	1.52
1	D	542	GLU	CG-CD	6.32	1.61	1.51
1	A	568	LYS	CD-CE	6.31	1.67	1.51
1	B	568	LYS	CD-CE	6.31	1.67	1.51
1	E	599	VAL	CB-CG1	6.29	1.66	1.52
1	B	614	LYS	CE-NZ	6.29	1.64	1.49
1	B	436	GLY	N-CA	6.25	1.55	1.46
1	B	418	LEU	CA-C	6.17	1.69	1.52
1	F	542	GLU	CG-CD	6.15	1.61	1.51
1	E	558	GLN	CG-CD	6.14	1.65	1.51
1	D	542	GLU	CD-OE1	6.13	1.32	1.25
1	F	540	LYS	CE-NZ	6.07	1.64	1.49
1	A	452	SER	CB-OG	6.06	1.50	1.42
1	F	554	GLU	CD-OE1	6.03	1.32	1.25
1	A	443	LEU	C-O	6.00	1.34	1.23
1	C	563	LYS	CE-NZ	5.97	1.64	1.49
1	F	568	LYS	CE-NZ	5.97	1.64	1.49
1	E	591	ARG	CZ-NH1	5.96	1.40	1.33
1	D	540	LYS	CD-CE	5.93	1.66	1.51
1	D	597	GLU	CD-OE2	5.92	1.32	1.25
1	A	457	GLU	CG-CD	5.91	1.60	1.51
1	B	498	PHE	CD2-CE2	-5.90	1.27	1.39
1	F	597	GLU	CG-CD	5.87	1.60	1.51
1	B	474	VAL	CB-CG2	5.84	1.65	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	438	SER	CB-OG	5.83	1.49	1.42
1	D	597	GLU	CD-OE1	5.81	1.32	1.25
1	D	509	SER	C-O	5.77	1.34	1.23
1	D	508	ASP	CG-OD2	5.74	1.38	1.25
1	C	585	GLU	CD-OE1	5.68	1.31	1.25
1	C	540	LYS	CE-NZ	5.67	1.63	1.49
1	F	476	ASN	CB-CG	5.66	1.64	1.51
1	A	542	GLU	CG-CD	5.63	1.60	1.51
1	F	597	GLU	CD-OE1	5.62	1.31	1.25
1	E	555	ALA	N-CA	5.61	1.57	1.46
1	A	562	LYS	CE-NZ	5.60	1.63	1.49
1	D	437	GLU	CD-OE2	5.60	1.31	1.25
1	B	614	LYS	CD-CE	5.57	1.65	1.51
1	C	472	GLU	CG-CD	5.55	1.60	1.51
1	F	472	GLU	CB-CG	5.53	1.62	1.52
1	D	465	ARG	CZ-NH1	5.52	1.40	1.33
1	A	585	GLU	CG-CD	5.52	1.60	1.51
1	D	530	SER	N-CA	5.51	1.57	1.46
1	D	563	LYS	CD-CE	5.49	1.65	1.51
1	E	558	GLN	CB-CG	5.47	1.67	1.52
1	F	498	PHE	CD1-CE1	5.45	1.50	1.39
1	A	468	GLU	CD-OE1	5.44	1.31	1.25
1	E	502	TYR	CE2-CZ	5.43	1.45	1.38
1	D	562	LYS	C-O	5.41	1.33	1.23
1	C	468	GLU	CD-OE1	5.40	1.31	1.25
1	A	429	VAL	CB-CG1	5.39	1.64	1.52
1	D	508	ASP	CA-C	5.39	1.67	1.52
1	A	422	GLU	CB-CG	-5.32	1.42	1.52
1	D	442	VAL	CB-CG1	-5.32	1.41	1.52
1	F	468	GLU	CG-CD	5.31	1.59	1.51
1	D	612	LYS	CD-CE	5.30	1.64	1.51
1	E	502	TYR	CD2-CE2	5.25	1.47	1.39
1	C	599	VAL	CB-CG1	-5.24	1.41	1.52
1	D	614	LYS	C-O	5.22	1.33	1.23
1	E	420	ILE	CA-CB	5.21	1.66	1.54
1	E	462	ALA	CA-CB	5.20	1.63	1.52
1	F	503	GLU	CG-CD	5.19	1.59	1.51
1	D	424	TYR	CG-CD1	5.17	1.45	1.39
1	E	522	ILE	CG1-CD1	5.17	1.86	1.50
1	C	601	GLU	CG-CD	-5.17	1.44	1.51
1	B	608	ARG	CB-CG	5.16	1.66	1.52
1	B	562	LYS	CD-CE	5.14	1.64	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	429	VAL	CB-CG2	5.13	1.63	1.52
1	A	436	GLY	C-O	5.11	1.31	1.23
1	D	608	ARG	CG-CD	5.08	1.64	1.51
1	D	551	GLN	C-O	5.08	1.33	1.23
1	D	506	GLU	CD-OE2	5.07	1.31	1.25
1	F	562	LYS	CE-NZ	5.05	1.61	1.49
1	B	503	GLU	CG-CD	5.05	1.59	1.51
1	D	533	MET	N-CA	-5.05	1.36	1.46
1	B	425	GLU	CG-CD	5.04	1.59	1.51
1	C	428	ARG	CZ-NH2	5.04	1.39	1.33
1	B	501	THR	CA-CB	5.03	1.66	1.53
1	D	538	SER	CB-OG	5.02	1.48	1.42
1	B	501	THR	C-O	5.01	1.32	1.23
1	B	518	VAL	CA-CB	5.01	1.65	1.54
1	C	568	LYS	CE-NZ	5.00	1.61	1.49

All (131) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	536	SER	O-C-N	-19.83	90.98	122.70
1	D	534	THR	CB-CA-C	-16.26	67.69	111.60
1	D	508	ASP	CB-CG-OD1	-16.15	103.77	118.30
1	D	534	THR	CA-CB-CG2	14.87	133.22	112.40
1	D	563	LYS	O-C-N	-14.79	99.03	122.70
1	D	537	LEU	CB-CG-CD1	13.30	133.60	111.00
1	D	508	ASP	OD1-CG-OD2	12.15	146.38	123.30
1	D	537	LEU	CB-CA-C	-11.82	87.74	110.20
1	D	465	ARG	NE-CZ-NH1	11.68	126.14	120.30
1	D	465	ARG	NE-CZ-NH2	-11.29	114.66	120.30
1	D	531	VAL	O-C-N	-11.29	104.64	122.70
1	D	602	ASP	CB-CG-OD2	10.60	127.84	118.30
1	D	508	ASP	CB-CG-OD2	-10.56	108.80	118.30
1	D	537	LEU	CA-C-O	10.40	141.94	120.10
1	B	428	ARG	NE-CZ-NH2	-9.87	115.36	120.30
1	D	563	LYS	CD-CE-NZ	-9.61	89.60	111.70
1	D	552	LYS	N-CA-C	9.55	136.78	111.00
1	C	609	LEU	CB-CG-CD2	-9.52	94.82	111.00
1	D	534	THR	CA-CB-OG1	-9.35	89.37	109.00
1	D	565	ILE	CB-CA-C	-9.29	93.02	111.60
1	D	508	ASP	N-CA-C	-9.17	86.25	111.00
1	D	537	LEU	CD1-CG-CD2	-9.14	83.08	110.50
1	C	428	ARG	NE-CZ-NH2	-8.97	115.81	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	465	ARG	NE-CZ-NH1	8.84	124.72	120.30
1	D	531	VAL	CA-CB-CG1	-8.54	98.09	110.90
1	D	536	SER	N-CA-CB	8.50	123.26	110.50
1	F	575	LEU	CA-CB-CG	8.44	134.72	115.30
1	F	591	ARG	NE-CZ-NH1	-8.32	116.14	120.30
1	D	532	ALA	CA-C-N	-8.26	99.03	117.20
1	B	460	VAL	N-CA-C	-8.16	88.97	111.00
1	D	509	SER	CB-CA-C	-8.01	94.89	110.10
1	D	532	ALA	N-CA-CB	7.92	121.19	110.10
1	E	591	ARG	NE-CZ-NH1	7.88	124.24	120.30
1	D	508	ASP	N-CA-CB	7.85	124.72	110.60
1	D	531	VAL	CA-C-O	7.84	136.57	120.10
1	C	465	ARG	NE-CZ-NH2	-7.71	116.44	120.30
1	D	471	ARG	NE-CZ-NH1	7.58	124.09	120.30
1	E	571	ILE	CB-CA-C	-7.55	96.49	111.60
1	D	565	ILE	CG1-CB-CG2	-7.50	94.89	111.40
1	B	422	GLU	N-CA-C	-7.40	91.03	111.00
1	C	540	LYS	CD-CE-NZ	7.39	128.69	111.70
1	D	508	ASP	O-C-N	-7.28	111.05	122.70
1	D	533	MET	N-CA-C	7.27	130.62	111.00
1	C	544	LEU	CB-CG-CD1	-7.24	98.70	111.00
1	A	585	GLU	OE1-CD-OE2	-7.20	114.66	123.30
1	D	602	ASP	CB-CG-OD1	-7.17	111.85	118.30
1	A	480	ILE	CB-CA-C	7.16	125.91	111.60
1	D	537	LEU	O-C-N	-7.11	111.32	122.70
1	D	443	LEU	N-CA-C	-7.03	92.03	111.00
1	F	544	LEU	CA-CB-CG	-6.76	99.74	115.30
1	D	544	LEU	CB-CG-CD1	-6.69	99.63	111.00
1	E	523	GLU	CB-CA-C	6.67	123.73	110.40
1	D	562	LYS	CD-CE-NZ	-6.62	96.46	111.70
1	D	531	VAL	N-CA-CB	6.61	126.05	111.50
1	F	446	ILE	CB-CA-C	-6.53	98.54	111.60
1	D	590	SER	CB-CA-C	-6.45	97.84	110.10
1	C	602	ASP	CB-CG-OD1	6.45	124.11	118.30
1	F	609	LEU	CA-CB-CG	-6.40	100.59	115.30
1	B	600	LEU	CB-CG-CD1	6.34	121.78	111.00
1	D	534	THR	O-C-N	-6.34	112.42	123.20
1	D	562	LYS	O-C-N	-6.25	112.71	122.70
1	D	532	ALA	O-C-N	6.24	132.69	122.70
1	D	552	LYS	N-CA-CB	-6.23	99.39	110.60
1	D	566	ILE	CB-CA-C	-6.20	99.20	111.60
1	D	536	SER	CB-CA-C	-6.19	98.33	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	479	ALA	N-CA-C	-6.18	94.30	111.00
1	F	475	MET	CG-SD-CE	6.13	110.02	100.20
1	A	596	LEU	CB-CG-CD1	-6.12	100.59	111.00
1	E	598	HIS	CB-CA-C	-6.10	98.21	110.40
1	B	541	GLY	N-CA-C	6.09	128.31	113.10
1	D	564	VAL	CA-C-O	6.09	132.88	120.10
1	E	591	ARG	NE-CZ-NH2	-6.06	117.27	120.30
1	E	573	ASP	CB-CG-OD1	6.06	123.75	118.30
1	F	471	ARG	NE-CZ-NH1	6.02	123.31	120.30
1	B	591	ARG	NE-CZ-NH1	6.01	123.31	120.30
1	C	591	ARG	NE-CZ-NH2	-5.95	117.33	120.30
1	C	608	ARG	NE-CZ-NH2	-5.93	117.34	120.30
1	A	544	LEU	C-N-CD	-5.86	107.71	120.60
1	F	476	ASN	CB-CA-C	5.86	122.11	110.40
1	B	593	ASN	N-CA-C	5.84	126.78	111.00
1	D	511	SER	CB-CA-C	5.84	121.19	110.10
1	F	445	ILE	CB-CA-C	-5.83	99.94	111.60
1	D	537	LEU	CB-CG-CD2	5.78	120.83	111.00
1	B	568	LYS	N-CA-CB	5.76	120.96	110.60
1	B	528	ASP	CB-CG-OD2	5.73	123.45	118.30
1	F	466	LEU	CA-CB-CG	-5.72	102.13	115.30
1	B	428	ARG	NE-CZ-NH1	5.71	123.16	120.30
1	D	589	VAL	CB-CA-C	-5.71	100.56	111.40
1	C	608	ARG	NE-CZ-NH1	5.68	123.14	120.30
1	D	452	SER	N-CA-C	5.66	126.27	111.00
1	E	532	ALA	N-CA-C	-5.62	95.84	111.00
1	E	572	ASP	CB-CG-OD1	5.59	123.33	118.30
1	B	575	LEU	CA-CB-CG	5.59	128.16	115.30
1	D	538	SER	CB-CA-C	-5.57	99.51	110.10
1	A	608	ARG	CG-CD-NE	5.56	123.47	111.80
1	A	612	LYS	CD-CE-NZ	5.53	124.42	111.70
1	F	441	ILE	CB-CA-C	-5.51	100.57	111.60
1	C	468	GLU	CB-CA-C	5.51	121.42	110.40
1	A	486	GLY	N-CA-C	5.50	126.86	113.10
1	D	537	LEU	CA-C-N	-5.49	105.12	117.20
1	D	587	ILE	C-N-CD	5.38	139.70	128.40
1	B	568	LYS	CA-CB-CG	5.37	125.21	113.40
1	D	534	THR	CA-C-O	5.35	131.34	120.10
1	C	452	SER	N-CA-C	5.35	125.43	111.00
1	E	563	LYS	N-CA-C	5.33	125.39	111.00
1	A	608	ARG	NE-CZ-NH2	-5.32	117.64	120.30
1	F	491	ASN	CB-CA-C	-5.32	99.77	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	564	VAL	CB-CA-C	-5.31	101.32	111.40
1	F	467	GLN	CA-CB-CG	5.30	125.06	113.40
1	C	437	GLU	N-CA-C	5.30	125.31	111.00
1	C	485	THR	N-CA-C	5.29	125.28	111.00
1	D	533	MET	N-CA-CB	5.28	120.11	110.60
1	E	554	GLU	CB-CA-C	5.28	120.95	110.40
1	D	533	MET	CA-CB-CG	-5.27	104.34	113.30
1	E	488	ASP	CB-CG-OD1	5.27	123.04	118.30
1	C	445	ILE	CB-CA-C	-5.26	101.08	111.60
1	C	468	GLU	CA-CB-CG	5.26	124.96	113.40
1	D	548	GLY	N-CA-C	5.25	126.23	113.10
1	F	512	ILE	CB-CA-C	-5.25	101.11	111.60
1	C	597	GLU	OE1-CD-OE2	5.20	129.54	123.30
1	D	587	ILE	CB-CA-C	-5.18	101.23	111.60
1	D	552	LYS	CB-CA-C	-5.18	100.04	110.40
1	D	531	VAL	CG1-CB-CG2	5.15	119.14	110.90
1	E	424	TYR	N-CA-C	-5.12	97.19	111.00
1	B	508	ASP	CB-CG-OD2	-5.10	113.71	118.30
1	A	569	ASP	CB-CG-OD1	5.10	122.89	118.30
1	E	459	ARG	N-CA-C	5.05	124.65	111.00
1	F	528	ASP	CB-CG-OD1	5.03	122.83	118.30
1	F	591	ARG	NE-CZ-NH2	5.02	122.81	120.30
1	E	451	PRO	N-CA-C	-5.02	99.04	112.10
1	D	564	VAL	O-C-N	-5.01	114.69	122.70

There are no chirality outliers.

All (18) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	485	THR	Peptide
1	B	417	LYS	Peptide
1	B	441	ILE	Peptide
1	B	451	PRO	Peptide
1	B	462	ALA	Peptide
1	B	585	GLU	Peptide
1	C	437	GLU	Peptide
1	D	457	GLU	Peptide
1	D	536	SER	Mainchain
1	D	552	LYS	Mainchain
1	D	563	LYS	Mainchain
1	D	580	HIS	Peptide
1	E	417	LYS	Peptide

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Mol	Chain	Res	Type	Group
1	E	434	VAL	Peptide
1	E	502	TYR	Peptide
1	F	484	TYR	Peptide
1	F	486	GLY	Peptide
1	F	577	ASP	Peptide

5.2 Too-close contacts (i)

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	160	0
1	B	1457	0	1523	229	0
1	C	1448	0	1510	136	0
1	D	1457	0	1523	129	0
1	E	1457	0	1523	147	0
1	F	1457	0	1523	154	1
2	A	78	0	0	12	0
2	B	74	0	0	13	0
2	C	104	0	0	5	0
2	D	99	0	0	10	0
2	E	69	0	0	13	0
2	F	79	0	0	11	0
All	All	9236	0	9125	906	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 51.

All (906) 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:C:445:ILE:CG1	1:C:445:ILE:CD1	1.78	1.56
1:A:483:LYS:NZ	1:A:483:LYS:CE	1.70	1.55
1:D:531:VAL:CA	1:D:531:VAL:N	1.68	1.55
1:A:568:LYS:NZ	1:A:568:LYS:CE	1.68	1.55
1:C:483:LYS:CG	1:C:483:LYS:CB	1.74	1.55
1:D:563:LYS:CA	1:D:563:LYS:N	1.71	1.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:562:LYS:CA	1:D:562:LYS:C	1.76	1.51
1:D:568:LYS:CE	1:D:568:LYS:NZ	1.74	1.51
1:D:562:LYS:CE	1:D:562:LYS:NZ	1.71	1.50
1:E:522:ILE:CD1	1:E:522:ILE:CG1	1.86	1.49
1:D:531:VAL:C	1:D:532:ALA:N	1.67	1.45
1:C:446:ILE:HD11	1:C:499:VAL:CG2	1.60	1.29
1:D:563:LYS:CE	1:D:563:LYS:NZ	2.01	1.24
1:B:481:ILE:HG23	1:B:485:THR:OG1	1.41	1.19
1:D:552:LYS:NZ	1:D:552:LYS:CE	2.08	1.17
1:F:428:ARG:HD2	1:F:446:ILE:HG23	1.28	1.13
1:A:487:ARG:HH11	1:A:487:ARG:HG3	1.07	1.12
1:B:563:LYS:HD3	1:B:587:ILE:HD11	1.31	1.12
1:D:537:LEU:HG	1:D:538:SER:N	1.49	1.11
1:B:449:VAL:HG13	1:B:521:ALA:HB1	1.15	1.11
1:A:540:LYS:HD2	2:A:689:HOH:O	1.51	1.10
1:B:492:MET:CE	1:B:522:ILE:HD11	1.81	1.10
1:A:544:LEU:HB3	1:A:545:PRO:HD2	1.33	1.10
1:B:431:GLY:HA2	1:B:533:MET:O	1.52	1.09
1:B:487:ARG:CG	1:B:487:ARG:HH11	1.65	1.09
1:B:487:ARG:HH11	1:B:487:ARG:HG3	0.91	1.06
1:B:531:VAL:HG21	1:B:599:VAL:HG12	1.33	1.06
1:A:428:ARG:HA	1:A:445:ILE:O	1.54	1.06
1:A:535:GLY:HA2	1:A:546:VAL:HG11	1.37	1.05
1:C:578:ALA:HA	1:C:581:GLU:OE2	1.57	1.04
1:B:424:TYR:HA	1:B:527:VAL:O	1.57	1.04
1:C:446:ILE:HD11	1:C:499:VAL:HG23	1.05	1.03
1:B:487:ARG:NH1	1:B:487:ARG:HG3	1.63	1.03
1:E:453:MET:HG2	1:F:482:LYS:HD3	1.40	1.02
1:A:568:LYS:HB2	1:A:588:PRO:HB3	1.37	1.02
1:B:481:ILE:HG22	1:B:487:ARG:HB2	1.42	1.02
1:E:563:LYS:HB3	1:E:585:GLU:HB3	1.43	1.00
1:B:526:PRO:HG2	1:B:601:GLU:HB3	1.43	1.00
1:A:595:VAL:O	1:A:599:VAL:HG13	1.58	1.00
1:F:446:ILE:HD12	1:F:497:GLN:HB2	1.44	1.00
1:A:452:SER:O	1:A:453:MET:HB2	1.58	0.99
1:D:487:ARG:HG3	1:D:487:ARG:HH11	1.21	0.99
1:A:481:ILE:HD12	1:A:489:ILE:HD11	1.04	0.99
1:B:449:VAL:HG13	1:B:521:ALA:CB	1.92	0.99
1:E:478:SER:OG	1:E:489:ILE:HD11	1.63	0.98
1:F:435:ILE:HG22	1:F:505:VAL:HG22	1.45	0.98
1:E:450:THR:HG22	1:E:493:ASP:HB2	1.44	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:419:PHE:CZ	1:B:559:ALA:HA	1.98	0.97
1:A:481:ILE:HD12	1:A:489:ILE:CD1	1.93	0.97
1:A:487:ARG:NH1	1:A:487:ARG:HG3	1.75	0.96
1:E:494:VAL:CG1	1:E:496:ILE:HD11	1.96	0.96
1:F:435:ILE:HG13	1:F:439:ALA:HB3	1.46	0.95
1:E:435:ILE:CG2	1:E:441:ILE:HG23	1.97	0.95
1:E:453:MET:HG2	1:F:482:LYS:CD	1.96	0.95
1:C:446:ILE:CD1	1:C:499:VAL:HG23	1.96	0.95
1:F:478:SER:HA	1:F:481:ILE:HB	1.47	0.95
1:E:453:MET:CG	1:F:482:LYS:HD3	1.97	0.94
1:E:568:LYS:O	1:E:571:ILE:HG13	1.65	0.94
1:C:465:ARG:HD3	1:C:503:GLU:OE2	1.66	0.94
1:E:494:VAL:HG12	1:E:496:ILE:HD11	1.48	0.94
1:C:465:ARG:HB3	1:C:465:ARG:CZ	1.95	0.94
1:D:537:LEU:HG	1:D:538:SER:H	1.29	0.94
1:F:537:LEU:HG	1:F:538:SER:O	1.69	0.93
1:F:489:ILE:CD1	1:F:489:ILE:H	1.81	0.93
1:E:522:ILE:HG22	1:E:523:GLU:HG2	1.51	0.92
1:A:467:GLN:HG3	1:A:471:ARG:NH1	1.85	0.92
1:F:568:LYS:O	1:F:571:ILE:HG12	1.68	0.92
1:C:472:GLU:HG3	1:C:473:ALA:H	1.30	0.92
1:C:501:THR:HG21	2:D:666:HOH:O	1.67	0.92
1:B:492:MET:HE1	1:B:522:ILE:HD11	1.49	0.91
1:C:446:ILE:CD1	1:C:499:VAL:CG2	2.47	0.91
1:D:424:TYR:CE1	1:D:528:ASP:HB2	2.06	0.90
1:D:542:GLU:OE2	1:D:591:ARG:HG3	1.72	0.90
1:E:577:ASP:OD1	1:E:580:HIS:N	2.05	0.89
1:F:553:ILE:O	1:F:556:ALA:HB3	1.72	0.89
1:C:578:ALA:HA	1:C:581:GLU:CD	1.93	0.88
1:F:489:ILE:HD13	1:F:489:ILE:H	1.36	0.88
1:A:481:ILE:CD1	1:A:489:ILE:HD11	1.98	0.88
1:D:542:GLU:OE2	1:D:591:ARG:CG	2.22	0.88
1:E:585:GLU:HG3	1:E:587:ILE:HD11	1.54	0.87
1:D:578:ALA:O	1:D:579:GLU:HB3	1.73	0.87
1:E:551:GLN:H	1:E:551:GLN:CD	1.75	0.87
1:E:597:GLU:HG2	1:E:610:MET:CE	2.04	0.87
1:B:463:THR:HG22	2:B:643:HOH:O	1.74	0.87
1:A:418:LEU:HD13	1:A:500:GLY:HA3	1.56	0.87
1:D:461:ILE:HD13	1:E:475:MET:SD	2.14	0.86
1:B:553:ILE:HG23	1:B:564:VAL:HG11	1.56	0.86
1:F:476:ASN:O	1:F:478:SER:N	2.06	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:568:LYS:CB	1:A:588:PRO:HB3	2.06	0.86
1:C:463:THR:HG22	2:D:648:HOH:O	1.74	0.86
1:E:435:ILE:HG21	1:E:441:ILE:HG23	1.54	0.86
1:B:474:VAL:HA	1:B:477:VAL:HG12	1.58	0.85
1:A:554:GLU:HG3	2:A:673:HOH:O	1.77	0.84
1:B:492:MET:HE3	1:B:522:ILE:HD11	1.57	0.84
1:B:419:PHE:HZ	1:B:559:ALA:HA	1.36	0.84
1:D:550:THR:O	1:D:554:GLU:HB2	1.76	0.84
1:E:417:LYS:HB3	1:E:419:PHE:H	1.41	0.84
1:E:487:ARG:HH11	1:E:487:ARG:HB3	1.43	0.84
1:D:465:ARG:HD2	1:D:465:ARG:H	1.42	0.84
1:E:597:GLU:HG2	1:E:610:MET:HE1	1.57	0.84
1:D:534:THR:HG23	1:D:534:THR:O	1.77	0.83
1:D:562:LYS:NZ	1:D:562:LYS:CG	2.41	0.83
1:C:472:GLU:HG3	1:C:473:ALA:N	1.93	0.83
1:B:502:TYR:HB2	1:B:505:VAL:CG2	2.09	0.82
1:B:449:VAL:CG1	1:B:521:ALA:HB1	2.06	0.82
1:B:568:LYS:HG3	1:B:590:SER:HB2	1.62	0.82
1:F:492:MET:CE	1:F:522:ILE:HG12	2.09	0.82
1:F:446:ILE:CD1	1:F:497:GLN:HB2	2.09	0.82
1:A:418:LEU:HD13	1:A:500:GLY:CA	2.10	0.81
1:A:577:ASP:HB3	2:A:682:HOH:O	1.80	0.81
1:B:418:LEU:HD22	1:C:545:PRO:HG2	1.62	0.81
1:B:481:ILE:CG2	1:B:485:THR:OG1	2.27	0.81
1:B:425:GLU:HB2	1:B:529:GLN:NE2	1.96	0.80
1:A:581:GLU:O	1:A:583:LYS:N	2.15	0.79
1:C:608:ARG:HD3	1:C:608:ARG:C	2.00	0.79
1:A:558:GLN:HB2	2:A:693:HOH:O	1.82	0.79
1:A:470:ALA:O	1:A:474:VAL:HG23	1.83	0.79
1:A:492:MET:SD	1:A:522:ILE:HD11	2.23	0.79
1:B:525:ILE:HG23	1:B:526:PRO:HD2	1.62	0.79
1:D:551:GLN:HG3	2:D:702:HOH:O	1.82	0.79
1:F:565:ILE:HA	1:F:587:ILE:O	1.82	0.79
1:A:542:GLU:OE2	1:A:542:GLU:HA	1.83	0.78
1:A:535:GLY:HA2	1:A:546:VAL:CG1	2.13	0.78
1:A:553:ILE:HG21	1:A:576:LEU:HD11	1.66	0.78
1:A:563:LYS:HG2	1:A:585:GLU:HB2	1.66	0.78
1:D:487:ARG:CG	1:D:487:ARG:HH11	1.96	0.78
1:F:434:VAL:O	1:F:505:VAL:HA	1.83	0.78
1:F:435:ILE:HG13	1:F:439:ALA:CB	2.13	0.78
1:A:534:THR:O	1:A:567:PRO:HD3	1.84	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:502:TYR:HB2	1:B:505:VAL:HG23	1.64	0.78
1:D:562:LYS:CD	1:D:562:LYS:NZ	2.45	0.77
1:D:489:ILE:HG21	1:D:522:ILE:CD1	2.14	0.77
1:A:519:ILE:HD13	1:A:596:LEU:HD11	1.66	0.77
1:C:465:ARG:CD	1:C:503:GLU:OE2	2.32	0.77
1:B:489:ILE:HA	1:B:492:MET:CE	2.15	0.77
1:B:449:VAL:CG1	1:B:521:ALA:CB	2.63	0.76
1:B:563:LYS:HD3	1:B:587:ILE:CD1	2.13	0.76
1:E:459:ARG:HG3	1:E:459:ARG:HH11	1.49	0.76
1:A:449:VAL:H	1:B:540:LYS:NZ	1.83	0.76
1:E:482:LYS:HD3	2:E:675:HOH:O	1.84	0.76
1:A:487:ARG:CG	1:A:487:ARG:HH11	1.92	0.76
1:D:534:THR:OG1	1:D:535:GLY:N	2.12	0.76
1:B:492:MET:CE	1:B:522:ILE:CD1	2.63	0.76
1:C:608:ARG:HD3	1:C:608:ARG:O	1.85	0.76
1:B:577:ASP:OD2	1:B:580:HIS:HE1	1.69	0.76
1:F:579:GLU:O	1:F:580:HIS:HB2	1.86	0.76
1:B:494:VAL:CG1	1:B:496:ILE:HD11	2.15	0.76
1:F:431:GLY:O	1:F:432:LEU:HD23	1.86	0.76
1:A:449:VAL:H	1:B:540:LYS:HZ1	1.33	0.75
1:C:428:ARG:CD	1:C:446:ILE:HG23	2.16	0.75
1:A:467:GLN:HG3	1:A:471:ARG:HH12	1.47	0.75
1:A:568:LYS:HB2	1:A:588:PRO:CB	2.15	0.75
1:C:448:GLU:OE2	1:D:539:VAL:HG13	1.87	0.75
1:C:437:GLU:HA	1:C:437:GLU:OE1	1.85	0.75
1:B:577:ASP:CG	1:B:580:HIS:HE1	1.90	0.75
1:B:531:VAL:CG2	1:B:599:VAL:HG12	2.13	0.75
1:F:435:ILE:HG22	1:F:505:VAL:CG2	2.17	0.75
1:E:478:SER:OG	1:E:489:ILE:CD1	2.33	0.74
1:B:425:GLU:H	1:B:529:GLN:HE21	1.35	0.74
1:F:587:ILE:HG21	1:F:598:HIS:CD2	2.22	0.74
1:E:435:ILE:HD12	2:E:642:HOH:O	1.85	0.74
1:E:435:ILE:HG22	1:E:441:ILE:HG23	1.69	0.74
1:F:473:ALA:HA	1:F:510:ALA:HA	1.69	0.74
1:F:566:ILE:HD13	1:F:586:VAL:CG1	2.17	0.74
1:B:492:MET:HE1	1:B:522:ILE:CD1	2.17	0.74
1:B:592:ILE:O	1:B:595:VAL:HB	1.87	0.74
1:C:475:MET:HB2	2:C:675:HOH:O	1.88	0.74
1:F:428:ARG:HD2	1:F:446:ILE:CG2	2.15	0.74
1:E:453:MET:HG2	1:F:482:LYS:CE	2.17	0.73
1:B:469:ILE:HD12	1:B:507:GLY:HA3	1.68	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:532:ALA:HB2	1:C:561:LEU:HD13	1.70	0.73
1:A:475:MET:SD	1:F:461:ILE:HD13	2.28	0.73
1:E:531:VAL:HA	1:E:563:LYS:O	1.88	0.73
1:A:544:LEU:CB	1:A:545:PRO:HD2	1.92	0.73
1:F:608:ARG:O	1:F:612:LYS:HG3	1.89	0.73
1:B:480:ILE:HD13	1:B:592:ILE:HG21	1.70	0.73
1:E:435:ILE:HG13	1:E:436:GLY:N	2.03	0.73
1:E:453:MET:CG	1:F:482:LYS:HE2	2.19	0.73
1:F:538:SER:OG	1:F:541:GLY:N	2.22	0.73
1:A:478:SER:HA	1:A:489:ILE:HD12	1.70	0.73
1:B:521:ALA:HA	2:B:645:HOH:O	1.88	0.73
1:C:489:ILE:C	1:C:491:ASN:H	1.88	0.73
1:A:452:SER:O	1:A:453:MET:CB	2.36	0.72
1:C:578:ALA:CA	1:C:581:GLU:OE2	2.37	0.72
1:A:542:GLU:HG3	2:A:649:HOH:O	1.89	0.72
1:D:534:THR:O	1:D:534:THR:CG2	2.35	0.72
1:E:450:THR:CG2	1:E:493:ASP:HB2	2.19	0.72
1:E:563:LYS:CB	1:E:585:GLU:HB3	2.18	0.72
1:B:537:LEU:HD11	1:B:592:ILE:HB	1.71	0.72
1:F:566:ILE:HD13	1:F:586:VAL:HG11	1.70	0.72
1:A:520:SER:O	1:A:524:GLY:N	2.22	0.72
1:B:482:LYS:HG2	2:B:667:HOH:O	1.88	0.72
1:C:446:ILE:N	1:C:446:ILE:HD13	2.05	0.72
1:C:428:ARG:HD3	1:C:446:ILE:HG23	1.71	0.72
1:F:442:VAL:HG12	1:F:444:PRO:HD3	1.71	0.71
1:E:587:ILE:HG22	1:E:589:VAL:CG1	2.19	0.71
1:B:438:SER:OG	1:B:551:GLN:HG2	1.89	0.71
1:D:562:LYS:NZ	1:D:562:LYS:HG3	2.04	0.71
1:B:595:VAL:O	1:B:599:VAL:HG22	1.91	0.71
1:F:435:ILE:CG1	1:F:439:ALA:HB3	2.20	0.71
1:A:478:SER:CA	1:A:489:ILE:HD12	2.21	0.71
1:E:452:SER:N	1:E:491:ASN:O	2.23	0.71
1:D:489:ILE:HG21	1:D:522:ILE:HD11	1.72	0.71
1:A:528:ASP:OD1	1:A:530:SER:OG	2.02	0.70
1:D:520:SER:O	1:D:524:GLY:N	2.24	0.70
1:B:531:VAL:CG1	1:B:565:ILE:HG13	2.22	0.70
1:E:505:VAL:HG12	1:E:506:GLU:H	1.55	0.70
1:D:563:LYS:HG2	1:D:585:GLU:HB3	1.74	0.70
1:D:487:ARG:HG3	1:D:487:ARG:NH1	2.02	0.70
1:D:431:GLY:HA2	1:D:533:MET:O	1.91	0.70
1:F:480:ILE:CD1	1:F:592:ILE:HG21	2.22	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:431:GLY:HA2	1:E:513:SER:OG	1.92	0.70
1:F:591:ARG:O	1:F:594:GLU:HB2	1.92	0.69
1:D:542:GLU:OE2	1:D:591:ARG:HG2	1.93	0.69
1:B:544:LEU:HB3	1:B:545:PRO:CD	2.22	0.69
1:B:508:ASP:HB2	1:B:511:SER:HB2	1.73	0.69
1:E:512:ILE:O	1:E:513:SER:C	2.31	0.69
1:E:450:THR:O	1:E:492:MET:HA	1.92	0.69
1:A:445:ILE:HD11	2:A:637:HOH:O	1.92	0.69
1:B:525:ILE:CG2	1:B:526:PRO:HD2	2.23	0.69
1:A:420:ILE:HD11	1:A:428:ARG:NH2	2.07	0.68
1:A:417:LYS:HB3	2:A:690:HOH:O	1.91	0.68
1:E:553:ILE:CD1	1:E:574:VAL:HG13	2.22	0.68
1:A:440:GLY:HA3	1:A:555:ALA:HB2	1.74	0.68
1:B:558:GLN:C	1:B:560:GLY:N	2.46	0.68
1:D:549:VAL:O	1:D:553:ILE:HG13	1.94	0.68
1:F:437:GLU:HA	1:F:437:GLU:OE2	1.94	0.68
1:B:435:ILE:CG2	1:B:503:GLU:O	2.42	0.68
1:E:553:ILE:HD12	1:E:574:VAL:HG13	1.76	0.68
1:B:470:ALA:HA	1:B:514:ILE:HD13	1.75	0.67
1:A:485:THR:HG23	1:A:485:THR:O	1.94	0.67
1:C:463:THR:CG2	1:D:469:ILE:HD11	2.25	0.67
1:B:418:LEU:HD13	1:C:545:PRO:O	1.93	0.67
1:E:481:ILE:HB	2:E:675:HOH:O	1.94	0.67
1:F:434:VAL:HB	1:F:439:ALA:O	1.95	0.67
1:D:429:VAL:HG22	1:D:527:VAL:HG11	1.76	0.67
1:D:435:ILE:HD11	1:D:439:ALA:HB3	1.77	0.67
1:A:532:ALA:O	1:A:564:VAL:HA	1.95	0.67
1:E:422:GLU:OE1	1:E:423:GLY:N	2.27	0.67
1:A:440:GLY:C	1:A:555:ALA:HB2	2.15	0.67
1:D:514:ILE:CG2	2:D:714:HOH:O	2.42	0.67
1:B:551:GLN:H	1:B:551:GLN:CD	1.98	0.67
1:C:472:GLU:OE1	1:C:509:SER:HB3	1.95	0.67
1:B:577:ASP:CG	1:B:580:HIS:CE1	2.68	0.67
1:E:460:VAL:HB	1:E:471:ARG:HG2	1.76	0.67
1:E:571:ILE:O	1:E:574:VAL:HG23	1.95	0.67
1:A:545:PRO:HG2	1:F:499:VAL:HG13	1.74	0.66
1:F:432:LEU:HB3	1:F:552:LYS:HG2	1.77	0.66
1:B:479:ALA:HA	1:B:482:LYS:HE3	1.76	0.66
1:F:462:ALA:HB2	1:F:496:ILE:HB	1.77	0.66
1:C:578:ALA:O	1:C:579:GLU:HB3	1.94	0.66
1:D:421:THR:HG22	1:D:561:LEU:HD21	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:532:ALA:O	1:D:565:ILE:N	2.24	0.66
1:C:482:LYS:HD3	1:C:488:ASP:HB2	1.78	0.66
1:A:581:GLU:O	1:A:583:LYS:HG3	1.96	0.66
1:D:563:LYS:CD	1:D:563:LYS:NZ	2.59	0.66
1:E:453:MET:HG3	1:F:482:LYS:HE2	1.76	0.66
1:B:435:ILE:HD11	1:B:441:ILE:CG2	2.26	0.66
1:F:535:GLY:HA2	1:F:546:VAL:HG11	1.76	0.66
1:A:478:SER:CB	1:A:489:ILE:HD12	2.26	0.66
1:B:568:LYS:HD2	1:B:569:ASP:H	1.61	0.66
1:B:596:LEU:HD13	1:B:609:LEU:HD21	1.78	0.66
1:C:445:ILE:CB	1:C:445:ILE:CD1	2.71	0.66
1:C:424:TYR:HA	1:C:527:VAL:O	1.96	0.65
1:D:519:ILE:HD13	1:D:596:LEU:HD11	1.79	0.65
1:E:491:ASN:HB3	1:E:492:MET:CE	2.26	0.65
1:F:489:ILE:HD13	1:F:489:ILE:N	2.10	0.65
1:F:492:MET:HE2	1:F:522:ILE:HG12	1.79	0.65
1:F:566:ILE:CD1	1:F:586:VAL:HG11	2.26	0.65
1:B:577:ASP:OD1	1:B:580:HIS:CE1	2.48	0.65
1:B:557:ILE:O	1:B:560:GLY:HA2	1.97	0.65
1:C:418:LEU:HD12	1:D:545:PRO:HB2	1.78	0.65
1:E:605:LYS:O	1:E:609:LEU:N	2.27	0.65
1:F:530:SER:HB2	1:F:562:LYS:HG3	1.77	0.65
1:B:545:PRO:HA	1:B:567:PRO:HG2	1.77	0.65
1:E:491:ASN:HB3	1:E:492:MET:HE3	1.78	0.65
1:B:487:ARG:CG	1:B:487:ARG:NH1	2.34	0.65
1:E:551:GLN:N	1:E:551:GLN:CD	2.49	0.65
1:D:467:GLN:HG3	1:D:471:ARG:NH2	2.12	0.65
1:A:485:THR:O	1:A:485:THR:CG2	2.43	0.64
1:E:433:ALA:HB3	1:E:441:ILE:CG1	2.26	0.64
1:B:464:GLY:O	1:B:467:GLN:HG2	1.98	0.64
1:B:556:ALA:HA	1:B:559:ALA:HB3	1.77	0.64
1:B:478:SER:HB2	1:B:489:ILE:HG12	1.80	0.64
1:F:477:VAL:CG2	1:F:515:ALA:HB1	2.27	0.64
1:A:566:ILE:HD11	1:A:571:ILE:HD12	1.80	0.64
1:D:424:TYR:HA	1:D:527:VAL:O	1.97	0.64
1:D:465:ARG:HD2	1:D:465:ARG:N	2.10	0.64
1:F:477:VAL:HG13	1:F:481:ILE:HD12	1.80	0.64
1:A:440:GLY:CA	1:A:555:ALA:HB2	2.28	0.63
1:C:489:ILE:C	1:C:491:ASN:N	2.51	0.63
1:D:548:GLY:O	1:D:552:LYS:HG3	1.98	0.63
1:B:477:VAL:HG21	1:B:515:ALA:HB1	1.78	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:537:LEU:HD12	1:C:542:GLU:O	1.98	0.63
1:D:568:LYS:HE3	2:D:669:HOH:O	1.97	0.63
1:E:489:ILE:HG22	1:E:492:MET:SD	2.39	0.63
1:B:580:HIS:O	1:B:583:LYS:HB2	1.99	0.63
1:A:581:GLU:C	1:A:583:LYS:H	2.01	0.63
1:B:431:GLY:CA	1:B:513:SER:HB3	2.28	0.63
1:F:488:ASP:HB3	1:F:491:ASN:ND2	2.14	0.63
1:B:483:LYS:HG3	1:B:484:TYR:N	2.15	0.62
1:D:514:ILE:HG23	2:D:714:HOH:O	1.97	0.62
1:B:492:MET:HE3	1:B:522:ILE:CD1	2.27	0.62
1:C:446:ILE:HD11	1:C:499:VAL:HG21	1.72	0.62
1:C:463:THR:CG2	1:C:464:GLY:N	2.61	0.62
1:D:531:VAL:HA	1:D:531:VAL:N	2.01	0.62
1:A:549:VAL:O	1:A:550:THR:C	2.37	0.62
1:B:489:ILE:HA	1:B:492:MET:HE2	1.81	0.62
1:D:465:ARG:NE	1:D:503:GLU:OE2	2.32	0.62
1:B:477:VAL:O	1:B:481:ILE:HD12	2.00	0.62
1:C:550:THR:O	1:C:554:GLU:HG3	1.99	0.62
1:D:562:LYS:HG3	1:D:562:LYS:HZ3	1.63	0.62
1:A:577:ASP:O	1:A:580:HIS:N	2.33	0.62
1:D:551:GLN:CD	1:D:551:GLN:H	2.03	0.62
1:B:467:GLN:HG3	2:B:629:HOH:O	2.00	0.61
1:B:580:HIS:HA	1:B:583:LYS:HB2	1.80	0.61
1:B:432:LEU:HB2	1:B:552:LYS:HD3	1.83	0.61
1:B:480:ILE:CD1	1:B:592:ILE:HG21	2.31	0.61
1:C:578:ALA:HA	1:C:581:GLU:OE1	2.01	0.61
1:E:523:GLU:O	1:E:525:ILE:HG13	2.00	0.61
1:A:474:VAL:HA	1:A:477:VAL:HG12	1.81	0.61
1:C:514:ILE:O	1:C:518:VAL:HG23	2.01	0.61
1:B:445:ILE:HD11	2:B:626:HOH:O	2.00	0.61
1:A:532:ALA:HB3	1:A:564:VAL:HB	1.83	0.61
1:B:553:ILE:O	1:B:556:ALA:HB3	2.00	0.61
1:F:435:ILE:CG2	1:F:505:VAL:HG22	2.27	0.61
1:A:548:GLY:O	1:A:552:LYS:HG3	2.00	0.60
1:E:420:ILE:H	1:E:428:ARG:HH21	1.49	0.60
1:B:503:GLU:OE1	1:B:503:GLU:HA	2.00	0.60
1:B:557:ILE:HD13	1:B:583:LYS:HB3	1.82	0.60
1:E:435:ILE:HB	2:E:642:HOH:O	2.00	0.60
1:E:435:ILE:HG23	1:E:439:ALA:O	2.01	0.60
1:A:425:GLU:H	1:A:527:VAL:H	1.48	0.60
1:C:467:GLN:O	1:C:470:ALA:HB3	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:428:ARG:HB2	1:A:529:GLN:OE1	2.00	0.60
1:E:494:VAL:HG12	1:E:496:ILE:CD1	2.29	0.60
1:F:467:GLN:CD	1:F:471:ARG:HH22	2.04	0.60
1:B:448:GLU:HB3	1:C:539:VAL:HG23	1.83	0.60
1:B:431:GLY:HA3	1:B:513:SER:CB	2.31	0.59
1:C:433:ALA:HB3	1:C:441:ILE:HD11	1.84	0.59
1:C:485:THR:OG1	1:C:486:GLY:N	2.35	0.59
1:B:557:ILE:HD12	1:B:580:HIS:HB3	1.84	0.59
1:C:578:ALA:O	1:C:579:GLU:CB	2.50	0.59
1:D:578:ALA:O	1:D:579:GLU:CB	2.48	0.59
1:A:512:ILE:HG12	1:A:535:GLY:N	2.16	0.59
1:B:438:SER:O	1:B:551:GLN:HG2	2.02	0.59
1:B:495:HIS:CD2	1:C:479:ALA:HB2	2.38	0.59
1:A:477:VAL:HG22	1:A:477:VAL:O	2.02	0.59
1:B:481:ILE:HG22	1:B:487:ARG:CB	2.24	0.59
1:D:489:ILE:HG21	1:D:522:ILE:HD13	1.84	0.59
1:E:451:PRO:HA	1:E:492:MET:HG3	1.85	0.59
1:C:554:GLU:HB3	2:C:706:HOH:O	2.01	0.59
1:E:432:LEU:HB2	1:E:552:LYS:HD3	1.84	0.59
1:F:477:VAL:HG23	1:F:515:ALA:HB1	1.85	0.59
1:A:427:GLY:O	1:A:446:ILE:HA	2.03	0.59
1:C:497:GLN:OE1	1:D:509:SER:HB3	2.02	0.59
1:E:453:MET:CG	1:F:482:LYS:CD	2.70	0.59
1:D:457:GLU:HG3	1:D:490:SER:O	2.03	0.59
1:F:535:GLY:HA2	1:F:546:VAL:CG1	2.33	0.58
1:B:418:LEU:HD12	2:B:693:HOH:O	2.03	0.58
1:B:445:ILE:HD12	1:B:498:PHE:CD1	2.38	0.58
1:B:564:VAL:HG12	1:B:584:ILE:HG12	1.83	0.58
1:C:549:VAL:HG21	1:C:570:ASN:HB3	1.84	0.58
1:A:472:GLU:HG2	1:A:510:ALA:HB2	1.85	0.58
1:B:558:GLN:C	1:B:560:GLY:H	2.05	0.58
1:B:580:HIS:CA	1:B:583:LYS:HB2	2.34	0.58
1:C:445:ILE:CD1	1:C:445:ILE:CG2	2.81	0.58
1:F:591:ARG:HD2	2:F:691:HOH:O	2.01	0.58
1:C:463:THR:HG21	1:D:469:ILE:HD11	1.85	0.58
1:C:571:ILE:HD11	1:C:588:PRO:HG3	1.85	0.58
1:E:453:MET:CG	1:F:482:LYS:CE	2.78	0.58
1:B:481:ILE:CG2	1:B:487:ARG:HB2	2.27	0.58
1:B:539:VAL:C	1:B:541:GLY:H	2.07	0.58
1:C:489:ILE:O	1:C:491:ASN:N	2.36	0.58
1:E:487:ARG:NH1	1:E:487:ARG:HB3	2.16	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:446:ILE:CD1	1:C:499:VAL:HG21	2.30	0.58
1:B:429:VAL:HG11	1:B:513:SER:HA	1.84	0.58
1:B:478:SER:O	1:B:482:LYS:HG3	2.03	0.58
1:F:435:ILE:CG1	1:F:439:ALA:CB	2.79	0.58
1:D:552:LYS:C	1:D:554:GLU:N	2.57	0.58
1:A:512:ILE:HG12	1:A:535:GLY:H	1.70	0.57
1:C:549:VAL:CG1	1:C:574:VAL:HG22	2.34	0.57
1:D:543:VAL:HB	1:D:590:SER:HA	1.85	0.57
1:F:427:GLY:O	1:F:446:ILE:HA	2.04	0.57
1:A:538:SER:OG	1:A:542:GLU:HB2	2.03	0.57
1:C:445:ILE:C	1:C:446:ILE:HD13	2.24	0.57
1:E:450:THR:O	1:E:493:ASP:N	2.34	0.57
1:C:438:SER:OG	1:C:551:GLN:CD	2.43	0.57
1:D:531:VAL:O	1:D:532:ALA:N	2.32	0.57
1:C:606:LYS:C	1:C:608:ARG:N	2.55	0.57
1:F:611:SER:O	1:F:614:LYS:HB3	2.05	0.57
1:A:568:LYS:CB	1:A:588:PRO:CB	2.78	0.57
1:B:494:VAL:HG12	1:B:496:ILE:HD11	1.84	0.57
1:D:452:SER:O	1:D:453:MET:SD	2.62	0.57
1:F:473:ALA:HB2	2:F:657:HOH:O	2.04	0.57
1:D:537:LEU:CG	1:D:538:SER:H	2.13	0.57
1:E:595:VAL:O	1:E:599:VAL:HG22	2.05	0.57
1:B:445:ILE:HD12	1:B:498:PHE:HD1	1.68	0.57
1:B:555:ALA:O	1:B:559:ALA:HB2	2.04	0.57
1:A:485:THR:HG22	1:A:487:ARG:H	1.69	0.57
1:B:451:PRO:HA	1:B:491:ASN:O	2.05	0.57
1:E:451:PRO:O	1:E:452:SER:C	2.43	0.57
1:C:489:ILE:HD12	1:C:492:MET:CE	2.35	0.56
1:E:459:ARG:CG	1:E:459:ARG:HH11	2.16	0.56
1:C:549:VAL:HG12	1:C:550:THR:N	2.20	0.56
1:C:608:ARG:NH2	1:C:612:LYS:HE3	2.20	0.56
1:D:564:VAL:CG2	1:D:565:ILE:N	2.67	0.56
1:E:420:ILE:H	1:E:428:ARG:NH2	2.03	0.56
1:B:431:GLY:HA3	1:B:513:SER:OG	2.04	0.56
1:B:593:ASN:O	1:B:597:GLU:HB2	2.05	0.56
1:D:487:ARG:NH1	1:D:487:ARG:CG	2.62	0.56
1:A:420:ILE:HD11	1:A:428:ARG:CZ	2.35	0.56
1:A:568:LYS:O	1:A:571:ILE:HG12	2.04	0.56
1:A:449:VAL:N	1:B:540:LYS:HZ1	2.02	0.56
1:D:489:ILE:HG22	1:D:492:MET:SD	2.46	0.56
1:F:492:MET:HE1	1:F:522:ILE:HG12	1.85	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:418:LEU:HD13	1:A:500:GLY:HA2	1.88	0.56
1:A:557:ILE:HG21	1:A:580:HIS:HD2	1.70	0.56
1:D:470:ALA:O	1:D:474:VAL:HG23	2.05	0.56
1:E:457:GLU:HG3	2:E:672:HOH:O	2.06	0.56
1:E:470:ALA:HA	1:E:514:ILE:HD13	1.87	0.56
1:F:588:PRO:C	1:F:589:VAL:CG1	2.74	0.56
1:A:441:ILE:HA	1:A:555:ALA:HB1	1.87	0.56
1:D:591:ARG:HB3	1:D:593:ASN:OD1	2.06	0.56
1:F:485:THR:OG1	1:F:609:LEU:HD11	2.05	0.56
1:A:446:ILE:O	1:A:446:ILE:HD13	2.06	0.56
1:A:566:ILE:HD11	1:A:571:ILE:CD1	2.35	0.56
1:B:428:ARG:HG3	1:B:445:ILE:O	2.06	0.56
1:C:480:ILE:HG21	2:C:707:HOH:O	2.06	0.56
1:D:563:LYS:HD3	1:D:563:LYS:NZ	2.21	0.56
1:B:500:GLY:HA2	2:B:693:HOH:O	2.06	0.56
1:D:570:ASN:ND2	1:D:573:ASP:OD2	2.34	0.56
1:A:419:PHE:HB3	1:A:444:PRO:HG3	1.88	0.55
1:B:495:HIS:NE2	1:C:479:ALA:HB2	2.21	0.55
1:E:563:LYS:HD3	1:E:587:ILE:HD11	1.87	0.55
1:F:588:PRO:C	1:F:589:VAL:HG13	2.26	0.55
1:A:539:VAL:HG13	1:F:448:GLU:CD	2.27	0.55
1:C:572:ASP:OD1	1:C:572:ASP:N	2.38	0.55
1:E:433:ALA:HB3	1:E:441:ILE:HG13	1.89	0.55
1:F:417:LYS:HD2	1:F:419:PHE:CE1	2.42	0.55
1:F:578:ALA:HA	1:F:581:GLU:OE1	2.06	0.55
1:B:431:GLY:CA	1:B:513:SER:CB	2.83	0.55
1:A:526:PRO:HD2	1:A:601:GLU:HB3	1.89	0.55
1:D:435:ILE:CG2	1:D:505:VAL:HG22	2.37	0.55
1:D:508:ASP:HB3	1:D:546:VAL:HG11	1.88	0.55
1:F:477:VAL:HG22	1:F:481:ILE:HG13	1.89	0.55
1:B:563:LYS:CD	1:B:587:ILE:HD11	2.22	0.55
1:C:446:ILE:N	1:C:446:ILE:CD1	2.67	0.55
1:C:611:SER:O	1:C:614:LYS:HE2	2.07	0.55
1:E:485:THR:HG21	1:E:523:GLU:OE2	2.07	0.55
1:E:545:PRO:HG3	1:E:569:ASP:HB2	1.89	0.55
1:A:568:LYS:HD3	1:A:569:ASP:N	2.23	0.54
1:D:533:MET:HG3	1:D:534:THR:N	2.20	0.54
1:E:558:GLN:NE2	1:E:580:HIS:HE1	2.05	0.54
1:F:452:SER:HA	1:F:493:ASP:OD2	2.07	0.54
1:E:433:ALA:HB3	1:E:441:ILE:HG12	1.88	0.54
1:E:587:ILE:HG22	1:E:589:VAL:HG13	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:470:ALA:O	1:A:473:ALA:HB3	2.08	0.54
1:B:525:ILE:HD13	1:B:600:LEU:HD13	1.88	0.54
1:B:580:HIS:C	1:B:583:LYS:HB2	2.27	0.54
1:E:492:MET:HG2	2:E:654:HOH:O	2.07	0.54
1:A:545:PRO:HG2	1:F:499:VAL:CG1	2.38	0.54
1:B:537:LEU:CD1	1:B:592:ILE:HB	2.36	0.54
1:D:421:THR:HG22	1:D:561:LEU:CD2	2.37	0.54
1:C:472:GLU:O	1:C:476:ASN:N	2.41	0.54
1:B:418:LEU:HD23	1:B:418:LEU:N	2.23	0.54
1:C:438:SER:HA	1:C:551:GLN:OE1	2.07	0.54
1:B:558:GLN:O	1:B:560:GLY:N	2.40	0.54
1:B:566:ILE:O	1:B:589:VAL:HG22	2.08	0.54
1:D:474:VAL:HA	1:D:477:VAL:HG12	1.89	0.54
1:E:463:THR:HG21	1:F:472:GLU:HB2	1.90	0.54
1:E:518:VAL:O	1:E:519:ILE:C	2.44	0.53
1:A:544:LEU:HB3	1:A:545:PRO:CD	2.22	0.53
1:B:544:LEU:CB	1:B:545:PRO:CD	2.85	0.53
1:A:596:LEU:HB3	1:A:600:LEU:CD1	2.39	0.53
1:B:432:LEU:HD23	1:B:442:VAL:HG22	1.89	0.53
1:B:448:GLU:OE2	1:B:449:VAL:N	2.42	0.53
1:B:531:VAL:HG11	1:B:565:ILE:CD1	2.38	0.53
1:D:421:THR:O	1:D:530:SER:HA	2.09	0.53
1:B:427:GLY:O	1:B:446:ILE:HA	2.08	0.53
1:B:481:ILE:HG23	1:B:485:THR:HG1	1.65	0.53
1:B:566:ILE:HD13	1:B:586:VAL:HG13	1.91	0.53
1:D:489:ILE:HD13	1:D:522:ILE:HD11	1.90	0.53
1:F:428:ARG:O	1:F:529:GLN:NE2	2.32	0.53
1:B:589:VAL:HB	1:B:594:GLU:HB2	1.90	0.53
1:B:453:MET:HB2	1:C:482:LYS:HE2	1.90	0.53
1:B:478:SER:HA	1:B:489:ILE:HG21	1.90	0.53
1:C:427:GLY:O	1:C:446:ILE:HA	2.08	0.53
1:C:608:ARG:CD	1:C:608:ARG:C	2.75	0.53
1:F:579:GLU:O	1:F:580:HIS:CB	2.54	0.53
1:B:423:GLY:O	1:B:529:GLN:HG2	2.07	0.53
1:B:512:ILE:O	1:B:513:SER:C	2.46	0.53
1:C:465:ARG:HB3	1:C:465:ARG:NH1	2.23	0.53
1:D:562:LYS:HZ2	1:D:562:LYS:CG	2.22	0.53
1:D:463:THR:HA	1:D:467:GLN:NE2	2.24	0.52
1:D:508:ASP:HB3	1:D:546:VAL:CG1	2.39	0.52
1:E:526:PRO:HG2	1:E:601:GLU:OE1	2.09	0.52
1:A:475:MET:HE1	1:F:459:ARG:HH22	1.73	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:424:TYR:CD1	1:B:601:GLU:HB2	2.44	0.52
1:A:544:LEU:CB	1:A:545:PRO:CD	2.76	0.52
1:B:558:GLN:O	1:B:559:ALA:C	2.48	0.52
1:F:523:GLU:O	1:F:525:ILE:HG13	2.09	0.52
1:C:433:ALA:HB3	1:C:441:ILE:CD1	2.40	0.52
1:E:482:LYS:HG3	1:E:488:ASP:HB2	1.91	0.52
1:A:565:ILE:HA	1:A:587:ILE:O	2.10	0.52
1:C:479:ALA:O	1:C:483:LYS:N	2.36	0.52
1:B:608:ARG:O	1:B:612:LYS:HE2	2.09	0.52
1:A:446:ILE:HD11	1:A:448:GLU:OE1	2.10	0.52
1:C:501:THR:HG22	2:D:638:HOH:O	2.09	0.52
1:F:418:LEU:O	1:F:499:VAL:HG11	2.10	0.52
1:F:428:ARG:CD	1:F:446:ILE:HG23	2.19	0.52
1:B:429:VAL:HG21	1:B:517:ALA:N	2.24	0.52
1:C:532:ALA:O	1:C:564:VAL:HA	2.09	0.52
1:B:563:LYS:HB3	1:B:587:ILE:HD12	1.91	0.51
1:D:480:ILE:HD13	1:D:592:ILE:HG21	1.91	0.51
1:E:520:SER:O	1:E:521:ALA:C	2.46	0.51
1:A:498:PHE:N	1:A:498:PHE:CD2	2.78	0.51
1:B:435:ILE:HD11	1:B:441:ILE:HG21	1.91	0.51
1:D:435:ILE:HG22	1:D:505:VAL:HG22	1.92	0.51
1:E:478:SER:HB3	1:E:482:LYS:HE3	1.92	0.51
1:A:570:ASN:HA	1:A:573:ASP:OD2	2.11	0.51
1:B:577:ASP:OD1	1:B:579:GLU:N	2.44	0.51
1:C:445:ILE:HG21	1:C:445:ILE:CD1	2.40	0.51
1:B:556:ALA:HA	1:B:559:ALA:CB	2.41	0.51
1:C:472:GLU:CG	1:C:473:ALA:N	2.71	0.51
1:F:488:ASP:OD1	1:F:489:ILE:HD13	2.11	0.51
1:A:467:GLN:CG	1:A:471:ARG:HH12	2.21	0.51
1:A:501:THR:HG23	2:A:634:HOH:O	2.09	0.51
1:A:543:VAL:N	1:A:590:SER:O	2.24	0.51
1:D:530:SER:C	1:D:531:VAL:CA	2.69	0.51
1:D:534:THR:HG23	1:D:567:PRO:HD3	1.92	0.51
1:D:532:ALA:O	1:D:564:VAL:HA	2.11	0.51
1:F:604:LYS:HD3	2:F:689:HOH:O	2.11	0.51
1:A:596:LEU:HB3	1:A:600:LEU:HG	1.92	0.51
1:B:557:ILE:CD1	1:B:580:HIS:HB3	2.41	0.51
1:A:573:ASP:OD2	1:F:417:LYS:N	2.44	0.51
1:A:475:MET:SD	1:F:461:ILE:CD1	2.99	0.51
1:A:563:LYS:HG2	1:A:585:GLU:CB	2.36	0.51
1:D:518:VAL:HG23	2:D:714:HOH:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:563:LYS:HD3	1:E:587:ILE:CD1	2.40	0.51
1:A:577:ASP:O	1:A:578:ALA:C	2.48	0.51
1:D:420:ILE:CG2	1:D:421:THR:N	2.74	0.51
1:C:428:ARG:HD2	1:C:446:ILE:HG23	1.93	0.51
1:E:459:ARG:CG	1:E:459:ARG:NH1	2.73	0.51
1:B:480:ILE:HD12	1:B:613:PHE:HE1	1.76	0.50
1:C:606:LYS:C	1:C:608:ARG:H	2.13	0.50
1:E:585:GLU:HG3	1:E:587:ILE:CD1	2.35	0.50
1:F:597:GLU:HB3	2:F:686:HOH:O	2.11	0.50
1:D:514:ILE:HG22	2:D:714:HOH:O	2.07	0.50
1:B:425:GLU:O	1:B:527:VAL:HB	2.11	0.50
1:F:478:SER:O	1:F:479:ALA:C	2.46	0.50
1:B:474:VAL:HG22	1:B:518:VAL:HG21	1.92	0.50
1:B:531:VAL:HG11	1:B:565:ILE:HG13	1.93	0.50
1:F:485:THR:OG1	1:F:486:GLY:N	2.43	0.50
1:B:479:ALA:HA	1:B:482:LYS:CE	2.41	0.50
1:B:601:GLU:HG3	2:B:659:HOH:O	2.11	0.50
1:D:563:LYS:HG2	1:D:585:GLU:CB	2.40	0.50
1:F:447:ALA:HA	1:F:495:HIS:O	2.11	0.50
1:B:434:VAL:HG12	1:B:439:ALA:O	2.11	0.50
1:C:477:VAL:HG22	1:C:481:ILE:HG13	1.93	0.50
1:D:435:ILE:CD1	1:D:439:ALA:HB3	2.42	0.50
1:D:595:VAL:O	1:D:599:VAL:HG22	2.11	0.50
1:B:451:PRO:HD3	1:B:492:MET:HG2	1.94	0.50
1:A:475:MET:CE	1:F:459:ARG:HH22	2.25	0.50
1:A:592:ILE:O	1:A:592:ILE:HG13	2.11	0.50
1:B:544:LEU:HB3	1:B:545:PRO:HD2	1.94	0.50
1:C:469:ILE:CG2	1:C:508:ASP:O	2.60	0.50
1:C:473:ALA:O	1:C:477:VAL:HG12	2.12	0.50
1:C:483:LYS:CD	1:C:483:LYS:CB	2.82	0.50
1:D:480:ILE:CD1	1:D:592:ILE:HG21	2.42	0.50
1:B:534:THR:OG1	1:B:546:VAL:HG21	2.12	0.49
1:A:448:GLU:CD	1:B:539:VAL:HG22	2.32	0.49
1:B:609:LEU:HD11	1:B:613:PHE:HE2	1.77	0.49
1:C:499:VAL:HG13	1:D:545:PRO:HG2	1.92	0.49
1:E:432:LEU:CB	1:E:552:LYS:HD3	2.42	0.49
1:F:424:TYR:C	1:F:425:GLU:HG2	2.26	0.49
1:B:550:THR:OG1	1:B:573:ASP:O	2.29	0.49
1:E:425:GLU:H	1:E:527:VAL:H	1.59	0.49
1:B:478:SER:CB	1:B:489:ILE:HG12	2.42	0.49
1:B:520:SER:OG	1:B:527:VAL:CG2	2.60	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:435:ILE:HG13	1:C:439:ALA:HB3	1.95	0.49
1:E:518:VAL:C	1:E:520:SER:N	2.63	0.49
1:C:489:ILE:HG22	1:C:490:SER:N	2.27	0.49
1:D:568:LYS:CB	1:D:588:PRO:HB2	2.42	0.49
1:E:486:GLY:HA2	2:E:644:HOH:O	2.12	0.49
1:E:579:GLU:O	1:E:583:LYS:NZ	2.32	0.49
1:F:566:ILE:O	1:F:588:PRO:HA	2.12	0.49
1:A:417:LYS:NZ	1:A:421:THR:HG23	2.26	0.49
1:A:484:TYR:O	1:A:612:LYS:HB3	2.12	0.49
1:B:489:ILE:HG13	1:B:490:SER:N	2.27	0.49
1:B:614:LYS:C	1:B:614:LYS:HD3	2.32	0.49
1:C:435:ILE:HG23	1:C:505:VAL:HG22	1.93	0.49
1:E:542:GLU:HB2	2:E:660:HOH:O	2.13	0.49
1:B:571:ILE:O	1:B:574:VAL:HG23	2.13	0.49
1:E:434:VAL:HA	1:E:439:ALA:O	2.12	0.49
1:F:477:VAL:HG21	1:F:515:ALA:HB1	1.94	0.49
1:F:568:LYS:N	1:F:589:VAL:O	2.42	0.49
1:F:488:ASP:HB3	1:F:491:ASN:HD21	1.77	0.49
1:B:480:ILE:HD12	1:B:613:PHE:CE1	2.47	0.49
1:B:551:GLN:H	1:B:551:GLN:NE2	2.09	0.49
1:F:467:GLN:HG3	1:F:471:ARG:NH2	2.28	0.49
1:A:435:ILE:HG23	1:A:505:VAL:HG22	1.95	0.48
1:B:420:ILE:O	1:B:421:THR:HG22	2.13	0.48
1:B:425:GLU:CB	1:B:529:GLN:NE2	2.72	0.48
1:E:475:MET:O	1:E:478:SER:HB2	2.13	0.48
1:E:419:PHE:HE1	1:E:559:ALA:HB1	1.78	0.48
1:F:516:THR:OG1	1:F:595:VAL:HG11	2.12	0.48
1:F:595:VAL:O	1:F:599:VAL:HG22	2.13	0.48
1:B:544:LEU:HB3	1:B:545:PRO:HD3	1.95	0.48
1:F:461:ILE:HD12	1:F:495:HIS:ND1	2.28	0.48
1:F:587:ILE:HG21	1:F:598:HIS:NE2	2.27	0.48
1:B:514:ILE:O	1:B:517:ALA:HB3	2.13	0.48
1:D:533:MET:HB2	1:D:565:ILE:HB	1.96	0.48
1:B:528:ASP:C	1:B:530:SER:H	2.17	0.48
1:C:445:ILE:HD12	1:C:514:ILE:HA	1.95	0.48
1:C:578:ALA:N	1:C:581:GLU:OE2	2.47	0.48
1:F:485:THR:HB	1:F:613:PHE:CE2	2.48	0.48
1:B:482:LYS:CG	2:B:667:HOH:O	2.56	0.48
1:D:551:GLN:CD	1:D:551:GLN:N	2.66	0.48
1:E:418:LEU:HD22	1:E:499:VAL:HG13	1.95	0.48
1:A:482:LYS:O	1:A:484:TYR:N	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:420:ILE:HG22	1:D:421:THR:N	2.29	0.48
1:E:450:THR:O	1:E:492:MET:CA	2.61	0.48
1:F:538:SER:HB2	2:F:630:HOH:O	2.14	0.48
1:F:571:ILE:HD11	1:F:588:PRO:HB2	1.95	0.48
1:A:443:LEU:HD21	1:A:466:LEU:HD13	1.96	0.48
1:B:417:LYS:HZ3	1:B:421:THR:CG2	2.27	0.48
1:C:463:THR:HG23	1:D:469:ILE:HD11	1.92	0.48
1:F:478:SER:O	1:F:479:ALA:O	2.32	0.48
1:F:562:LYS:CG	2:F:626:HOH:O	2.61	0.48
1:F:531:VAL:HA	1:F:563:LYS:O	2.13	0.48
1:C:419:PHE:HB3	1:C:444:PRO:HG3	1.95	0.48
1:B:601:GLU:HG2	1:B:602:ASP:N	2.28	0.48
1:A:549:VAL:O	1:A:552:LYS:N	2.47	0.47
1:F:432:LEU:HB2	1:F:534:THR:HB	1.95	0.47
1:F:578:ALA:C	1:F:579:GLU:O	2.52	0.47
1:A:429:VAL:HG21	1:A:513:SER:O	2.13	0.47
1:B:478:SER:OG	1:B:482:LYS:HD3	2.14	0.47
1:F:512:ILE:HG13	1:F:533:MET:HG3	1.96	0.47
1:A:428:ARG:CB	1:A:529:GLN:OE1	2.62	0.47
1:A:557:ILE:HG21	1:A:580:HIS:CD2	2.49	0.47
1:B:424:TYR:CA	1:B:527:VAL:O	2.47	0.47
1:B:553:ILE:HG23	1:B:564:VAL:CG1	2.35	0.47
1:B:419:PHE:CE1	1:B:559:ALA:HA	2.48	0.47
1:C:435:ILE:HG13	1:C:439:ALA:O	2.15	0.47
1:D:614:LYS:HB3	1:D:614:LYS:HE2	1.64	0.47
1:E:577:ASP:OD1	1:E:580:HIS:HB2	2.14	0.47
1:F:466:LEU:HB2	1:F:498:PHE:CD2	2.50	0.47
1:B:489:ILE:HA	1:B:492:MET:HE1	1.90	0.47
1:C:610:MET:HA	1:C:610:MET:CE	2.45	0.47
1:A:554:GLU:C	1:A:556:ALA:N	2.68	0.47
1:B:480:ILE:CD1	1:B:613:PHE:CE1	2.98	0.47
1:E:546:VAL:HG22	1:E:567:PRO:HG2	1.97	0.47
1:A:441:ILE:HD11	1:A:505:VAL:HG21	1.97	0.47
1:A:568:LYS:C	1:A:568:LYS:HD3	2.35	0.47
1:B:417:LYS:HE2	1:B:417:LYS:HB2	1.38	0.47
1:C:502:TYR:HD2	1:C:505:VAL:HG21	1.80	0.47
1:F:435:ILE:N	1:F:439:ALA:O	2.48	0.47
1:F:489:ILE:N	1:F:489:ILE:CD1	2.58	0.47
1:A:420:ILE:O	1:A:529:GLN:HB3	2.15	0.47
1:B:568:LYS:HE2	1:B:590:SER:OG	2.15	0.47
1:A:435:ILE:HG23	1:A:505:VAL:CG2	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:480:ILE:CD1	1:B:613:PHE:HE1	2.27	0.46
1:B:543:VAL:N	1:B:590:SER:O	2.43	0.46
1:D:513:SER:CB	2:D:657:HOH:O	2.63	0.46
1:B:468:GLU:HG2	2:B:629:HOH:O	2.15	0.46
1:A:447:ALA:O	1:A:521:ALA:HB2	2.14	0.46
1:C:571:ILE:HD13	1:C:571:ILE:HA	1.81	0.46
1:E:453:MET:SD	1:F:482:LYS:HD3	2.54	0.46
1:E:571:ILE:HG23	2:E:688:HOH:O	2.15	0.46
1:F:523:GLU:O	1:F:524:GLY:C	2.53	0.46
1:A:478:SER:C	1:A:480:ILE:N	2.68	0.46
1:D:533:MET:CG	1:D:534:THR:N	2.70	0.46
1:E:417:LYS:HB3	1:E:419:PHE:N	2.22	0.46
1:D:489:ILE:C	1:D:491:ASN:H	2.19	0.46
1:F:571:ILE:HD11	1:F:588:PRO:CB	2.45	0.46
1:C:489:ILE:HD12	1:C:492:MET:HE2	1.96	0.46
1:E:563:LYS:HB3	1:E:585:GLU:CB	2.30	0.46
1:F:419:PHE:CD2	1:F:419:PHE:N	2.84	0.46
1:A:417:LYS:HD3	2:A:690:HOH:O	2.15	0.46
1:C:435:ILE:O	1:C:436:GLY:C	2.54	0.46
1:E:576:LEU:HA	2:E:671:HOH:O	2.16	0.46
1:B:463:THR:HB	2:B:627:HOH:O	2.16	0.46
1:B:598:HIS:O	1:B:599:VAL:CG1	2.64	0.46
1:E:547:GLY:O	1:E:552:LYS:NZ	2.48	0.46
1:E:450:THR:CG2	1:F:482:LYS:NZ	2.79	0.46
1:A:444:PRO:HD2	1:A:502:TYR:OH	2.16	0.45
1:A:546:VAL:HG13	1:A:567:PRO:HG2	1.98	0.45
1:C:463:THR:HG23	1:C:464:GLY:H	1.79	0.45
1:F:609:LEU:HD12	1:F:609:LEU:HA	1.43	0.45
1:F:420:ILE:HD13	1:F:425:GLU:OE2	2.16	0.45
1:A:444:PRO:HB2	1:A:499:VAL:HB	1.99	0.45
1:E:457:GLU:N	2:E:676:HOH:O	2.49	0.45
1:E:477:VAL:HG23	1:E:515:ALA:HB1	1.97	0.45
1:A:424:TYR:CD1	1:A:528:ASP:N	2.84	0.45
1:A:599:VAL:CG2	1:A:600:LEU:N	2.79	0.45
1:E:573:ASP:O	1:E:575:LEU:HD12	2.15	0.45
1:E:600:LEU:HB2	1:E:606:LYS:HZ2	1.81	0.45
1:B:426:VAL:CG1	1:B:427:GLY:H	2.29	0.45
1:C:478:SER:N	2:C:629:HOH:O	2.50	0.45
1:D:435:ILE:HG13	1:D:435:ILE:H	1.50	0.45
1:A:420:ILE:CD1	1:A:428:ARG:NH2	2.76	0.45
1:A:513:SER:HA	1:A:533:MET:SD	2.57	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:482:LYS:HD2	2:F:700:HOH:O	2.16	0.45
1:F:525:ILE:HA	1:F:526:PRO:HD3	1.81	0.45
1:B:510:ALA:O	1:B:511:SER:C	2.55	0.45
1:A:501:THR:HB	2:B:653:HOH:O	2.16	0.45
1:B:418:LEU:HD23	1:B:418:LEU:H	1.81	0.45
1:C:592:ILE:O	1:C:595:VAL:HB	2.17	0.45
1:B:449:VAL:HG21	1:B:522:ILE:HD12	1.99	0.45
1:A:571:ILE:HD11	1:A:588:PRO:HG3	1.98	0.45
1:B:531:VAL:HG13	1:B:563:LYS:HB2	1.98	0.45
1:C:463:THR:HG23	1:C:464:GLY:N	2.31	0.45
1:D:467:GLN:O	1:D:470:ALA:HB3	2.17	0.45
1:C:418:LEU:CD1	1:D:545:PRO:HB2	2.46	0.45
1:D:461:ILE:CD1	1:E:475:MET:SD	2.97	0.45
1:E:482:LYS:HD2	1:E:488:ASP:HA	1.98	0.45
1:E:545:PRO:HA	1:E:567:PRO:CG	2.46	0.45
1:E:563:LYS:HA	1:E:584:ILE:HG13	1.99	0.45
1:B:431:GLY:CA	1:B:533:MET:O	2.44	0.44
1:E:420:ILE:HG13	1:E:428:ARG:NE	2.31	0.44
1:F:477:VAL:CG2	1:F:515:ALA:CB	2.94	0.44
1:F:592:ILE:CG2	1:F:593:ASN:N	2.79	0.44
1:D:611:SER:O	1:D:614:LYS:HE2	2.17	0.44
1:E:603:GLY:O	1:E:607:ASN:ND2	2.50	0.44
1:F:418:LEU:HB3	1:F:499:VAL:HG12	1.98	0.44
1:F:523:GLU:HB2	1:F:525:ILE:HD12	2.00	0.44
1:A:518:VAL:O	1:A:519:ILE:C	2.56	0.44
1:B:502:TYR:C	1:B:503:GLU:O	2.55	0.44
1:E:417:LYS:N	1:E:417:LYS:HD2	2.31	0.44
1:D:564:VAL:HG22	1:D:565:ILE:N	2.27	0.44
1:D:583:LYS:HB2	1:D:583:LYS:HE3	1.67	0.44
1:E:601:GLU:HG2	2:E:690:HOH:O	2.16	0.44
1:A:592:ILE:C	1:A:594:GLU:N	2.64	0.44
1:B:611:SER:HA	1:B:614:LYS:HD3	2.00	0.44
1:C:537:LEU:HG	1:C:538:SER:N	2.33	0.44
1:D:563:LYS:HD3	1:D:563:LYS:HZ2	1.82	0.44
1:B:505:VAL:CG1	1:B:506:GLU:N	2.80	0.44
1:C:499:VAL:CG1	1:D:545:PRO:HG2	2.48	0.44
1:E:505:VAL:HG12	1:E:506:GLU:N	2.27	0.44
1:F:452:SER:O	1:F:453:MET:HG2	2.17	0.44
1:F:478:SER:HA	1:F:481:ILE:CB	2.34	0.44
1:A:580:HIS:C	1:A:581:GLU:O	2.55	0.44
1:B:554:GLU:C	1:B:556:ALA:N	2.69	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:489:ILE:HD12	1:C:492:MET:HE1	1.99	0.44
1:F:608:ARG:C	1:F:612:LYS:HZ2	2.21	0.44
1:A:472:GLU:HG3	2:A:626:HOH:O	2.18	0.44
1:D:432:LEU:HD21	1:D:532:ALA:HB1	2.00	0.44
1:F:432:LEU:HA	1:F:432:LEU:HD23	1.67	0.44
1:F:576:LEU:HA	1:F:576:LEU:HD23	1.89	0.44
1:E:545:PRO:HA	1:E:567:PRO:CB	2.47	0.43
1:F:562:LYS:HG2	2:F:626:HOH:O	2.17	0.43
1:F:581:GLU:H	1:F:581:GLU:CD	2.21	0.43
1:B:435:ILE:HG22	1:B:503:GLU:O	2.17	0.43
1:A:501:THR:HG22	1:B:547:GLY:H	1.82	0.43
1:D:565:ILE:HD13	1:D:565:ILE:HG21	1.54	0.43
1:B:418:LEU:CD2	1:B:418:LEU:N	2.81	0.43
1:D:440:GLY:O	1:D:441:ILE:HG23	2.18	0.43
1:F:474:VAL:O	1:F:477:VAL:HG12	2.18	0.43
1:A:426:VAL:CG1	1:A:524:GLY:HA2	2.48	0.43
1:A:468:GLU:O	1:A:469:ILE:C	2.54	0.43
1:B:430:ASN:HB3	1:B:442:VAL:CG1	2.48	0.43
1:C:469:ILE:HG21	1:C:508:ASP:O	2.19	0.43
1:D:476:ASN:ND2	1:D:537:LEU:O	2.44	0.43
1:E:550:THR:HB	1:E:551:GLN:OE1	2.19	0.43
1:A:571:ILE:HD11	1:A:588:PRO:HB3	2.01	0.43
1:F:466:LEU:HA	1:F:466:LEU:HD23	1.61	0.43
1:A:428:ARG:HD2	1:A:446:ILE:HB	2.00	0.43
1:A:512:ILE:HG13	1:A:513:SER:N	2.33	0.43
1:B:426:VAL:CG2	1:B:526:PRO:HA	2.49	0.43
1:B:550:THR:HB	1:B:551:GLN:NE2	2.33	0.43
1:C:463:THR:CG2	1:D:469:ILE:CD1	2.94	0.43
1:C:537:LEU:HD11	1:C:592:ILE:HB	2.01	0.43
1:E:477:VAL:CG1	1:E:478:SER:N	2.82	0.43
1:F:561:LEU:HA	2:F:626:HOH:O	2.17	0.43
1:A:554:GLU:HA	2:A:695:HOH:O	2.18	0.43
1:B:417:LYS:NZ	1:B:419:PHE:CE1	2.78	0.43
1:E:427:GLY:O	1:E:446:ILE:HA	2.19	0.43
1:A:526:PRO:HG2	1:A:601:GLU:OE1	2.18	0.43
1:B:580:HIS:O	1:B:583:LYS:CB	2.67	0.43
1:E:477:VAL:O	1:E:480:ILE:HB	2.19	0.43
1:F:467:GLN:OE1	1:F:471:ARG:NH2	2.41	0.43
1:F:467:GLN:CG	1:F:471:ARG:HH22	2.32	0.43
1:D:463:THR:HG22	1:E:468:GLU:HB3	2.00	0.42
1:A:601:GLU:O	1:A:606:LYS:HD2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:477:VAL:CG2	1:C:477:VAL:O	2.67	0.42
1:E:432:LEU:HD21	1:E:556:ALA:HB2	2.01	0.42
1:F:562:LYS:HG3	2:F:626:HOH:O	2.18	0.42
1:B:494:VAL:HG13	1:B:496:ILE:HD11	1.98	0.42
1:B:426:VAL:HG12	1:B:427:GLY:N	2.34	0.42
1:B:435:ILE:CG1	1:B:441:ILE:HG23	2.50	0.42
1:E:450:THR:HG21	1:F:482:LYS:NZ	2.35	0.42
1:B:420:ILE:HG22	1:B:421:THR:H	1.84	0.42
1:B:426:VAL:HG12	1:B:427:GLY:H	1.84	0.42
1:B:515:ALA:O	1:B:519:ILE:HG13	2.19	0.42
1:B:528:ASP:O	1:B:530:SER:N	2.52	0.42
1:B:565:ILE:HD11	1:B:599:VAL:HG13	2.00	0.42
1:E:539:VAL:C	1:E:541:GLY:H	2.22	0.42
1:E:551:GLN:HG3	2:E:641:HOH:O	2.19	0.42
1:E:533:MET:HB3	1:E:565:ILE:HB	2.02	0.42
1:F:444:PRO:HB2	1:F:499:VAL:HB	1.99	0.42
1:B:577:ASP:C	1:B:577:ASP:OD1	2.58	0.42
1:C:462:ALA:HB2	1:C:496:ILE:HB	2.02	0.42
1:C:473:ALA:HA	1:C:476:ASN:HD22	1.85	0.42
1:C:527:VAL:HG12	1:C:528:ASP:N	2.34	0.42
1:E:549:VAL:HG21	1:E:570:ASN:CG	2.40	0.42
1:F:548:GLY:O	1:F:551:GLN:HB2	2.20	0.42
1:A:440:GLY:C	1:A:555:ALA:CB	2.87	0.42
1:A:483:LYS:NZ	1:A:483:LYS:CD	2.71	0.42
1:A:432:LEU:HD13	1:A:552:LYS:HB3	2.02	0.42
1:B:429:VAL:HG23	1:B:517:ALA:HA	2.01	0.42
1:B:482:LYS:HA	1:B:487:ARG:O	2.19	0.42
1:B:532:ALA:HB2	1:B:561:LEU:HD13	2.00	0.42
1:C:581:GLU:OE2	1:C:581:GLU:N	2.53	0.42
1:E:438:SER:O	1:E:439:ALA:C	2.58	0.42
1:E:568:LYS:CE	1:E:569:ASP:OD1	2.67	0.42
1:F:447:ALA:O	1:F:521:ALA:HB2	2.19	0.42
1:F:608:ARG:HB3	1:F:608:ARG:HE	1.23	0.42
1:B:512:ILE:HG22	1:B:537:LEU:HB2	2.02	0.42
1:C:463:THR:HG21	1:D:469:ILE:CD1	2.50	0.42
1:C:606:LYS:HG2	1:C:610:MET:HG2	2.01	0.42
1:D:443:LEU:HD21	1:D:466:LEU:HD13	2.01	0.42
1:F:421:THR:HA	1:F:561:LEU:HD21	2.01	0.42
1:A:587:ILE:HA	1:A:588:PRO:HD3	1.91	0.42
1:E:514:ILE:O	1:E:518:VAL:HG23	2.19	0.42
1:E:528:ASP:HB3	1:E:531:VAL:HG23	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:440:GLY:C	1:B:555:ALA:HB2	2.40	0.42
1:C:587:ILE:HA	1:C:588:PRO:HD3	1.76	0.42
1:A:535:GLY:HA3	1:A:567:PRO:HG3	2.02	0.41
1:B:481:ILE:CG2	1:B:485:THR:HG1	2.26	0.41
1:B:512:ILE:CG2	1:B:537:LEU:HB2	2.50	0.41
1:C:483:LYS:O	1:C:483:LYS:HD2	2.19	0.41
1:D:498:PHE:N	1:D:498:PHE:CD2	2.88	0.41
1:E:574:VAL:HG12	1:E:576:LEU:HB2	2.01	0.41
1:F:466:LEU:CB	1:F:498:PHE:CE2	3.02	0.41
1:F:483:LYS:O	1:F:483:LYS:HG3	2.19	0.41
1:F:538:SER:OG	1:F:540:LYS:N	2.53	0.41
1:F:546:VAL:N	1:F:570:ASN:OD1	2.35	0.41
1:C:445:ILE:CG2	1:C:445:ILE:HD13	2.50	0.41
1:A:478:SER:HA	1:A:489:ILE:CD1	2.45	0.41
1:B:477:VAL:CG2	1:B:515:ALA:HB1	2.45	0.41
1:C:433:ALA:HB1	1:C:506:GLU:O	2.20	0.41
1:C:488:ASP:O	1:C:491:ASN:HB2	2.20	0.41
1:B:448:GLU:HB3	1:C:539:VAL:CG2	2.47	0.41
1:E:474:VAL:O	1:E:477:VAL:HG12	2.20	0.41
1:A:469:ILE:HA	1:A:469:ILE:HD12	1.70	0.41
1:A:516:THR:HG21	1:A:533:MET:HE1	2.03	0.41
1:A:549:VAL:H	1:A:549:VAL:HG23	1.60	0.41
1:C:445:ILE:HG21	1:C:445:ILE:HD13	2.02	0.41
1:E:463:THR:HG21	1:F:472:GLU:CB	2.50	0.41
1:A:484:TYR:CD1	1:A:613:PHE:HA	2.56	0.41
1:E:531:VAL:HG21	1:E:599:VAL:HG12	2.02	0.41
1:B:570:ASN:O	1:B:571:ILE:C	2.57	0.41
1:C:480:ILE:CG2	2:C:707:HOH:O	2.67	0.41
1:E:417:LYS:HG3	1:E:419:PHE:CE2	2.56	0.41
1:E:446:ILE:HG12	2:F:630:HOH:O	2.20	0.41
1:F:464:GLY:O	1:F:467:GLN:HB3	2.21	0.41
1:D:448:GLU:OE2	1:E:540:LYS:NZ	2.53	0.41
1:E:483:LYS:HE3	1:E:484:TYR:CZ	2.55	0.41
1:E:540:LYS:NZ	1:E:540:LYS:HB2	2.36	0.41
1:F:537:LEU:HD11	1:F:541:GLY:HA2	2.03	0.41
1:A:581:GLU:HB3	1:A:582:GLY:H	1.70	0.41
1:B:466:LEU:HG	1:B:466:LEU:H	1.68	0.41
1:B:531:VAL:HG12	1:B:565:ILE:HG13	2.00	0.41
1:B:448:GLU:HG2	1:C:539:VAL:O	2.20	0.41
1:C:608:ARG:CZ	1:C:612:LYS:HE3	2.51	0.41
1:D:542:GLU:HA	1:D:542:GLU:OE2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:609:LEU:HD11	1:B:613:PHE:CE2	2.56	0.41
1:D:463:THR:HB	1:D:464:GLY:H	1.67	0.41
1:D:528:ASP:OD2	1:D:531:VAL:HG23	2.21	0.41
1:D:596:LEU:O	1:D:600:LEU:HG	2.21	0.41
1:E:441:ILE:HD12	1:E:502:TYR:CE1	2.56	0.41
1:A:478:SER:O	1:A:479:ALA:C	2.58	0.41
1:B:442:VAL:HB	2:B:663:HOH:O	2.20	0.41
1:F:478:SER:CA	1:F:481:ILE:HB	2.35	0.41
1:F:538:SER:HG	1:F:541:GLY:N	2.18	0.41
1:F:592:ILE:HG23	1:F:593:ASN:N	2.35	0.41
1:A:482:LYS:O	1:A:483:LYS:C	2.59	0.41
1:A:581:GLU:C	1:A:583:LYS:N	2.65	0.41
1:B:531:VAL:HG11	1:B:565:ILE:HD11	2.03	0.41
1:C:511:SER:HB3	1:C:514:ILE:HB	2.03	0.41
1:C:563:LYS:HD3	1:C:587:ILE:HD11	2.02	0.41
1:E:545:PRO:HA	1:E:567:PRO:HG2	2.02	0.41
1:F:429:VAL:O	1:F:445:ILE:HG12	2.21	0.41
1:A:512:ILE:O	1:A:513:SER:C	2.59	0.40
1:B:427:GLY:HA3	1:B:447:ALA:O	2.21	0.40
1:B:512:ILE:C	1:B:514:ILE:N	2.75	0.40
1:C:467:GLN:HB2	1:C:471:ARG:CZ	2.51	0.40
1:C:476:ASN:O	1:C:476:ASN:CG	2.58	0.40
1:C:465:ARG:HD2	1:C:503:GLU:OE2	2.19	0.40
1:F:477:VAL:HG21	1:F:515:ALA:CB	2.51	0.40
1:A:558:GLN:CB	2:A:693:HOH:O	2.54	0.40
1:B:428:ARG:C	1:B:429:VAL:HG23	2.41	0.40
1:B:518:VAL:O	1:B:519:ILE:C	2.60	0.40
1:C:429:VAL:HG22	1:C:527:VAL:HG11	2.03	0.40
1:D:424:TYR:CD1	1:D:528:ASP:N	2.89	0.40
1:D:555:ALA:O	1:D:558:GLN:HB2	2.21	0.40
1:E:491:ASN:HB3	1:E:492:MET:HE2	2.01	0.40
1:F:429:VAL:CG1	1:F:430:ASN:N	2.83	0.40
1:C:445:ILE:HG12	1:C:445:ILE:H	1.59	0.40
1:C:482:LYS:O	1:C:485:THR:N	2.55	0.40
1:E:557:ILE:HG12	1:E:584:ILE:HG21	2.02	0.40
1:B:420:ILE:C	1:B:421:THR:CG2	2.90	0.40
1:B:469:ILE:HD13	1:B:508:ASP:O	2.22	0.40
1:B:609:LEU:CD1	1:B:613:PHE:HE2	2.35	0.40
1:D:549:VAL:H	1:D:549:VAL:HG23	1.48	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:486:GLY:O	1:F:578:ALA:CB[1_455]	1.65	0.55

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	191/205 (93%)	164 (86%)	16 (8%)	11 (6%)	1 10
1	B	191/205 (93%)	140 (73%)	35 (18%)	16 (8%)	1 4
1	C	190/205 (93%)	162 (85%)	18 (10%)	10 (5%)	2 11
1	D	191/205 (93%)	169 (88%)	16 (8%)	6 (3%)	4 23
1	E	191/205 (93%)	151 (79%)	35 (18%)	5 (3%)	5 27
1	F	191/205 (93%)	155 (81%)	25 (13%)	11 (6%)	1 10
All	All	1145/1230 (93%)	941 (82%)	145 (13%)	59 (5%)	2 12

All (59) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	486	GLY
1	A	549	VAL
1	A	578	ALA
1	A	581	GLU
1	A	582	GLY
1	B	559	ALA
1	B	569	ASP
1	B	586	VAL
1	C	439	ALA
1	C	465	ARG
1	C	549	VAL
1	C	578	ALA
1	C	579	GLU
1	F	476	ASN
1	F	477	VAL

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Mol	Chain	Res	Type
1	F	486	GLY
1	F	579	GLU
1	A	436	GLY
1	A	483	LYS
1	A	613	PHE
1	B	427	GLY
1	B	436	GLY
1	B	484	TYR
1	B	529	GLN
1	C	436	GLY
1	C	483	LYS
1	C	572	ASP
1	C	607	ASN
1	D	579	GLU
1	E	435	ILE
1	E	524	GLY
1	F	436	GLY
1	F	437	GLU
1	F	510	ALA
1	F	549	VAL
1	B	418	LEU
1	C	490	SER
1	D	490	SER
1	D	509	SER
1	E	439	ALA
1	E	510	ALA
1	A	509	SER
1	A	510	ALA
1	B	421	THR
1	B	490	SER
1	D	553	ILE
1	A	451	PRO
1	B	435	ILE
1	B	437	GLU
1	B	451	PRO
1	D	499	VAL
1	E	513	SER
1	F	597	GLU
1	B	540	LYS
1	D	510	ALA
1	B	599	VAL
1	F	458	GLY

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Mol	Chain	Res	Type
1	F	499	VAL
1	B	571	ILE

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	160/168 (95%)	116 (72%)	44 (28%)	0 2
1	B	160/168 (95%)	115 (72%)	45 (28%)	0 2
1	C	159/168 (95%)	125 (79%)	34 (21%)	1 5
1	D	160/168 (95%)	133 (83%)	27 (17%)	2 11
1	E	160/168 (95%)	122 (76%)	38 (24%)	0 3
1	F	160/168 (95%)	131 (82%)	29 (18%)	1 9
All	All	959/1008 (95%)	742 (77%)	217 (23%)	1 4

All (217) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	422	GLU
1	A	424	TYR
1	A	426	VAL
1	A	435	ILE
1	A	446	ILE
1	A	453	MET
1	A	457	GLU
1	A	459	ARG
1	A	467	GLN
1	A	468	GLU
1	A	469	ILE
1	A	471	ARG
1	A	475	MET
1	A	478	SER
1	A	480	ILE
1	A	482	LYS

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Mol	Chain	Res	Type
1	A	483	LYS
1	A	485	THR
1	A	487	ARG
1	A	488	ASP
1	A	492	MET
1	A	493	ASP
1	A	501	THR
1	A	503	GLU
1	A	508	ASP
1	A	509	SER
1	A	516	THR
1	A	529	GLN
1	A	533	MET
1	A	539	VAL
1	A	540	LYS
1	A	542	GLU
1	A	562	LYS
1	A	568	LYS
1	A	569	ASP
1	A	571	ILE
1	A	579	GLU
1	A	590	SER
1	A	592	ILE
1	A	598	HIS
1	A	599	VAL
1	A	602	ASP
1	A	608	ARG
1	A	612	LYS
1	B	417	LYS
1	B	418	LEU
1	B	420	ILE
1	B	425	GLU
1	B	428	ARG
1	B	434	VAL
1	B	435	ILE
1	B	437	GLU
1	B	443	LEU
1	B	449	VAL
1	B	451	PRO
1	B	463	THR
1	B	466	LEU
1	B	478	SER

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Mol	Chain	Res	Type
1	B	480	ILE
1	B	482	LYS
1	B	483	LYS
1	B	487	ARG
1	B	492	MET
1	B	496	ILE
1	B	502	TYR
1	B	503	GLU
1	B	506	GLU
1	B	518	VAL
1	B	520	SER
1	B	522	ILE
1	B	534	THR
1	B	542	GLU
1	B	546	VAL
1	B	549	VAL
1	B	550	THR
1	B	562	LYS
1	B	568	LYS
1	B	570	ASN
1	B	573	ASP
1	B	575	LEU
1	B	579	GLU
1	B	580	HIS
1	B	583	LYS
1	B	584	ILE
1	B	597	GLU
1	B	605	LYS
1	B	608	ARG
1	B	609	LEU
1	B	614	LYS
1	C	420	ILE
1	C	425	GLU
1	C	435	ILE
1	C	437	GLU
1	C	438	SER
1	C	441	ILE
1	C	445	ILE
1	C	446	ILE
1	C	463	THR
1	C	465	ARG
1	C	472	GLU

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Mol	Chain	Res	Type
1	C	476	ASN
1	C	477	VAL
1	C	480	ILE
1	C	482	LYS
1	C	483	LYS
1	C	485	THR
1	C	488	ASP
1	C	489	ILE
1	C	501	THR
1	C	506	GLU
1	C	508	ASP
1	C	509	SER
1	C	519	ILE
1	C	558	GLN
1	C	568	LYS
1	C	570	ASN
1	C	572	ASP
1	C	577	ASP
1	C	580	HIS
1	C	581	GLU
1	C	597	GLU
1	C	608	ARG
1	C	614	LYS
1	D	417	LYS
1	D	418	LEU
1	D	435	ILE
1	D	442	VAL
1	D	443	LEU
1	D	453	MET
1	D	457	GLU
1	D	459	ARG
1	D	465	ARG
1	D	468	GLU
1	D	480	ILE
1	D	487	ARG
1	D	506	GLU
1	D	509	SER
1	D	533	MET
1	D	539	VAL
1	D	540	LYS
1	D	551	GLN
1	D	562	LYS

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Mol	Chain	Res	Type
1	D	564	VAL
1	D	579	GLU
1	D	597	GLU
1	D	604	LYS
1	D	608	ARG
1	D	610	MET
1	D	612	LYS
1	D	614	LYS
1	E	419	PHE
1	E	420	ILE
1	E	421	THR
1	E	422	GLU
1	E	425	GLU
1	E	434	VAL
1	E	435	ILE
1	E	443	LEU
1	E	450	THR
1	E	453	MET
1	E	457	GLU
1	E	459	ARG
1	E	461	ILE
1	E	463	THR
1	E	475	MET
1	E	477	VAL
1	E	482	LYS
1	E	487	ARG
1	E	488	ASP
1	E	489	ILE
1	E	491	ASN
1	E	492	MET
1	E	502	TYR
1	E	503	GLU
1	E	508	ASP
1	E	531	VAL
1	E	536	SER
1	E	540	LYS
1	E	551	GLN
1	E	558	GLN
1	E	562	LYS
1	E	563	LYS
1	E	579	GLU
1	E	599	VAL

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Mol	Chain	Res	Type
1	E	605	LYS
1	E	608	ARG
1	E	609	LEU
1	E	613	PHE
1	F	420	ILE
1	F	425	GLU
1	F	428	ARG
1	F	437	GLU
1	F	445	ILE
1	F	446	ILE
1	F	459	ARG
1	F	467	GLN
1	F	469	ILE
1	F	472	GLU
1	F	480	ILE
1	F	482	LYS
1	F	489	ILE
1	F	501	THR
1	F	527	VAL
1	F	540	LYS
1	F	546	VAL
1	F	549	VAL
1	F	550	THR
1	F	558	GLN
1	F	562	LYS
1	F	566	ILE
1	F	572	ASP
1	F	575	LEU
1	F	580	HIS
1	F	581	GLU
1	F	593	ASN
1	F	605	LYS
1	F	614	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	467	GLN
1	B	529	GLN
1	B	551	GLN
1	B	580	HIS
1	D	598	HIS

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Mol	Chain	Res	Type
1	E	558	GLN
1	E	580	HIS
1	F	558	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	D	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	531:VAL	C	532:ALA	N	1.67
1	D	532:ALA	C	533:MET	N	1.66

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, 95^{th} 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%)	-0.42	0 100 100	5, 17, 35, 47	0
1	B	195/205 (95%)	-0.02	4 (2%) 63 34	11, 25, 43, 61	0
1	C	194/205 (94%)	-0.69	0 100 100	2, 10, 27, 35	0
1	D	195/205 (95%)	-0.71	0 100 100	2, 8, 24, 34	0
1	E	195/205 (95%)	-0.35	1 (0%) 91 75	5, 17, 42, 57	0
1	F	195/205 (95%)	-0.50	0 100 100	2, 17, 36, 50	0
All	All	1169/1230 (95%)	-0.45	5 (0%) 92 79	2, 16, 37, 61	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	501	THR	2.7
1	B	608	ARG	2.2
1	E	458	GLY	2.2
1	B	483	LYS	2.2
1	B	579	GLU	2.1

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

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.