



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 11:55 PM GMT

PDB ID : 1Z0T
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
<http://wwpdb.org/validation/2016/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
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

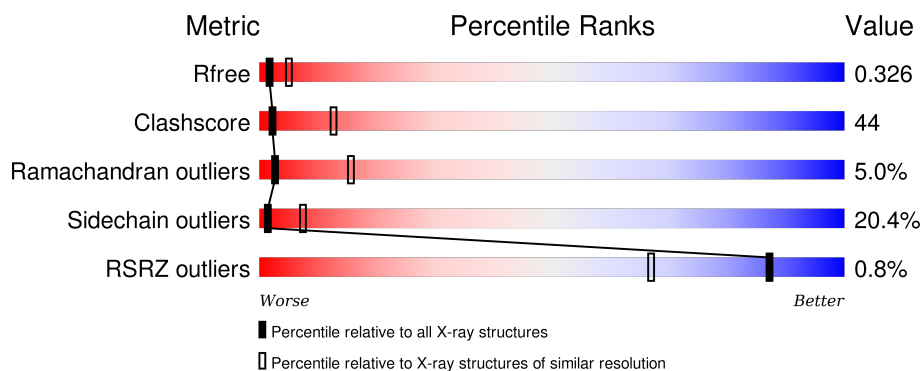
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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}	91344	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (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. 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>43%</div> <div>34%</div> <div>14%</div> <div>5%</div> </div>
1	B	205	<div>2%</div> <div>29%</div> <div>40%</div> <div>20%</div> <div>7%</div> <div>•</div>
1	C	205	<div>42%</div> <div>33%</div> <div>15%</div> <div>5%</div> <div>•</div>
1	D	205	<div>41%</div> <div>35%</div> <div>14%</div> <div>6%</div> <div>•</div>
1	E	205	<div>%</div> <div>25%</div> <div>40%</div> <div>21%</div> <div>9%</div> <div>5%</div>

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Mol	Chain	Length	Quality of chain
1	F	205	<div><div></div><div>34%</div><div>40%</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 9870 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			

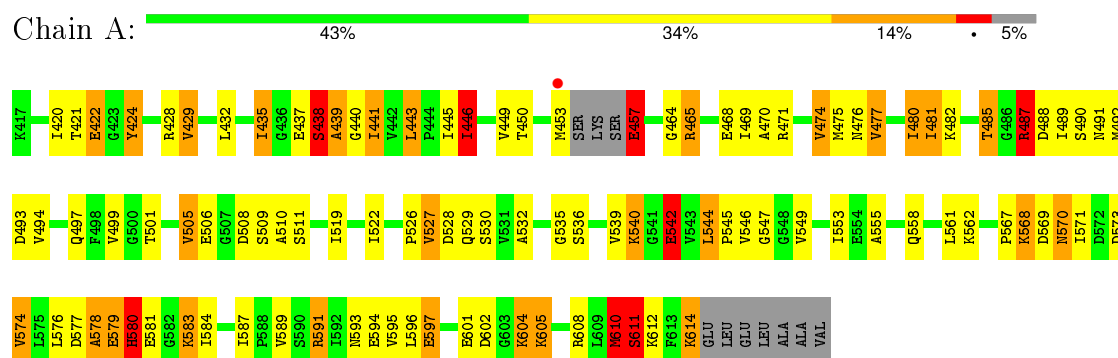
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	159	Total	O	0	0
			159	159		
2	B	164	Total	O	0	0
			164	164		
2	C	208	Total	O	0	0
			208	208		
2	D	190	Total	O	0	0
			190	190		
2	E	145	Total	O	0	0
			145	145		
2	F	226	Total	O	0	0
			226	226		

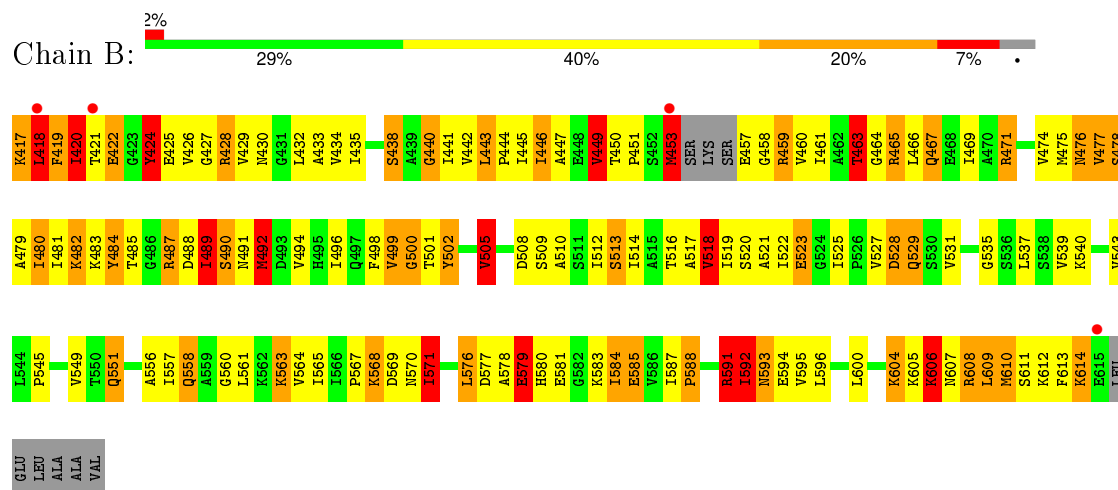
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

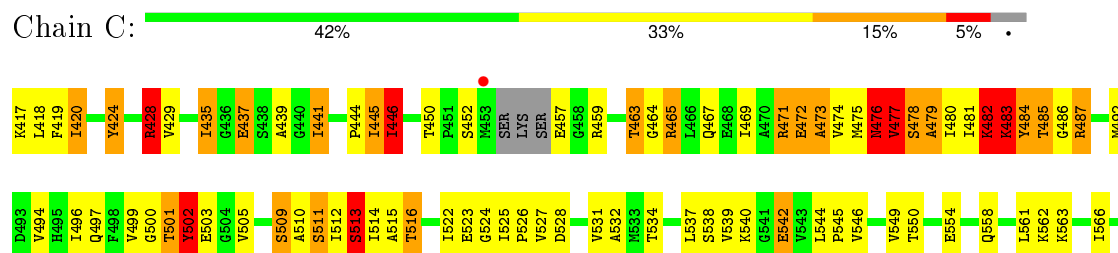
• Molecule 1: Putative protease La homolog type

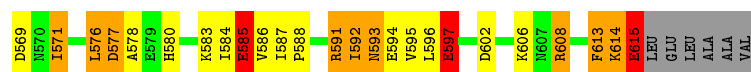


• Molecule 1: Putative protease La homolog type

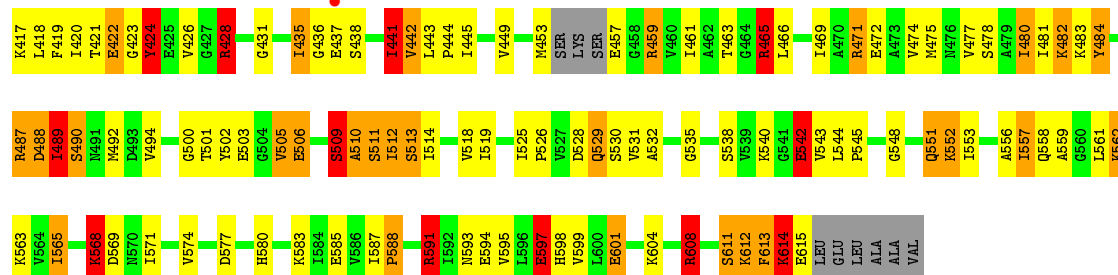


• Molecule 1: Putative protease La homolog type

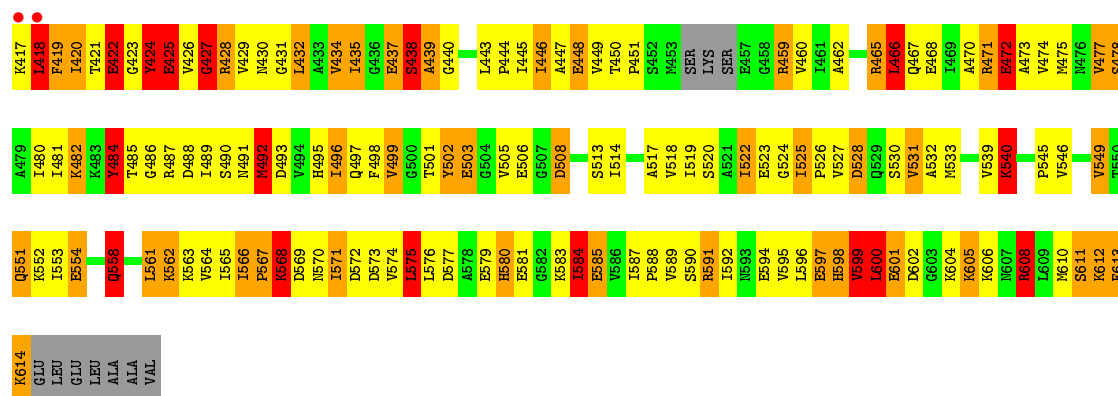
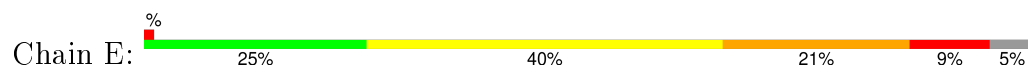




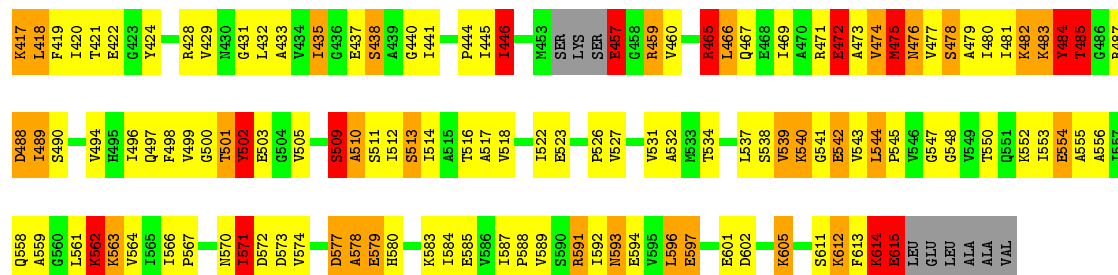
• Molecule 1: Putative protease La homolog type



• 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	86.25Å 90.55Å 147.95Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 3.00 14.98 – 3.00	Depositor EDS
% Data completeness (in resolution range)	100.0 (15.00-3.00) 100.0 (14.98-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.94 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.200 , 0.330 0.200 , 0.326	Depositor DCC
R_{free} test set	1210 reflections (5.40%)	DCC
Wilson B-factor (Å ²)	41.7	Xtriage
Anisotropy	0.218	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 48.7	EDS
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.55$, $\langle L^2 \rangle = 0.39$	Xtriage
Outliers	2 of 23617 reflections (0.008%)	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9870	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 54.90 % 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 3.4165e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	1.93	32/1470 (2.2%)	1.58	26/1983 (1.3%)
1	B	1.90	27/1479 (1.8%)	1.54	14/1995 (0.7%)
1	C	1.98	34/1479 (2.3%)	1.49	18/1995 (0.9%)
1	D	1.94	36/1479 (2.4%)	1.58	17/1995 (0.9%)
1	E	1.91	35/1470 (2.4%)	1.64	28/1983 (1.4%)
1	F	1.88	26/1479 (1.8%)	1.53	16/1995 (0.8%)
All	All	1.92	190/8856 (2.1%)	1.56	119/11946 (1.0%)

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	2
1	C	0	1
1	D	0	2
1	E	0	2
1	F	0	1
All	All	0	8

All (190) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	612	LYS	CE-NZ	13.53	1.82	1.49
1	C	597	GLU	CG-CD	11.91	1.69	1.51
1	F	484	TYR	CB-CG	10.78	1.67	1.51
1	A	597	GLU	CG-CD	10.61	1.67	1.51
1	C	472	GLU	CB-CG	10.32	1.71	1.52
1	C	597	GLU	CD-OE2	10.07	1.36	1.25
1	A	604	LYS	CE-NZ	9.87	1.73	1.49
1	D	422	GLU	CG-CD	9.61	1.66	1.51
1	C	477	VAL	CB-CG2	9.37	1.72	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	511	SER	CB-OG	9.32	1.54	1.42
1	D	422	GLU	CD-OE2	9.20	1.35	1.25
1	A	605	LYS	CE-NZ	9.16	1.72	1.49
1	A	583	LYS	CE-NZ	9.10	1.71	1.49
1	C	542	GLU	CB-CG	9.02	1.69	1.52
1	A	597	GLU	CD-OE2	8.86	1.35	1.25
1	A	597	GLU	CB-CG	8.84	1.69	1.52
1	F	438	SER	CB-OG	8.72	1.53	1.42
1	A	579	GLU	CG-CD	8.63	1.64	1.51
1	D	437	GLU	CG-CD	8.59	1.64	1.51
1	D	612	LYS	CE-NZ	8.52	1.70	1.49
1	A	424	TYR	CD1-CE1	8.43	1.51	1.39
1	F	612	LYS	CD-CE	8.43	1.72	1.51
1	C	420	ILE	CB-CG2	8.33	1.78	1.52
1	A	422	GLU	CD-OE2	8.29	1.34	1.25
1	D	568	LYS	CD-CE	8.24	1.71	1.51
1	A	540	LYS	CD-CE	8.19	1.71	1.51
1	C	615	GLU	CG-CD	8.15	1.64	1.51
1	E	591	ARG	CG-CD	8.12	1.72	1.51
1	C	503	GLU	CG-CD	8.06	1.64	1.51
1	C	479	ALA	CA-CB	7.99	1.69	1.52
1	D	591	ARG	CG-CD	7.93	1.71	1.51
1	D	484	TYR	CE2-CZ	7.85	1.48	1.38
1	B	478	SER	CB-OG	7.70	1.52	1.42
1	D	509	SER	CB-OG	7.64	1.52	1.42
1	C	484	TYR	CD2-CE2	7.63	1.50	1.39
1	C	542	GLU	CG-CD	7.57	1.63	1.51
1	D	597	GLU	CD-OE1	7.52	1.33	1.25
1	C	473	ALA	CA-CB	-7.45	1.36	1.52
1	D	608	ARG	CG-CD	7.43	1.70	1.51
1	D	422	GLU	CB-CG	7.37	1.66	1.52
1	B	585	GLU	CB-CG	7.36	1.66	1.52
1	D	437	GLU	CB-CG	7.34	1.66	1.52
1	E	466	LEU	C-O	7.31	1.37	1.23
1	E	558	GLN	CG-CD	7.24	1.67	1.51
1	D	608	ARG	CB-CG	7.23	1.72	1.52
1	E	589	VAL	CB-CG1	7.22	1.68	1.52
1	B	585	GLU	CG-CD	7.17	1.62	1.51
1	F	474	VAL	CB-CG1	7.15	1.67	1.52
1	E	546	VAL	CB-CG2	7.14	1.67	1.52
1	B	449	VAL	CB-CG1	7.12	1.67	1.52
1	C	554	GLU	CG-CD	7.07	1.62	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	457	GLU	CB-CG	6.96	1.65	1.52
1	B	523	GLU	CG-CD	6.96	1.62	1.51
1	C	483	LYS	N-CA	6.91	1.60	1.46
1	E	462	ALA	CA-CB	-6.87	1.38	1.52
1	F	597	GLU	CD-OE2	6.85	1.33	1.25
1	C	542	GLU	CD-OE1	6.82	1.33	1.25
1	A	424	TYR	CG-CD1	6.79	1.48	1.39
1	B	463	THR	CB-CG2	6.78	1.74	1.52
1	E	502	TYR	CE2-CZ	6.74	1.47	1.38
1	A	542	GLU	CG-CD	6.73	1.62	1.51
1	F	502	TYR	CB-CG	6.72	1.61	1.51
1	B	608	ARG	CG-CD	6.71	1.68	1.51
1	D	484	TYR	CE1-CZ	6.70	1.47	1.38
1	C	503	GLU	CD-OE2	6.64	1.32	1.25
1	F	542	GLU	CG-CD	6.62	1.61	1.51
1	B	442	VAL	CB-CG2	-6.62	1.39	1.52
1	C	503	GLU	CB-CG	6.61	1.64	1.52
1	C	597	GLU	CD-OE1	6.50	1.32	1.25
1	D	601	GLU	CD-OE1	6.46	1.32	1.25
1	C	513	SER	CB-OG	6.46	1.50	1.42
1	B	499	VAL	CB-CG1	6.44	1.66	1.52
1	B	608	ARG	CB-CG	6.41	1.69	1.52
1	B	594	GLU	CG-CD	-6.37	1.42	1.51
1	F	457	GLU	CD-OE1	6.31	1.32	1.25
1	A	542	GLU	CB-CG	6.29	1.64	1.52
1	C	478	SER	CB-OG	6.28	1.50	1.42
1	E	613	PHE	CB-CG	6.28	1.62	1.51
1	C	511	SER	CB-OG	6.27	1.50	1.42
1	F	422	GLU	CD-OE2	6.27	1.32	1.25
1	C	585	GLU	CD-OE2	6.26	1.32	1.25
1	F	472	GLU	CG-CD	6.22	1.61	1.51
1	B	579	GLU	CG-CD	6.20	1.61	1.51
1	F	457	GLU	CD-OE2	6.20	1.32	1.25
1	B	477	VAL	CB-CG1	6.14	1.65	1.52
1	D	482	LYS	CE-NZ	6.14	1.64	1.49
1	A	579	GLU	C-O	6.08	1.34	1.23
1	E	428	ARG	CZ-NH1	6.06	1.41	1.33
1	A	453	MET	CG-SD	6.06	1.97	1.81
1	F	559	ALA	CA-CB	6.06	1.65	1.52
1	B	426	VAL	CB-CG1	6.04	1.65	1.52
1	F	483	LYS	CE-NZ	6.04	1.64	1.49
1	E	540	LYS	CB-CG	5.98	1.68	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	509	SER	CB-OG	5.95	1.50	1.42
1	A	422	GLU	CG-CD	5.95	1.60	1.51
1	B	471	ARG	CG-CD	5.94	1.66	1.51
1	C	420	ILE	CG1-CD1	5.94	1.91	1.50
1	F	605	LYS	CE-NZ	5.94	1.63	1.49
1	E	506	GLU	CG-CD	5.93	1.60	1.51
1	A	577	ASP	CB-CG	5.89	1.64	1.51
1	E	493	ASP	CB-CG	5.88	1.64	1.51
1	D	506	GLU	C-O	5.87	1.34	1.23
1	D	594	GLU	CD-OE2	5.87	1.32	1.25
1	E	604	LYS	CD-CE	5.86	1.65	1.51
1	A	597	GLU	CD-OE1	5.86	1.32	1.25
1	A	437	GLU	CB-CG	5.84	1.63	1.52
1	F	554	GLU	CD-OE2	5.81	1.32	1.25
1	F	471	ARG	CG-CD	5.80	1.66	1.51
1	B	424	TYR	CD1-CE1	5.79	1.48	1.39
1	D	543	VAL	N-CA	-5.77	1.34	1.46
1	A	438	SER	CB-OG	5.76	1.49	1.42
1	E	422	GLU	CD-OE2	5.75	1.31	1.25
1	D	489	ILE	CB-CG2	5.70	1.70	1.52
1	D	437	GLU	CD-OE1	5.69	1.31	1.25
1	A	546	VAL	CA-CB	5.67	1.66	1.54
1	B	476	ASN	CB-CG	5.66	1.64	1.51
1	F	457	GLU	CG-CD	5.65	1.60	1.51
1	F	615	GLU	CG-CD	5.63	1.60	1.51
1	B	484	TYR	CD1-CE1	-5.62	1.30	1.39
1	C	615	GLU	CB-CG	5.62	1.62	1.52
1	D	428	ARG	CG-CD	5.62	1.66	1.51
1	E	459	ARG	CB-CG	5.61	1.67	1.52
1	D	490	SER	CB-OG	5.60	1.49	1.42
1	C	586	VAL	CB-CG2	-5.57	1.41	1.52
1	E	597	GLU	CG-CD	5.56	1.60	1.51
1	A	424	TYR	CZ-OH	5.55	1.47	1.37
1	A	429	VAL	C-O	5.55	1.33	1.23
1	E	496	ILE	CB-CG2	5.54	1.70	1.52
1	E	554	GLU	CB-CG	5.53	1.62	1.52
1	C	594	GLU	CG-CD	5.53	1.60	1.51
1	E	424	TYR	CB-CG	5.53	1.59	1.51
1	C	424	TYR	CG-CD1	5.51	1.46	1.39
1	E	424	TYR	CG-CD2	5.50	1.46	1.39
1	A	465	ARG	CB-CG	5.49	1.67	1.52
1	E	424	TYR	CD2-CE2	5.49	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	597	GLU	CG-CD	5.49	1.60	1.51
1	C	583	LYS	CE-NZ	5.48	1.62	1.49
1	E	506	GLU	CD-OE1	5.48	1.31	1.25
1	D	542	GLU	CD-OE1	5.48	1.31	1.25
1	E	520	SER	CB-OG	5.46	1.49	1.42
1	A	440	GLY	C-O	5.44	1.32	1.23
1	D	552	LYS	CB-CG	5.44	1.67	1.52
1	E	427	GLY	N-CA	5.43	1.54	1.46
1	D	597	GLU	CD-OE2	5.42	1.31	1.25
1	A	580	HIS	N-CA	5.42	1.57	1.46
1	E	554	GLU	CG-CD	5.39	1.60	1.51
1	D	613	PHE	CE2-CZ	5.39	1.47	1.37
1	B	505	VAL	CB-CG2	5.38	1.64	1.52
1	F	562	LYS	CG-CD	5.38	1.70	1.52
1	C	457	GLU	CD-OE2	5.38	1.31	1.25
1	E	477	VAL	CB-CG2	-5.34	1.41	1.52
1	A	587	ILE	C-O	5.33	1.33	1.23
1	D	484	TYR	CD1-CE1	5.31	1.47	1.39
1	D	542	GLU	CG-CD	5.30	1.59	1.51
1	E	424	TYR	CE2-CZ	5.28	1.45	1.38
1	D	574	VAL	C-O	5.28	1.33	1.23
1	A	594	GLU	CG-CD	5.26	1.59	1.51
1	D	562	LYS	CD-CE	5.25	1.64	1.51
1	D	424	TYR	CG-CD1	5.25	1.46	1.39
1	B	425	GLU	CD-OE1	5.24	1.31	1.25
1	A	611	SER	CB-OG	5.21	1.49	1.42
1	E	590	SER	CB-OG	5.20	1.49	1.42
1	E	552	LYS	CE-NZ	5.20	1.62	1.49
1	E	471	ARG	CZ-NH1	5.18	1.39	1.33
1	F	589	VAL	CB-CG2	5.16	1.63	1.52
1	C	515	ALA	C-O	5.15	1.33	1.23
1	A	437	GLU	CG-CD	5.14	1.59	1.51
1	E	484	TYR	CE2-CZ	5.14	1.45	1.38
1	B	505	VAL	CA-CB	5.13	1.65	1.54
1	E	419	PHE	CB-CG	5.12	1.60	1.51
1	F	562	LYS	CE-NZ	5.11	1.61	1.49
1	E	425	GLU	CG-CD	5.09	1.59	1.51
1	C	613	PHE	CB-CG	5.09	1.59	1.51
1	C	472	GLU	CG-CD	5.08	1.59	1.51
1	B	429	VAL	CB-CG2	5.07	1.63	1.52
1	D	484	TYR	CD2-CE2	5.06	1.47	1.39
1	B	420	ILE	CA-CB	5.06	1.66	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	420	ILE	N-CA	5.06	1.56	1.46
1	C	558	GLN	CG-CD	5.06	1.62	1.51
1	D	542	GLU	CD-OE2	5.05	1.31	1.25
1	B	422	GLU	CB-CG	5.05	1.61	1.52
1	B	518	VAL	CA-CB	5.05	1.65	1.54
1	E	525	ILE	C-O	5.04	1.32	1.23
1	C	484	TYR	CE2-CZ	5.03	1.45	1.38
1	B	568	LYS	N-CA	5.03	1.56	1.46
1	F	544	LEU	CG-CD2	5.02	1.70	1.51
1	F	484	TYR	CG-CD2	5.02	1.45	1.39
1	A	527	VAL	CA-CB	-5.02	1.44	1.54
1	D	562	LYS	CE-NZ	5.01	1.61	1.49
1	E	568	LYS	CE-NZ	5.00	1.61	1.49

All (119) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	471	ARG	NE-CZ-NH2	-16.20	112.20	120.30
1	D	587	ILE	C-N-CD	11.68	152.92	128.40
1	F	563	LYS	CD-CE-NZ	-11.20	85.94	111.70
1	A	471	ARG	NE-CZ-NH1	9.81	125.20	120.30
1	D	465	ARG	NE-CZ-NH2	-9.72	115.44	120.30
1	A	604	LYS	CD-CE-NZ	9.01	132.42	111.70
1	A	508	ASP	CB-CG-OD2	-8.51	110.65	118.30
1	F	465	ARG	NE-CZ-NH1	-8.48	116.06	120.30
1	D	465	ARG	NE-CZ-NH1	8.46	124.53	120.30
1	A	471	ARG	NE-CZ-NH2	-8.44	116.08	120.30
1	F	577	ASP	CB-CG-OD1	8.24	125.72	118.30
1	B	418	LEU	CA-CB-CG	7.99	133.68	115.30
1	F	466	LEU	CB-CG-CD1	7.84	124.34	111.00
1	E	471	ARG	NE-CZ-NH1	7.83	124.22	120.30
1	E	438	SER	N-CA-C	-7.82	89.89	111.00
1	C	484	TYR	CB-CA-C	7.78	125.96	110.40
1	A	597	GLU	OE1-CD-OE2	-7.62	114.15	123.30
1	E	508	ASP	CB-CG-OD1	7.52	125.07	118.30
1	E	428	ARG	NE-CZ-NH2	-7.34	116.63	120.30
1	C	583	LYS	CD-CE-NZ	7.31	128.52	111.70
1	B	428	ARG	CG-CD-NE	-7.28	96.51	111.80
1	C	446	ILE	CB-CA-C	-7.27	97.06	111.60
1	D	428	ARG	NE-CZ-NH1	7.19	123.89	120.30
1	E	418	LEU	CA-CB-CG	7.18	131.81	115.30
1	E	460	VAL	N-CA-C	-7.09	91.84	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	600	LEU	CA-CB-CG	7.06	131.53	115.30
1	F	466	LEU	CA-CB-CG	-7.06	99.06	115.30
1	C	516	THR	CA-CB-CG2	-7.06	102.52	112.40
1	E	528	ASP	CB-CG-OD1	-7.03	111.98	118.30
1	A	602	ASP	CB-CG-OD2	7.02	124.62	118.30
1	D	428	ARG	NE-CZ-NH2	-7.01	116.80	120.30
1	F	502	TYR	N-CA-C	6.93	129.71	111.00
1	D	569	ASP	CB-CG-OD1	6.91	124.52	118.30
1	E	575	LEU	N-CA-C	-6.89	92.39	111.00
1	B	453	MET	CG-SD-CE	6.88	111.22	100.20
1	C	502	TYR	CB-CG-CD2	-6.87	116.88	121.00
1	A	610	MET	CG-SD-CE	6.85	111.16	100.20
1	C	441	ILE	CB-CA-C	-6.79	98.02	111.60
1	C	502	TYR	CA-CB-CG	-6.78	100.51	113.40
1	B	446	ILE	CG1-CB-CG2	-6.69	96.68	111.40
1	A	583	LYS	CD-CE-NZ	6.67	127.03	111.70
1	F	446	ILE	CB-CA-C	-6.65	98.30	111.60
1	D	587	ILE	C-N-CA	-6.63	94.15	122.00
1	A	493	ASP	CB-CG-OD1	6.58	124.22	118.30
1	C	576	LEU	CB-CG-CD2	6.57	122.17	111.00
1	E	432	LEU	CA-CB-CG	-6.55	100.24	115.30
1	E	561	LEU	CA-CB-CG	6.51	130.28	115.30
1	E	492	MET	CG-SD-CE	-6.48	89.83	100.20
1	A	487	ARG	NE-CZ-NH1	6.44	123.52	120.30
1	F	465	ARG	NE-CZ-NH2	6.38	123.49	120.30
1	F	596	LEU	CB-CG-CD2	-6.34	100.22	111.00
1	E	499	VAL	CB-CA-C	-6.28	99.47	111.40
1	E	482	LYS	CD-CE-NZ	6.25	126.07	111.70
1	C	502	TYR	N-CA-C	6.23	127.82	111.00
1	F	475	MET	CG-SD-CE	6.19	110.10	100.20
1	B	591	ARG	NE-CZ-NH1	6.17	123.38	120.30
1	E	598	HIS	CB-CA-C	-6.15	98.09	110.40
1	F	485	THR	N-CA-CB	6.14	121.97	110.30
1	F	571	ILE	CG1-CB-CG2	-6.12	97.94	111.40
1	A	605	LYS	CD-CE-NZ	6.11	125.76	111.70
1	D	512	ILE	CB-CA-C	-6.10	99.41	111.60
1	E	443	LEU	C-N-CD	6.07	141.15	128.40
1	A	505	VAL	CB-CA-C	-6.07	99.86	111.40
1	A	453	MET	CG-SD-CE	6.07	109.91	100.20
1	E	591	ARG	CG-CD-NE	6.07	124.55	111.80
1	A	597	GLU	CB-CG-CD	-6.04	97.89	114.20
1	A	443	LEU	CB-CG-CD2	6.00	121.20	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	441	ILE	CB-CA-C	-5.99	99.62	111.60
1	E	599	VAL	CB-CA-C	-5.97	100.05	111.40
1	D	608	ARG	CD-NE-CZ	5.89	131.84	123.60
1	F	488	ASP	CB-CG-OD1	-5.88	113.01	118.30
1	A	465	ARG	CB-CG-CD	5.88	126.88	111.60
1	A	443	LEU	CA-CB-CG	5.79	128.61	115.30
1	E	424	TYR	CB-CG-CD2	5.78	124.47	121.00
1	E	572	ASP	CB-CG-OD1	5.78	123.50	118.30
1	B	492	MET	CG-SD-CE	5.77	109.42	100.20
1	B	585	GLU	CA-CB-CG	5.75	126.05	113.40
1	A	465	ARG	CA-CB-CG	5.74	126.03	113.40
1	D	608	ARG	CG-CD-NE	5.74	123.86	111.80
1	C	445	ILE	CG1-CB-CG2	-5.71	98.83	111.40
1	D	442	VAL	CG1-CB-CG2	-5.70	101.79	110.90
1	C	465	ARG	NE-CZ-NH1	-5.69	117.45	120.30
1	D	597	GLU	CA-CB-CG	-5.68	100.90	113.40
1	B	434	VAL	N-CA-C	-5.68	95.67	111.00
1	C	471	ARG	NE-CZ-NH2	-5.67	117.47	120.30
1	E	432	LEU	CB-CG-CD2	-5.67	101.37	111.00
1	C	445	ILE	CB-CA-C	-5.66	100.28	111.60
1	D	441	ILE	CB-CA-C	-5.62	100.35	111.60
1	D	488	ASP	CB-CG-OD1	-5.50	113.35	118.30
1	A	453	MET	CB-CG-SD	5.49	128.88	112.40
1	F	602	ASP	CB-CG-OD1	5.49	123.24	118.30
1	B	465	ARG	NE-CZ-NH2	-5.46	117.57	120.30
1	C	602	ASP	CB-CG-OD1	5.40	123.16	118.30
1	E	466	LEU	N-CA-C	5.36	125.47	111.00
1	A	544	LEU	CB-CG-CD2	-5.34	101.92	111.00
1	C	608	ARG	NE-CZ-NH1	5.33	122.97	120.30
1	A	474	VAL	CB-CA-C	-5.29	101.35	111.40
1	C	615	GLU	OE1-CD-OE2	-5.28	116.97	123.30
1	F	500	GLY	N-CA-C	-5.24	99.99	113.10
1	B	489	ILE	CG1-CB-CG2	5.24	122.93	111.40
1	C	487	ARG	CG-CD-NE	-5.24	100.80	111.80
1	E	528	ASP	CB-CG-OD2	5.22	123.00	118.30
1	B	443	LEU	CA-CB-CG	5.21	127.29	115.30
1	C	428	ARG	NE-CZ-NH2	-5.19	117.70	120.30
1	E	472	GLU	OE1-CD-OE2	-5.12	117.16	123.30
1	B	428	ARG	CD-NE-CZ	5.11	130.75	123.60
1	B	463	THR	CA-CB-CG2	5.11	119.55	112.40
1	E	608	ARG	NE-CZ-NH2	-5.10	117.75	120.30
1	A	578	ALA	N-CA-CB	5.08	117.21	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	591	ARG	CB-CG-CD	-5.08	98.40	111.60
1	A	450	THR	C-N-CD	5.07	139.05	128.40
1	E	508	ASP	OD1-CG-OD2	-5.07	113.66	123.30
1	E	443	LEU	CA-CB-CG	5.02	126.86	115.30
1	D	591	ARG	CG-CD-NE	5.01	122.33	111.80
1	A	580	HIS	N-CA-C	5.01	124.53	111.00
1	B	466	LEU	CB-CG-CD1	-5.01	102.48	111.00
1	A	446	ILE	CB-CA-C	-5.01	101.58	111.60
1	D	505	VAL	CB-CA-C	-5.00	101.89	111.40
1	D	484	TYR	CB-CG-CD1	-5.00	118.00	121.00

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	500	GLY	Peptide
1	B	606	LYS	Peptide
1	C	452	SER	Peptide
1	D	438	SER	Peptide
1	D	614	LYS	Peptide
1	E	424	TYR	Peptide
1	E	567	PRO	Peptide
1	F	484	TYR	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	100	0
1	B	1466	0	1529	178	0
1	C	1466	0	1529	135	0
1	D	1466	0	1529	96	0
1	E	1457	0	1523	172	0
1	F	1466	0	1529	140	0
2	A	159	0	0	13	0
2	B	164	0	0	33	0
2	C	208	0	0	36	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	190	0	0	17	0
2	E	145	0	0	31	0
2	F	226	0	0	35	0
All	All	9870	0	9162	795	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 44.

All (795) 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:435:ILE:CG1	1:C:435:ILE:CD1	1.76	1.61
1:C:420:ILE:CB	1:C:420:ILE:CG2	1.78	1.60
1:F:522:ILE:CG1	1:F:522:ILE:CD1	1.79	1.58
1:B:463:THR:CG2	1:B:463:THR:CB	1.74	1.54
1:D:612:LYS:CE	1:D:612:LYS:NZ	1.70	1.54
1:A:605:LYS:CE	1:A:605:LYS:NZ	1.71	1.52
1:A:604:LYS:NZ	1:A:604:LYS:CE	1.73	1.50
1:A:583:LYS:NZ	1:A:583:LYS:CE	1.71	1.48
1:C:420:ILE:CD1	1:C:420:ILE:CG1	1.91	1.46
1:F:612:LYS:CE	1:F:612:LYS:NZ	1.82	1.42
1:C:502:TYR:CD1	2:C:701:HOH:O	1.68	1.33
1:E:576:LEU:HD22	1:E:580:HIS:CB	1.57	1.33
1:C:614:LYS:HG2	2:C:713:HOH:O	1.27	1.30
1:F:502:TYR:CE2	1:F:503:GLU:O	1.89	1.24
1:F:502:TYR:CD2	1:F:503:GLU:O	1.93	1.22
1:B:509:SER:N	2:B:633:HOH:O	1.71	1.21
1:C:497:GLN:HB2	2:C:826:HOH:O	1.04	1.21
1:E:426:VAL:HG11	2:E:647:HOH:O	1.39	1.20
1:E:576:LEU:HD22	1:E:580:HIS:HB3	1.22	1.17
1:E:451:PRO:HD3	2:E:639:HOH:O	1.46	1.16
1:E:450:THR:CG2	2:F:803:HOH:O	1.94	1.15
1:C:501:THR:HG21	2:D:676:HOH:O	1.43	1.15
1:E:450:THR:HG21	2:F:803:HOH:O	1.43	1.14
1:E:478:SER:HB3	1:E:489:ILE:HG12	1.23	1.13
1:C:459:ARG:HB3	2:C:825:HOH:O	1.49	1.13
1:E:437:GLU:HB2	2:E:735:HOH:O	1.44	1.12
1:A:470:ALA:O	1:A:474:VAL:HG23	1.47	1.12
1:E:422:GLU:OE2	1:E:423:GLY:N	1.84	1.09
1:D:428:ARG:CG	2:D:811:HOH:O	2.03	1.06
1:E:576:LEU:HD22	1:E:580:HIS:HB2	1.33	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:563:LYS:HG3	1:B:585:GLU:HB2	1.37	1.05
1:C:597:GLU:HB3	2:C:775:HOH:O	1.54	1.05
1:B:604:LYS:HB2	2:B:753:HOH:O	1.55	1.05
1:F:597:GLU:HB3	2:F:817:HOH:O	1.55	1.04
1:E:576:LEU:CD2	1:E:580:HIS:CB	2.36	1.03
1:D:428:ARG:HG2	2:D:811:HOH:O	1.56	1.02
1:F:502:TYR:CD2	1:F:505:VAL:HG23	1.94	1.02
1:B:563:LYS:HG2	1:B:587:ILE:HD11	1.43	1.01
1:B:453:MET:HG2	1:C:482:LYS:NZ	1.75	1.00
1:E:551:GLN:HB2	2:E:739:HOH:O	1.62	0.99
1:E:530:SER:HB3	1:E:562:LYS:HB2	1.43	0.99
1:E:418:LEU:HD13	1:E:419:PHE:HD2	1.27	0.97
1:E:601:GLU:HG2	1:E:602:ASP:H	1.27	0.96
1:E:496:ILE:C	2:E:744:HOH:O	2.04	0.96
1:E:450:THR:HG23	2:E:731:HOH:O	1.63	0.95
1:A:487:ARG:HG2	1:A:487:ARG:HH11	1.33	0.94
1:F:473:ALA:O	1:F:477:VAL:HG12	1.66	0.94
1:E:549:VAL:HB	2:E:734:HOH:O	1.69	0.92
1:B:585:GLU:HB3	2:B:653:HOH:O	1.70	0.91
1:B:480:ILE:HG13	1:B:481:ILE:N	1.83	0.90
1:A:438:SER:O	1:A:439:ALA:O	1.90	0.90
1:B:453:MET:HG2	1:C:482:LYS:HZ1	1.36	0.90
1:E:540:LYS:HG3	2:E:657:HOH:O	1.71	0.89
1:C:476:ASN:ND2	1:C:477:VAL:N	2.20	0.89
1:E:576:LEU:CD2	1:E:580:HIS:HB3	1.97	0.88
1:E:449:VAL:HG21	1:E:522:ILE:HG13	1.56	0.87
1:C:472:GLU:CG	1:C:473:ALA:N	2.36	0.87
1:B:523:GLU:HG3	1:B:609:LEU:HD22	1.56	0.87
1:D:428:ARG:HH11	1:D:428:ARG:HG2	1.38	0.86
1:B:549:VAL:HG23	2:B:643:HOH:O	1.73	0.86
1:D:611:SER:O	1:D:614:LYS:HG3	1.75	0.86
1:D:488:ASP:OD1	1:D:490:SER:HB2	1.75	0.86
1:A:477:VAL:O	1:A:481:ILE:HG23	1.74	0.86
1:C:445:ILE:CG2	2:C:645:HOH:O	2.24	0.85
1:A:469:ILE:HG21	2:A:777:HOH:O	1.76	0.85
1:D:465:ARG:HG3	1:D:465:ARG:HH11	1.42	0.85
1:C:420:ILE:CG2	1:C:420:ILE:CG1	2.55	0.85
1:D:459:ARG:NH2	2:D:678:HOH:O	2.04	0.85
1:E:496:ILE:N	2:E:744:HOH:O	2.10	0.84
1:B:489:ILE:HG13	1:B:492:MET:CG	2.07	0.84
1:F:563:LYS:HD2	1:F:587:ILE:HD11	1.59	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:568:LYS:HD3	2:A:725:HOH:O	1.77	0.83
1:B:529:GLN:HA	2:B:639:HOH:O	1.78	0.83
1:E:435:ILE:HG21	2:E:751:HOH:O	1.77	0.83
1:B:478:SER:HB3	1:B:482:LYS:HE3	1.60	0.83
1:C:445:ILE:HG22	2:C:645:HOH:O	1.79	0.82
1:D:568:LYS:O	1:D:571:ILE:HG13	1.79	0.82
1:E:577:ASP:O	1:E:581:GLU:HG2	1.80	0.82
1:B:484:TYR:CD2	1:B:613:PHE:CD2	2.68	0.81
1:F:562:LYS:HE3	2:F:680:HOH:O	1.80	0.81
1:B:450:THR:HG21	1:C:483:LYS:HB2	1.61	0.81
1:E:611:SER:O	1:E:614:LYS:HD3	1.80	0.80
1:D:571:ILE:HD11	1:D:588:PRO:HG3	1.60	0.80
1:C:420:ILE:HG13	2:C:774:HOH:O	1.80	0.80
1:F:469:ILE:HG21	2:F:815:HOH:O	1.82	0.80
1:C:476:ASN:HD22	1:C:477:VAL:N	1.76	0.80
1:F:485:THR:HA	2:F:762:HOH:O	1.81	0.80
1:B:418:LEU:HD23	2:B:658:HOH:O	1.82	0.80
1:B:484:TYR:CD2	1:B:613:PHE:HD2	1.99	0.80
1:E:599:VAL:HG23	1:E:600:LEU:H	1.46	0.79
1:B:478:SER:O	1:B:482:LYS:HD3	1.81	0.79
1:B:489:ILE:HG13	1:B:492:MET:HG3	1.65	0.79
1:D:422:GLU:HG2	1:D:423:GLY:N	1.98	0.79
1:E:425:GLU:H	1:E:526:PRO:HB2	1.48	0.79
1:B:563:LYS:HG3	1:B:585:GLU:CB	2.11	0.79
1:E:601:GLU:HG2	1:E:602:ASP:N	1.96	0.79
1:D:428:ARG:HG3	2:D:811:HOH:O	1.75	0.78
1:B:531:VAL:HG22	1:B:563:LYS:HB2	1.66	0.78
1:E:496:ILE:CA	2:E:744:HOH:O	2.29	0.78
1:C:424:TYR:HB3	1:C:526:PRO:HB2	1.65	0.78
1:D:558:GLN:NE2	2:D:744:HOH:O	2.16	0.78
1:F:571:ILE:HD11	1:F:588:PRO:HG3	1.66	0.78
1:C:472:GLU:HG2	1:C:473:ALA:H	1.47	0.77
1:E:425:GLU:H	1:E:526:PRO:CB	1.96	0.77
1:E:470:ALA:O	1:E:474:VAL:HG23	1.84	0.77
1:F:485:THR:HG23	1:F:523:GLU:OE2	1.84	0.77
1:B:480:ILE:CD1	1:B:613:PHE:HE2	1.97	0.76
1:B:430:ASN:ND2	2:B:639:HOH:O	2.18	0.76
1:F:419:PHE:HB3	1:F:444:PRO:HG3	1.65	0.76
1:B:568:LYS:O	1:B:571:ILE:HB	1.85	0.76
1:A:446:ILE:HD11	1:A:497:GLN:HB2	1.66	0.76
1:C:502:TYR:CE1	2:C:701:HOH:O	2.10	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:421:THR:HG22	1:A:561:LEU:HD21	1.67	0.76
1:C:476:ASN:HD22	1:C:477:VAL:H	1.34	0.75
1:E:427:GLY:O	1:E:447:ALA:N	2.15	0.75
1:D:568:LYS:HA	1:D:588:PRO:HB2	1.69	0.75
1:D:418:LEU:HD23	1:E:545:PRO:HB2	1.67	0.75
1:B:459:ARG:NH2	1:B:461:ILE:HD11	2.01	0.74
1:B:453:MET:HG2	1:C:482:LYS:HZ2	1.52	0.74
1:B:480:ILE:HD11	1:B:613:PHE:CE2	2.21	0.74
1:E:485:THR:HG22	1:E:487:ARG:H	1.50	0.74
1:A:421:THR:HG22	1:A:561:LEU:CD2	2.16	0.74
1:C:501:THR:HG22	2:D:653:HOH:O	1.86	0.74
1:A:476:ASN:O	1:A:480:ILE:HG22	1.87	0.74
1:C:474:VAL:CG2	1:C:496:ILE:HD11	2.18	0.74
1:C:428:ARG:HH11	1:C:428:ARG:HG3	1.53	0.74
1:C:614:LYS:HA	1:C:615:GLU:O	1.86	0.74
1:C:474:VAL:HG21	1:C:496:ILE:HD11	1.70	0.73
1:F:466:LEU:CD2	1:F:469:ILE:HD12	2.18	0.73
1:B:525:ILE:HG22	1:B:600:LEU:HD22	1.69	0.73
1:B:492:MET:O	2:B:631:HOH:O	2.06	0.73
1:C:472:GLU:HG2	1:C:473:ALA:N	2.03	0.73
1:A:443:LEU:HG	2:A:761:HOH:O	1.87	0.73
1:E:554:GLU:HG2	1:E:580:HIS:CD2	2.23	0.73
1:B:489:ILE:CD1	1:B:492:MET:HG2	2.19	0.73
1:B:482:LYS:HE2	1:B:489:ILE:H	1.54	0.73
1:C:615:GLU:C	2:C:818:HOH:O	2.27	0.72
1:C:445:ILE:HD11	2:C:787:HOH:O	1.87	0.72
1:E:478:SER:HB3	1:E:489:ILE:CG1	2.11	0.72
1:E:562:LYS:C	1:E:563:LYS:HG3	2.10	0.72
1:B:543:VAL:O	2:B:744:HOH:O	2.06	0.72
1:C:531:VAL:HG22	1:C:563:LYS:HB2	1.70	0.72
1:F:446:ILE:CD1	1:F:497:GLN:HB2	2.20	0.72
1:E:576:LEU:CD2	1:E:580:HIS:HB2	2.08	0.72
1:B:451:PRO:CA	1:B:492:MET:HE2	2.20	0.72
1:B:576:LEU:HB3	1:B:580:HIS:HB2	1.70	0.72
1:B:453:MET:CG	1:C:482:LYS:NZ	2.53	0.71
1:C:497:GLN:CB	2:C:826:HOH:O	1.83	0.71
1:C:420:ILE:HG23	1:C:420:ILE:HD12	1.72	0.71
1:B:451:PRO:HA	1:B:492:MET:HE2	1.72	0.71
1:A:553:ILE:HG21	1:A:576:LEU:HD11	1.72	0.71
1:B:417:LYS:HD2	1:B:419:PHE:CE1	2.24	0.71
1:E:466:LEU:HD12	2:E:718:HOH:O	1.91	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:469:ILE:O	1:F:472:GLU:HG3	1.90	0.71
1:E:595:VAL:O	1:E:599:VAL:HG22	1.91	0.71
1:E:553:ILE:HD11	1:E:566:ILE:HD11	1.73	0.71
1:B:489:ILE:HG13	1:B:492:MET:HG2	1.73	0.70
1:C:577:ASP:OD2	1:C:580:HIS:HB2	1.92	0.70
1:E:551:GLN:CB	2:E:739:HOH:O	2.30	0.70
1:B:459:ARG:CZ	1:B:461:ILE:HD11	2.21	0.70
1:F:477:VAL:HG22	1:F:481:ILE:HG13	1.73	0.69
1:B:484:TYR:HD2	1:B:613:PHE:CE2	2.09	0.69
1:F:502:TYR:HD2	1:F:505:VAL:HG23	1.52	0.69
1:F:482:LYS:HG3	2:F:832:HOH:O	1.92	0.69
1:F:578:ALA:C	1:F:580:HIS:N	2.46	0.69
1:B:477:VAL:HG11	1:B:518:VAL:CG1	2.22	0.69
1:E:481:ILE:O	1:E:486:GLY:N	2.26	0.69
1:E:601:GLU:O	1:E:606:LYS:HD2	1.92	0.69
1:B:428:ARG:HA	1:B:445:ILE:O	1.93	0.69
1:B:453:MET:CG	1:C:482:LYS:HZ2	2.06	0.68
1:A:481:ILE:HG13	1:A:482:LYS:N	2.07	0.68
1:E:495:HIS:C	2:E:744:HOH:O	2.32	0.68
1:B:463:THR:CG2	1:B:463:THR:HB	2.15	0.68
1:E:562:LYS:O	1:E:563:LYS:HG3	1.93	0.68
1:B:523:GLU:CG	1:B:609:LEU:HD22	2.23	0.68
1:B:571:ILE:HD13	1:B:571:ILE:O	1.93	0.68
1:F:476:ASN:ND2	2:F:666:HOH:O	2.25	0.68
1:D:538:SER:OG	1:D:542:GLU:HG2	1.93	0.68
1:B:609:LEU:O	1:B:612:LYS:HB2	1.93	0.68
1:B:545:PRO:HA	1:B:567:PRO:HG2	1.74	0.68
1:D:595:VAL:O	1:D:599:VAL:HG22	1.94	0.68
1:F:592:ILE:CG2	1:F:593:ASN:N	2.56	0.68
1:C:450:THR:HB	2:C:781:HOH:O	1.94	0.68
1:C:450:THR:CB	2:C:781:HOH:O	2.43	0.67
1:E:418:LEU:HD13	1:E:419:PHE:CD2	2.19	0.67
1:E:429:VAL:HG12	1:E:430:ASN:N	2.09	0.67
1:C:502:TYR:CE2	1:C:505:VAL:HG21	2.29	0.67
1:F:460:VAL:HG13	1:F:494:VAL:HG22	1.77	0.67
1:A:428:ARG:HD3	1:A:446:ILE:CG2	2.24	0.66
1:B:487:ARG:HD2	1:B:489:ILE:HD13	1.76	0.66
1:C:435:ILE:CB	1:C:435:ILE:CD1	2.72	0.66
1:E:528:ASP:HB3	1:E:531:VAL:HG23	1.78	0.66
1:F:554:GLU:OE1	2:F:807:HOH:O	2.13	0.66
1:B:484:TYR:HD2	1:B:613:PHE:CD2	2.13	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:480:ILE:CD1	1:B:613:PHE:CE2	2.77	0.66
1:C:418:LEU:HD23	1:C:499:VAL:O	1.94	0.66
1:A:424:TYR:HB3	1:A:526:PRO:HB3	1.79	0.66
1:A:574:VAL:HG12	1:A:574:VAL:O	1.97	0.65
1:B:501:THR:HG22	2:C:679:HOH:O	1.95	0.65
1:B:465:ARG:NE	2:B:747:HOH:O	2.27	0.65
1:C:467:GLN:OE1	1:C:471:ARG:NH2	2.29	0.65
1:B:453:MET:HB2	2:B:673:HOH:O	1.95	0.65
1:D:478:SER:HA	1:D:481:ILE:HD12	1.79	0.65
1:E:420:ILE:HG21	2:E:675:HOH:O	1.97	0.65
1:D:613:PHE:C	1:D:615:GLU:H	1.98	0.65
1:F:578:ALA:C	1:F:580:HIS:H	2.00	0.65
1:C:420:ILE:CD1	1:C:420:ILE:CB	2.74	0.65
2:A:693:HOH:O	1:F:501:THR:HG21	1.95	0.65
1:C:571:ILE:HD11	1:C:588:PRO:HG3	1.79	0.65
1:A:475:MET:CE	1:F:459:ARG:HH22	2.10	0.65
1:A:477:VAL:HA	1:A:480:ILE:HG23	1.79	0.64
1:F:593:ASN:HB3	1:F:613:PHE:CD1	2.31	0.64
1:B:549:VAL:HG21	1:B:570:ASN:HB3	1.78	0.64
1:C:446:ILE:HD11	1:D:544:LEU:HD13	1.80	0.64
1:D:562:LYS:HG2	2:D:632:HOH:O	1.97	0.64
1:A:489:ILE:HD11	1:A:522:ILE:HD11	1.78	0.64
1:C:428:ARG:NH1	1:C:428:ARG:HG3	2.13	0.64
1:F:532:ALA:HB2	1:F:561:LEU:HD13	1.80	0.64
1:A:475:MET:CE	1:F:459:ARG:NH2	2.61	0.64
1:D:445:ILE:HD12	1:D:513:SER:HB2	1.79	0.64
1:E:499:VAL:HG22	2:E:727:HOH:O	1.98	0.63
1:C:545:PRO:HG3	1:C:569:ASP:HB2	1.79	0.63
1:F:483:LYS:O	1:F:484:TYR:CD1	2.52	0.63
1:C:597:GLU:HG2	2:C:775:HOH:O	1.97	0.63
1:E:614:LYS:HA	2:E:666:HOH:O	1.97	0.63
1:D:548:GLY:HA2	1:D:551:GLN:HE22	1.63	0.63
1:B:488:ASP:O	1:B:489:ILE:HD13	1.98	0.63
1:B:489:ILE:CG1	1:B:492:MET:HG2	2.27	0.63
1:E:608:ARG:O	1:E:612:LYS:HG2	1.98	0.63
1:A:428:ARG:HD3	1:A:446:ILE:HG22	1.81	0.63
1:A:424:TYR:HB3	1:A:526:PRO:CB	2.29	0.63
1:C:597:GLU:CG	2:C:775:HOH:O	2.47	0.63
1:C:550:THR:HG23	2:C:816:HOH:O	1.97	0.63
1:A:570:ASN:ND2	1:A:573:ASP:OD2	2.29	0.62
1:C:467:GLN:HB2	1:C:471:ARG:HH21	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:604:LYS:N	2:B:753:HOH:O	2.25	0.62
1:E:531:VAL:HA	1:E:563:LYS:O	2.00	0.62
1:C:472:GLU:HG3	1:C:473:ALA:N	2.13	0.62
1:D:428:ARG:NH1	1:D:428:ARG:HG2	2.14	0.62
1:F:563:LYS:HG2	1:F:585:GLU:HB3	1.82	0.61
1:D:435:ILE:HG23	1:D:505:VAL:HG22	1.81	0.61
1:F:579:GLU:N	2:F:802:HOH:O	2.04	0.61
1:E:519:ILE:HD13	1:E:596:LEU:HD11	1.82	0.61
1:F:421:THR:HB	2:F:769:HOH:O	2.00	0.61
1:E:495:HIS:NE2	1:F:479:ALA:HB2	2.15	0.61
1:A:481:ILE:CD1	1:A:485:THR:HG22	2.30	0.61
1:D:484:TYR:HB3	1:D:612:LYS:O	2.00	0.61
1:B:483:LYS:HD3	1:B:484:TYR:CE1	2.36	0.61
1:C:477:VAL:HG22	1:C:481:ILE:CD1	2.31	0.61
1:F:577:ASP:O	1:F:578:ALA:O	2.17	0.61
1:A:477:VAL:O	1:A:481:ILE:CG2	2.47	0.61
1:D:565:ILE:HD11	1:D:598:HIS:HB3	1.82	0.61
1:E:570:ASN:CG	2:E:734:HOH:O	2.39	0.61
1:F:467:GLN:OE1	2:F:784:HOH:O	2.16	0.61
1:C:485:THR:OG1	1:C:486:GLY:N	2.34	0.61
1:E:491:ASN:C	1:E:492:MET:HG2	2.20	0.61
1:A:475:MET:HE1	1:F:459:ARG:NH2	2.15	0.61
1:F:517:ALA:HB3	2:F:701:HOH:O	2.00	0.61
1:A:470:ALA:O	1:A:474:VAL:CG2	2.37	0.61
1:A:567:PRO:O	1:A:570:ASN:HB2	2.01	0.61
1:D:443:LEU:HD21	1:D:466:LEU:HD13	1.81	0.61
1:D:480:ILE:HD11	1:D:613:PHE:HE1	1.66	0.60
1:B:487:ARG:HD2	1:B:488:ASP:O	2.01	0.60
1:E:599:VAL:HG23	1:E:600:LEU:N	2.16	0.60
1:E:611:SER:O	1:E:614:LYS:CD	2.48	0.60
1:E:496:ILE:HD11	1:E:518:VAL:CG2	2.31	0.60
1:D:571:ILE:CD1	1:D:588:PRO:HG3	2.31	0.60
1:F:511:SER:OG	1:F:514:ILE:HD12	2.00	0.60
1:C:577:ASP:OD2	1:C:580:HIS:CB	2.50	0.60
1:B:592:ILE:HG23	1:B:593:ASN:N	2.16	0.60
1:B:418:LEU:HD11	2:C:808:HOH:O	2.01	0.60
1:B:563:LYS:CG	1:B:587:ILE:HD11	2.26	0.60
1:B:558:GLN:HE21	1:B:558:GLN:N	1.99	0.60
1:E:575:LEU:HB2	2:E:635:HOH:O	2.02	0.59
1:B:482:LYS:HD2	2:B:784:HOH:O	2.01	0.59
1:A:449:VAL:HG12	1:A:494:VAL:HG22	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:547:GLY:O	1:F:552:LYS:HE3	2.02	0.59
1:B:508:ASP:HA	2:B:633:HOH:O	2.01	0.59
1:C:550:THR:HA	2:C:816:HOH:O	2.01	0.59
1:E:528:ASP:HB3	1:E:531:VAL:CG2	2.33	0.59
1:C:477:VAL:HG22	1:C:481:ILE:HD12	1.83	0.59
1:C:472:GLU:CG	1:C:473:ALA:H	2.09	0.59
1:B:525:ILE:CG2	1:B:600:LEU:HD22	2.31	0.59
1:C:420:ILE:CG2	1:C:420:ILE:CA	2.78	0.59
1:E:425:GLU:N	1:E:526:PRO:CB	2.65	0.59
1:E:440:GLY:N	2:E:739:HOH:O	2.36	0.59
1:E:540:LYS:CD	2:E:657:HOH:O	2.51	0.59
1:F:558:GLN:HG3	2:F:842:HOH:O	2.01	0.58
1:E:596:LEU:O	1:E:597:GLU:C	2.42	0.58
1:B:551:GLN:H	1:B:551:GLN:CD	2.06	0.58
1:A:429:VAL:HG22	1:A:527:VAL:HG11	1.85	0.58
1:A:432:LEU:HG	1:A:532:ALA:HB1	1.84	0.58
1:A:487:ARG:HG2	1:A:487:ARG:NH1	2.08	0.58
1:A:428:ARG:HA	1:A:445:ILE:O	2.02	0.58
1:F:514:ILE:O	1:F:518:VAL:HG23	2.03	0.58
1:F:612:LYS:HG2	2:F:699:HOH:O	2.03	0.58
1:E:553:ILE:HD11	1:E:566:ILE:CD1	2.33	0.58
1:A:420:ILE:HB	1:A:529:GLN:HG3	1.86	0.58
1:A:428:ARG:CD	1:A:446:ILE:CG2	2.82	0.58
1:F:571:ILE:O	1:F:574:VAL:HG23	2.04	0.58
2:C:755:HOH:O	1:D:540:LYS:HE3	2.04	0.57
1:E:428:ARG:HG2	1:E:429:VAL:N	2.20	0.57
1:B:467:GLN:HG3	2:B:762:HOH:O	2.05	0.57
1:F:435:ILE:HG23	1:F:505:VAL:HG22	1.85	0.57
1:B:592:ILE:CG2	1:B:593:ASN:N	2.67	0.57
1:E:588:PRO:HG2	2:E:760:HOH:O	2.05	0.57
1:A:468:GLU:OE1	2:A:649:HOH:O	2.18	0.57
1:C:502:TYR:CD2	1:C:505:VAL:HG21	2.39	0.57
1:F:475:MET:HB2	2:F:705:HOH:O	2.04	0.57
1:D:422:GLU:HG2	1:D:423:GLY:H	1.67	0.57
1:F:483:LYS:O	1:F:484:TYR:HD1	1.88	0.57
1:A:555:ALA:O	1:A:558:GLN:HB3	2.05	0.57
1:F:469:ILE:CG2	2:F:815:HOH:O	2.48	0.57
1:A:589:VAL:HG21	1:A:595:VAL:HG23	1.87	0.56
1:B:513:SER:HB2	2:B:769:HOH:O	2.05	0.56
1:B:449:VAL:HG13	1:B:521:ALA:HB1	1.86	0.56
1:B:609:LEU:HD12	1:B:609:LEU:O	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:457:GLU:HG2	2:B:689:HOH:O	2.05	0.56
1:A:549:VAL:HG13	1:A:553:ILE:CD1	2.35	0.56
1:A:435:ILE:HG12	1:A:441:ILE:HG23	1.87	0.56
1:A:481:ILE:HD11	1:A:487:ARG:HB2	1.87	0.56
1:B:545:PRO:HA	1:B:567:PRO:CB	2.36	0.56
1:D:472:GLU:HB2	2:D:777:HOH:O	2.06	0.56
1:B:489:ILE:HG12	1:B:522:ILE:HD12	1.87	0.56
1:C:428:ARG:HG2	1:C:446:ILE:HG23	1.86	0.56
1:E:525:ILE:HG21	1:E:600:LEU:HD13	1.87	0.56
1:F:538:SER:O	1:F:541:GLY:N	2.31	0.56
1:C:420:ILE:CD1	1:C:420:ILE:HG23	2.36	0.55
1:F:472:GLU:O	1:F:473:ALA:C	2.44	0.55
1:F:446:ILE:HD12	1:F:497:GLN:HB2	1.88	0.55
1:B:474:VAL:HG22	1:B:518:VAL:HG21	1.88	0.55
1:B:478:SER:C	1:B:482:LYS:HD3	2.26	0.55
1:C:428:ARG:HD3	1:C:446:ILE:HG12	1.87	0.55
1:B:480:ILE:HD12	1:B:613:PHE:HE2	1.71	0.55
1:A:428:ARG:CD	1:A:446:ILE:HG23	2.37	0.55
1:B:419:PHE:HA	1:B:428:ARG:NH2	2.21	0.55
1:B:509:SER:O	1:B:510:ALA:C	2.45	0.55
1:E:610:MET:O	1:E:613:PHE:HB2	2.07	0.55
1:C:469:ILE:O	1:C:472:GLU:HG2	2.07	0.55
1:D:474:VAL:HG22	1:D:518:VAL:HG21	1.88	0.55
1:E:434:VAL:HG12	1:E:439:ALA:O	2.06	0.55
1:E:551:GLN:CD	1:E:551:GLN:H	2.10	0.55
1:E:484:TYR:CB	1:E:613:PHE:HD1	2.20	0.55
1:B:545:PRO:HA	1:B:567:PRO:CG	2.37	0.55
1:E:495:HIS:HE2	1:F:479:ALA:HB2	1.72	0.55
1:D:441:ILE:HD11	1:D:505:VAL:HG13	1.89	0.55
1:A:438:SER:O	1:A:439:ALA:C	2.45	0.55
1:E:540:LYS:CG	2:E:657:HOH:O	2.41	0.54
1:B:449:VAL:HG21	1:B:522:ILE:HD13	1.89	0.54
1:A:558:GLN:HB3	2:A:636:HOH:O	2.06	0.54
1:E:527:VAL:HG13	1:E:599:VAL:HB	1.89	0.54
1:B:477:VAL:HG13	1:B:477:VAL:O	2.05	0.54
1:C:516:THR:HG23	1:C:596:LEU:CD2	2.37	0.54
1:B:600:LEU:HB2	1:B:606:LYS:HG3	1.88	0.54
1:B:444:PRO:HD2	1:B:499:VAL:O	2.07	0.54
1:A:611:SER:O	1:A:614:LYS:HD3	2.07	0.54
1:F:466:LEU:HD23	1:F:469:ILE:HD12	1.89	0.54
1:B:428:ARG:HH11	1:B:446:ILE:HD11	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:465:ARG:HD3	2:B:687:HOH:O	2.07	0.54
1:D:424:TYR:HB3	1:D:526:PRO:HB2	1.89	0.54
1:F:429:VAL:HG22	1:F:527:VAL:HG11	1.89	0.54
1:D:548:GLY:O	1:D:552:LYS:HG3	2.07	0.54
1:B:484:TYR:CD2	1:B:613:PHE:CE2	2.94	0.54
1:B:428:ARG:NH1	1:B:446:ILE:HD11	2.22	0.54
1:A:570:ASN:HA	1:A:573:ASP:OD2	2.08	0.54
1:B:610:MET:C	2:B:648:HOH:O	2.45	0.54
1:C:532:ALA:HB2	1:C:561:LEU:HD13	1.90	0.54
1:F:553:ILE:HG23	1:F:584:ILE:HG21	1.89	0.54
1:C:435:ILE:HD13	1:C:435:ILE:HG21	1.89	0.54
1:B:508:ASP:C	2:B:633:HOH:O	2.28	0.54
1:B:535:GLY:HA2	1:B:567:PRO:HG3	1.89	0.54
1:C:435:ILE:HG21	1:C:435:ILE:CD1	2.38	0.54
1:B:558:GLN:HE21	1:B:558:GLN:H	1.56	0.54
1:D:478:SER:HB3	1:D:489:ILE:HD12	1.89	0.53
1:B:424:TYR:HA	1:B:527:VAL:O	2.08	0.53
1:C:511:SER:N	2:C:719:HOH:O	2.37	0.53
1:E:425:GLU:N	1:E:526:PRO:HB2	2.20	0.53
1:E:606:LYS:O	1:E:610:MET:HG2	2.08	0.53
1:C:577:ASP:OD2	1:C:580:HIS:ND1	2.41	0.53
1:B:489:ILE:O	1:B:489:ILE:HG23	2.08	0.53
1:A:457:GLU:HG2	1:A:490:SER:O	2.08	0.53
1:F:592:ILE:HG23	1:F:593:ASN:N	2.22	0.53
1:D:445:ILE:CD1	1:D:513:SER:HB2	2.39	0.53
1:C:464:GLY:O	1:C:467:GLN:HG2	2.09	0.53
1:F:543:VAL:HG12	1:F:567:PRO:HB3	1.90	0.53
1:F:433:ALA:O	1:F:440:GLY:HA2	2.09	0.53
1:B:489:ILE:CG1	1:B:492:MET:CG	2.82	0.53
1:F:475:MET:HG3	2:F:723:HOH:O	2.08	0.53
1:B:469:ILE:HG22	1:B:514:ILE:HD12	1.90	0.53
1:E:428:ARG:HG3	1:E:446:ILE:HG13	1.91	0.53
1:E:592:ILE:O	1:E:595:VAL:HB	2.07	0.53
1:E:576:LEU:CD2	1:E:580:HIS:CG	2.92	0.53
1:E:568:LYS:O	1:E:571:ILE:HG12	2.08	0.53
1:D:444:PRO:HD2	1:D:502:TYR:OH	2.08	0.53
1:C:577:ASP:OD2	1:C:580:HIS:CG	2.62	0.52
1:D:538:SER:OG	1:D:542:GLU:CG	2.56	0.52
1:E:484:TYR:CB	1:E:613:PHE:CD1	2.92	0.52
1:D:465:ARG:NH1	1:D:465:ARG:HG3	2.16	0.52
1:C:500:GLY:N	2:C:641:HOH:O	2.33	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:430:ASN:O	1:E:533:MET:N	2.42	0.52
1:E:614:LYS:N	2:E:666:HOH:O	2.41	0.52
1:A:568:LYS:O	1:A:571:ILE:HD12	2.09	0.52
1:E:539:VAL:O	1:E:539:VAL:HG12	2.08	0.52
1:E:430:ASN:HB2	1:E:532:ALA:HA	1.91	0.52
1:F:483:LYS:HG2	1:F:484:TYR:CE1	2.43	0.52
1:E:570:ASN:OD1	2:E:734:HOH:O	2.19	0.52
1:D:535:GLY:N	2:D:749:HOH:O	2.08	0.52
1:F:472:GLU:HG3	1:F:473:ALA:H	1.75	0.52
1:C:516:THR:HG23	1:C:596:LEU:HD23	1.92	0.52
1:C:566:ILE:O	1:C:588:PRO:HA	2.10	0.52
1:A:591:ARG:NE	2:A:753:HOH:O	2.42	0.52
1:D:420:ILE:HB	1:D:529:GLN:HG3	1.91	0.52
2:A:628:HOH:O	1:F:501:THR:HG22	2.10	0.52
1:E:422:GLU:OE2	1:E:422:GLU:CA	2.59	0.51
1:C:597:GLU:CB	2:C:775:HOH:O	2.27	0.51
1:A:481:ILE:CD1	1:A:485:THR:CG2	2.87	0.51
1:E:499:VAL:O	1:E:502:TYR:HE1	1.94	0.51
1:F:445:ILE:HD12	1:F:513:SER:HB2	1.91	0.51
1:F:488:ASP:OD2	1:F:490:SER:OG	2.25	0.51
1:E:579:GLU:O	1:E:580:HIS:ND1	2.44	0.51
1:B:435:ILE:HD11	1:B:502:TYR:HB3	1.90	0.51
1:C:472:GLU:OE1	1:C:509:SER:HA	2.11	0.51
1:F:531:VAL:HG22	1:F:563:LYS:HB2	1.93	0.51
1:B:457:GLU:HG3	1:B:458:GLY:H	1.75	0.51
1:E:438:SER:O	1:E:439:ALA:HB2	2.10	0.51
1:B:585:GLU:CG	2:B:653:HOH:O	2.58	0.51
1:D:548:GLY:HA2	1:D:551:GLN:NE2	2.25	0.51
1:D:540:LYS:HG2	1:D:540:LYS:O	2.11	0.51
1:E:421:THR:HG22	1:E:421:THR:O	2.11	0.51
1:E:445:ILE:HG22	1:E:446:ILE:N	2.26	0.51
1:E:565:ILE:HG12	1:E:587:ILE:HB	1.92	0.51
1:B:459:ARG:HH11	1:B:459:ARG:HB3	1.76	0.51
1:F:418:LEU:HG	1:F:499:VAL:O	2.10	0.51
1:B:477:VAL:HG11	1:B:518:VAL:HG11	1.93	0.51
1:A:421:THR:HG22	1:A:561:LEU:HD23	1.92	0.51
1:F:445:ILE:HD11	2:F:813:HOH:O	2.10	0.51
1:B:457:GLU:CD	2:B:689:HOH:O	2.49	0.51
1:C:592:ILE:O	1:C:595:VAL:HB	2.10	0.51
1:F:446:ILE:HD11	1:F:497:GLN:HB2	1.91	0.51
1:B:479:ALA:HA	2:B:775:HOH:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:545:PRO:HA	1:B:567:PRO:HB2	1.93	0.50
1:D:568:LYS:CA	1:D:588:PRO:HB2	2.40	0.50
1:B:512:ILE:O	1:B:513:SER:C	2.50	0.50
1:E:451:PRO:HA	1:E:492:MET:HA	1.92	0.50
1:E:496:ILE:HD11	1:E:518:VAL:HG22	1.92	0.50
1:D:613:PHE:O	1:D:615:GLU:N	2.36	0.50
1:E:499:VAL:O	1:E:502:TYR:CE1	2.65	0.50
1:A:545:PRO:HG3	1:A:569:ASP:HB3	1.93	0.50
1:D:591:ARG:HB2	1:D:593:ASN:OD1	2.10	0.50
1:F:570:ASN:ND2	1:F:573:ASP:OD2	2.40	0.50
1:E:417:LYS:HD2	1:E:419:PHE:O	2.11	0.50
1:E:614:LYS:CA	2:E:666:HOH:O	2.56	0.50
1:A:421:THR:O	1:A:530:SER:HB3	2.10	0.50
1:A:475:MET:HE1	1:F:459:ARG:HH22	1.73	0.50
1:B:438:SER:CA	1:B:551:GLN:HG2	2.42	0.50
1:B:577:ASP:O	1:B:578:ALA:C	2.50	0.50
1:C:435:ILE:CD1	1:C:435:ILE:CG2	2.90	0.50
1:A:475:MET:HE2	1:F:459:ARG:NH2	2.25	0.50
1:C:562:LYS:O	1:C:584:ILE:HG13	2.11	0.50
1:B:474:VAL:CG2	1:B:496:ILE:HD11	2.41	0.50
1:C:537:LEU:HG	1:C:538:SER:O	2.11	0.50
1:F:432:LEU:HD21	1:F:556:ALA:HB2	1.92	0.50
1:D:477:VAL:HG21	1:D:519:ILE:HG13	1.93	0.50
1:D:502:TYR:HB3	1:D:505:VAL:HG21	1.94	0.50
1:F:417:LYS:HG3	1:F:418:LEU:N	2.26	0.50
1:C:592:ILE:HG23	1:C:593:ASN:N	2.27	0.50
1:B:613:PHE:O	1:B:614:LYS:HB3	2.12	0.50
1:A:477:VAL:HG22	1:A:519:ILE:HD11	1.93	0.49
1:A:475:MET:HE2	1:F:459:ARG:HH22	1.74	0.49
1:C:593:ASN:HB3	1:C:613:PHE:CD1	2.47	0.49
1:B:583:LYS:O	1:B:584:ILE:HB	2.12	0.49
1:F:475:MET:HB2	2:F:751:HOH:O	2.12	0.49
1:E:492:MET:HE1	1:E:522:ILE:HG12	1.93	0.49
1:A:446:ILE:H	1:A:446:ILE:HD13	1.78	0.49
1:B:512:ILE:HG13	1:B:513:SER:H	1.78	0.49
1:D:532:ALA:HB2	1:D:561:LEU:HD13	1.95	0.49
1:E:584:ILE:HG12	1:E:585:GLU:N	2.27	0.49
1:B:477:VAL:HG13	1:B:481:ILE:HD12	1.95	0.49
1:D:417:LYS:HG2	2:D:768:HOH:O	2.12	0.49
1:A:481:ILE:HD12	1:A:485:THR:HG22	1.93	0.49
1:D:571:ILE:HD11	1:D:588:PRO:CG	2.37	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:438:SER:HB2	1:B:551:GLN:HG2	1.93	0.49
1:D:563:LYS:HE2	1:D:585:GLU:OE2	2.13	0.49
1:E:422:GLU:OE2	1:E:422:GLU:C	2.50	0.49
1:E:420:ILE:HD12	1:E:425:GLU:OE1	2.12	0.49
1:B:489:ILE:HD12	1:B:492:MET:HG2	1.91	0.49
1:F:591:ARG:N	1:F:594:GLU:OE1	2.43	0.49
1:A:428:ARG:HD3	1:A:446:ILE:HG23	1.94	0.49
1:E:444:PRO:O	1:E:499:VAL:HG23	2.12	0.49
1:A:610:MET:C	1:A:612:LYS:H	2.16	0.49
1:D:484:TYR:HB2	2:D:778:HOH:O	2.12	0.49
1:A:464:GLY:HA3	2:A:652:HOH:O	2.13	0.49
1:D:614:LYS:O	1:D:615:GLU:HB2	2.12	0.48
1:D:613:PHE:C	1:D:615:GLU:N	2.66	0.48
1:B:461:ILE:N	1:B:494:VAL:O	2.36	0.48
1:C:424:TYR:CE1	1:C:528:ASP:HB2	2.48	0.48
1:A:591:ARG:HD2	1:A:593:ASN:OD1	2.12	0.48
1:E:591:ARG:N	1:E:594:GLU:OE1	2.46	0.48
1:A:509:SER:O	1:A:510:ALA:C	2.51	0.48
1:E:450:THR:HG23	2:F:803:HOH:O	1.89	0.48
1:E:601:GLU:CG	1:E:602:ASP:H	2.13	0.48
1:B:427:GLY:O	1:B:447:ALA:N	2.43	0.48
1:E:592:ILE:O	1:E:595:VAL:N	2.46	0.48
1:B:508:ASP:CA	2:B:633:HOH:O	2.56	0.48
1:E:564:VAL:HG12	1:E:584:ILE:CD1	2.43	0.48
1:B:480:ILE:HD11	1:B:613:PHE:CZ	2.48	0.48
1:E:451:PRO:HA	1:E:492:MET:HB3	1.95	0.48
1:F:424:TYR:HB3	1:F:526:PRO:HB2	1.96	0.48
1:D:577:ASP:O	1:D:580:HIS:N	2.42	0.48
1:F:566:ILE:HG13	1:F:567:PRO:O	2.13	0.48
1:F:578:ALA:O	1:F:580:HIS:N	2.31	0.48
1:D:489:ILE:HA	1:D:492:MET:HE2	1.96	0.48
1:D:444:PRO:C	1:D:445:ILE:HG13	2.34	0.48
1:D:419:PHE:CE1	1:D:559:ALA:HB1	2.49	0.48
1:E:425:GLU:N	1:E:526:PRO:HB3	2.27	0.47
1:C:563:LYS:HD2	2:C:802:HOH:O	2.14	0.47
1:E:579:GLU:O	1:E:580:HIS:CG	2.67	0.47
1:C:471:ARG:O	1:C:475:MET:HB2	2.13	0.47
1:C:512:ILE:HD11	1:C:534:THR:O	2.13	0.47
1:A:578:ALA:HA	1:A:581:GLU:HB2	1.96	0.47
1:E:531:VAL:HG13	1:E:563:LYS:HB2	1.95	0.47
1:C:445:ILE:HG21	2:C:645:HOH:O	1.99	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:487:ARG:CD	1:B:489:ILE:HD13	2.42	0.47
1:A:569:ASP:O	1:F:417:LYS:N	2.47	0.47
1:C:476:ASN:O	1:C:478:SER:N	2.47	0.47
1:B:489:ILE:CD1	1:B:492:MET:CG	2.90	0.47
1:F:553:ILE:HG12	1:F:564:VAL:HG11	1.96	0.47
1:F:489:ILE:N	1:F:489:ILE:HD13	2.28	0.47
1:E:444:PRO:HD2	1:E:499:VAL:HB	1.95	0.47
1:B:438:SER:CB	1:B:551:GLN:HG2	2.45	0.47
1:C:420:ILE:CD1	1:C:420:ILE:CG2	2.92	0.47
1:E:448:GLU:HG3	1:E:448:GLU:O	2.10	0.47
1:B:482:LYS:HA	1:B:487:ARG:O	2.14	0.47
1:C:484:TYR:HD1	1:C:484:TYR:HA	1.58	0.47
1:E:565:ILE:HG21	1:E:595:VAL:HG22	1.95	0.47
1:C:476:ASN:ND2	1:C:477:VAL:CA	2.77	0.47
1:C:477:VAL:O	1:C:478:SER:C	2.52	0.47
1:C:424:TYR:HA	1:C:527:VAL:O	2.14	0.47
1:F:445:ILE:CG2	2:F:701:HOH:O	2.62	0.47
1:F:472:GLU:OE1	1:F:510:ALA:N	2.48	0.47
1:E:472:GLU:O	1:E:473:ALA:C	2.52	0.47
1:C:497:GLN:C	2:C:826:HOH:O	2.52	0.47
1:D:431:GLY:N	1:D:443:LEU:O	2.45	0.47
1:D:424:TYR:CE1	1:D:528:ASP:HB2	2.50	0.47
1:F:431:GLY:HA3	2:F:813:HOH:O	2.14	0.47
1:A:492:MET:HE1	1:A:522:ILE:HD13	1.97	0.46
1:D:445:ILE:HD13	1:D:514:ILE:HG12	1.97	0.46
1:E:497:GLN:NE2	1:F:539:VAL:HG22	2.30	0.46
1:E:562:LYS:N	1:E:562:LYS:HD2	2.26	0.46
1:E:568:LYS:C	1:E:570:ASN:H	2.18	0.46
1:D:469:ILE:HG22	1:D:514:ILE:HD12	1.96	0.46
1:F:477:VAL:HG22	1:F:481:ILE:CG1	2.44	0.46
1:B:424:TYR:CE1	1:B:528:ASP:HB2	2.51	0.46
1:E:431:GLY:HA2	1:E:513:SER:OG	2.16	0.46
1:D:597:GLU:H	1:D:597:GLU:HG3	1.37	0.46
1:C:420:ILE:HA	1:C:420:ILE:HD13	1.96	0.46
1:F:597:GLU:CG	2:F:817:HOH:O	2.60	0.46
1:B:478:SER:HB2	2:B:759:HOH:O	2.15	0.46
1:A:428:ARG:CD	1:A:446:ILE:HG22	2.42	0.46
1:C:538:SER:HB3	1:C:544:LEU:HD11	1.98	0.46
1:A:589:VAL:HG12	2:A:765:HOH:O	2.15	0.46
1:F:555:ALA:HA	2:F:781:HOH:O	2.15	0.46
1:D:568:LYS:HG3	2:D:626:HOH:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:463:THR:CG2	2:D:773:HOH:O	2.63	0.46
1:E:429:VAL:HG23	1:E:517:ALA:HB2	1.97	0.46
1:E:484:TYR:CG	1:E:613:PHE:HD1	2.34	0.46
1:B:484:TYR:HA	1:B:484:TYR:HD1	1.62	0.46
1:F:550:THR:HG22	2:F:838:HOH:O	2.16	0.46
1:C:494:VAL:HG23	2:C:626:HOH:O	2.15	0.46
1:E:568:LYS:O	1:E:570:ASN:N	2.49	0.45
1:D:489:ILE:CG1	1:D:492:MET:HE3	2.46	0.45
1:B:464:GLY:O	1:B:467:GLN:NE2	2.42	0.45
1:D:553:ILE:O	1:D:556:ALA:HB3	2.16	0.45
1:C:428:ARG:CG	1:C:428:ARG:HH11	2.26	0.45
1:A:424:TYR:CE1	1:A:528:ASP:HB2	2.51	0.45
1:B:457:GLU:OE2	1:B:490:SER:OG	2.35	0.45
1:F:611:SER:O	1:F:614:LYS:HE2	2.16	0.45
1:F:466:LEU:HB3	1:F:498:PHE:CE2	2.50	0.45
1:E:429:VAL:CG1	1:E:430:ASN:N	2.77	0.45
1:A:489:ILE:HG12	1:A:492:MET:CE	2.46	0.45
1:B:433:ALA:HB3	1:B:441:ILE:CG1	2.46	0.45
1:E:424:TYR:HB3	1:E:526:PRO:HB2	1.97	0.45
1:E:477:VAL:O	1:E:481:ILE:HG13	2.16	0.45
1:A:446:ILE:O	1:A:446:ILE:HG12	2.17	0.45
1:B:563:LYS:CG	1:B:585:GLU:CB	2.91	0.45
1:B:451:PRO:HA	1:B:492:MET:CE	2.44	0.45
1:B:476:ASN:O	1:B:479:ALA:HB3	2.17	0.45
1:B:460:VAL:HG11	1:B:471:ARG:HA	1.98	0.45
1:E:605:LYS:HE2	1:E:605:LYS:HB3	1.81	0.45
1:B:459:ARG:HH11	1:B:459:ARG:CB	2.28	0.45
1:B:440:GLY:H	1:B:551:GLN:HB3	1.80	0.45
1:F:566:ILE:HB	1:F:567:PRO:HD2	1.98	0.45
1:D:461:ILE:N	1:D:461:ILE:HD12	2.31	0.45
1:A:568:LYS:HB2	2:A:725:HOH:O	2.16	0.45
1:C:522:ILE:HG23	2:C:750:HOH:O	2.16	0.45
1:F:596:LEU:HD23	1:F:596:LEU:HA	1.70	0.45
1:B:591:ARG:NH2	2:B:677:HOH:O	2.50	0.45
1:C:502:TYR:HE1	2:C:625:HOH:O	1.97	0.45
1:E:598:HIS:O	1:E:599:VAL:HG13	2.17	0.45
1:E:418:LEU:HA	1:F:545:PRO:HG2	1.99	0.45
1:A:481:ILE:HD12	1:A:485:THR:CG2	2.47	0.45
1:C:546:VAL:HG12	2:C:733:HOH:O	2.16	0.45
1:C:576:LEU:HD22	1:C:580:HIS:HB3	1.99	0.45
1:F:475:MET:O	1:F:478:SER:HB3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:538:SER:HB2	1:F:544:LEU:HD11	1.97	0.45
1:B:432:LEU:HD11	1:B:564:VAL:HG23	1.99	0.45
1:B:557:ILE:O	1:B:560:GLY:N	2.48	0.45
1:E:613:PHE:HB3	2:E:745:HOH:O	2.15	0.44
1:F:489:ILE:HA	1:F:489:ILE:HD12	1.50	0.44
1:C:525:ILE:HD13	1:C:606:LYS:N	2.32	0.44
1:B:587:ILE:HA	1:B:588:PRO:HD2	1.61	0.44
1:E:531:VAL:HG21	1:E:599:VAL:HG12	1.99	0.44
1:B:523:GLU:CB	1:B:609:LEU:HD22	2.46	0.44
1:C:563:LYS:HE2	1:C:585:GLU:OE1	2.17	0.44
1:F:577:ASP:C	1:F:578:ALA:O	2.55	0.44
1:D:553:ILE:HG22	1:D:557:ILE:CD1	2.48	0.44
1:C:465:ARG:HD2	1:C:465:ARG:HA	1.78	0.44
1:D:480:ILE:HD11	1:D:613:PHE:CE1	2.49	0.44
1:E:474:VAL:HA	1:E:477:VAL:HG12	1.99	0.44
1:C:563:LYS:HG2	1:C:585:GLU:HB2	2.00	0.44
1:C:492:MET:HE1	1:C:522:ILE:HD11	1.98	0.44
1:B:517:ALA:O	1:B:520:SER:HB3	2.17	0.44
1:D:449:VAL:HG12	1:D:494:VAL:HA	1.99	0.44
1:C:428:ARG:CG	1:C:446:ILE:HG23	2.48	0.44
1:E:563:LYS:HG2	1:E:585:GLU:HB3	1.99	0.44
1:C:463:THR:HG23	1:C:464:GLY:N	2.33	0.44
1:A:596:LEU:HD23	1:A:596:LEU:HA	1.78	0.44
1:E:448:GLU:CD	2:E:731:HOH:O	2.56	0.44
1:E:435:ILE:H	1:E:435:ILE:HG13	1.35	0.44
1:B:419:PHE:CE2	2:B:679:HOH:O	2.56	0.44
1:B:537:LEU:HD13	1:B:592:ILE:HD13	1.99	0.44
1:D:571:ILE:HD13	1:D:571:ILE:HG21	1.77	0.44
1:F:571:ILE:HD13	1:F:571:ILE:HA	1.73	0.44
1:B:445:ILE:HD12	1:B:498:PHE:CD1	2.52	0.44
1:D:471:ARG:O	1:D:475:MET:HB2	2.16	0.44
1:E:577:ASP:OD2	1:E:577:ASP:C	2.56	0.44
1:C:499:VAL:CG1	1:D:545:PRO:HG2	2.47	0.44
1:D:531:VAL:HG13	1:D:563:LYS:HB2	1.99	0.44
1:B:545:PRO:HB2	1:B:570:ASN:ND2	2.33	0.44
1:D:530:SER:O	1:D:562:LYS:N	2.51	0.44
1:A:468:GLU:HG3	2:A:706:HOH:O	2.18	0.44
1:D:556:ALA:O	1:D:557:ILE:C	2.54	0.44
1:E:601:GLU:O	1:E:606:LYS:CD	2.63	0.43
1:A:480:ILE:HD13	1:A:481:ILE:N	2.33	0.43
1:B:489:ILE:O	1:B:489:ILE:CG2	2.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:580:HIS:N	1:A:580:HIS:ND1	2.65	0.43
1:B:427:GLY:O	1:B:446:ILE:HA	2.17	0.43
1:C:420:ILE:CD1	1:C:420:ILE:HA	2.48	0.43
1:F:512:ILE:HD11	1:F:534:THR:O	2.18	0.43
1:E:484:TYR:HB3	1:E:613:PHE:CD1	2.54	0.43
1:C:463:THR:HG22	1:D:509:SER:HB3	2.00	0.43
1:A:476:ASN:O	1:A:480:ILE:CG2	2.63	0.43
1:B:489:ILE:HD11	1:B:492:MET:SD	2.59	0.43
1:F:593:ASN:HB3	1:F:613:PHE:HD1	1.80	0.43
1:F:445:ILE:CD1	1:F:513:SER:HB2	2.48	0.43
1:E:508:ASP:HB2	2:E:697:HOH:O	2.18	0.43
1:F:457:GLU:CG	2:F:772:HOH:O	2.67	0.43
1:B:450:THR:HG22	1:C:483:LYS:HE3	2.00	0.43
1:F:612:LYS:CG	2:F:699:HOH:O	2.63	0.43
1:B:484:TYR:HD2	1:B:613:PHE:HE2	1.61	0.43
1:B:570:ASN:HD22	1:B:570:ASN:HA	1.64	0.43
1:D:419:PHE:HD1	1:D:421:THR:HG23	1.84	0.43
1:E:465:ARG:NH2	1:E:503:GLU:HG2	2.33	0.43
1:D:608:ARG:HH11	1:D:608:ARG:HG3	1.83	0.43
1:B:604:LYS:CB	2:B:753:HOH:O	2.34	0.43
1:F:563:LYS:HE2	2:F:698:HOH:O	2.19	0.43
1:F:417:LYS:HE3	1:F:417:LYS:HB2	1.42	0.43
1:B:565:ILE:HA	1:B:587:ILE:O	2.19	0.43
1:E:429:VAL:HG12	1:E:430:ASN:H	1.82	0.43
1:A:542:GLU:OE2	1:A:591:ARG:HG3	2.18	0.43
1:E:605:LYS:HG3	2:E:699:HOH:O	2.18	0.43
1:D:483:LYS:HD2	2:D:754:HOH:O	2.19	0.43
1:F:494:VAL:HG23	1:F:496:ILE:HG13	2.00	0.43
1:C:446:ILE:HD12	2:C:826:HOH:O	2.18	0.43
1:B:418:LEU:CD1	1:C:544:LEU:HB3	2.49	0.43
1:D:442:VAL:HG23	2:D:654:HOH:O	2.18	0.43
1:F:477:VAL:HA	1:F:480:ILE:HD12	2.01	0.42
1:B:596:LEU:HD22	1:B:600:LEU:HD11	2.02	0.42
1:A:424:TYR:HB3	1:A:526:PRO:HB2	2.01	0.42
1:B:512:ILE:O	1:B:516:THR:N	2.38	0.42
1:F:614:LYS:HA	2:F:836:HOH:O	2.19	0.42
1:E:601:GLU:CG	1:E:602:ASP:N	2.73	0.42
1:A:489:ILE:O	1:A:489:ILE:CG2	2.66	0.42
1:F:516:THR:HG23	1:F:596:LEU:CD2	2.49	0.42
1:C:418:LEU:CD2	1:C:500:GLY:HA3	2.49	0.42
1:D:489:ILE:HA	1:D:492:MET:CE	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:488:ASP:OD1	1:A:489:ILE:N	2.52	0.42
1:F:548:GLY:O	1:F:552:LYS:HG3	2.19	0.42
1:E:432:LEU:HD23	1:E:432:LEU:HA	1.66	0.42
1:C:437:GLU:N	1:C:437:GLU:OE2	2.52	0.42
1:F:522:ILE:CD1	1:F:522:ILE:CB	2.85	0.42
1:E:480:ILE:O	1:E:484:TYR:HD2	2.02	0.42
1:F:561:LEU:HA	2:F:645:HOH:O	2.19	0.42
1:F:457:GLU:HG2	2:F:772:HOH:O	2.19	0.42
1:C:509:SER:O	1:C:510:ALA:C	2.57	0.42
1:D:542:GLU:HG2	1:D:542:GLU:H	1.24	0.42
1:F:424:TYR:CD1	1:F:601:GLU:HB2	2.54	0.42
1:B:592:ILE:HD12	1:B:592:ILE:HA	1.70	0.42
1:F:424:TYR:HA	1:F:527:VAL:O	2.19	0.42
1:E:437:GLU:HB3	1:E:438:SER:H	1.58	0.42
1:B:579:GLU:OE1	1:B:579:GLU:HA	2.19	0.42
1:C:444:PRO:HD2	2:C:625:HOH:O	2.18	0.42
1:E:564:VAL:HG12	1:E:584:ILE:HD13	2.01	0.42
1:B:494:VAL:HG23	2:B:631:HOH:O	2.20	0.42
1:B:418:LEU:HD21	2:C:733:HOH:O	2.20	0.42
1:B:525:ILE:HD13	1:B:525:ILE:HG21	1.84	0.42
1:D:489:ILE:HG12	1:D:492:MET:HE3	2.02	0.42
1:D:426:VAL:HB	2:D:745:HOH:O	2.19	0.42
1:E:611:SER:C	1:E:613:PHE:H	2.21	0.42
1:C:445:ILE:CD1	1:C:513:SER:HB2	2.50	0.42
1:C:429:VAL:HG22	1:C:527:VAL:HG11	2.02	0.42
1:E:481:ILE:HG22	1:E:487:ARG:HB3	2.02	0.42
1:E:434:VAL:HA	1:E:439:ALA:O	2.19	0.41
1:D:510:ALA:O	1:D:511:SER:C	2.58	0.41
1:C:435:ILE:HB	2:C:824:HOH:O	2.20	0.41
1:F:518:VAL:HG12	1:F:522:ILE:HD12	2.02	0.41
1:B:418:LEU:HD13	1:C:545:PRO:HD2	2.02	0.41
1:F:550:THR:O	1:F:554:GLU:HB2	2.20	0.41
1:D:512:ILE:HG13	1:D:513:SER:N	2.35	0.41
1:B:438:SER:HB2	1:B:551:GLN:CG	2.50	0.41
1:A:438:SER:HB2	1:A:439:ALA:H	1.72	0.41
1:F:571:ILE:HG22	1:F:572:ASP:N	2.35	0.41
1:B:576:LEU:HB2	1:B:581:GLU:HG2	2.02	0.41
1:D:525:ILE:HA	1:D:526:PRO:HD3	1.92	0.41
1:A:511:SER:HA	1:A:535:GLY:O	2.20	0.41
1:E:420:ILE:HG13	1:E:428:ARG:CZ	2.50	0.41
1:E:435:ILE:CG2	2:E:751:HOH:O	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:547:GLY:HA3	1:F:501:THR:CG2	2.50	0.41
1:F:552:LYS:O	1:F:553:ILE:C	2.58	0.41
1:C:435:ILE:N	1:C:439:ALA:O	2.49	0.41
1:F:509:SER:O	1:F:510:ALA:C	2.59	0.41
1:F:509:SER:O	1:F:511:SER:N	2.53	0.41
1:E:450:THR:HG22	2:F:808:HOH:O	2.20	0.41
1:C:545:PRO:HG3	1:C:569:ASP:CB	2.47	0.41
1:A:570:ASN:HD22	1:A:570:ASN:HA	1.76	0.41
1:F:538:SER:C	1:F:540:LYS:N	2.72	0.41
1:E:561:LEU:C	1:E:562:LYS:HD2	2.41	0.41
1:E:484:TYR:HB3	1:E:613:PHE:HD1	1.83	0.41
1:B:474:VAL:HG21	1:B:496:ILE:HD11	2.02	0.41
1:C:473:ALA:HA	1:C:510:ALA:HA	2.02	0.41
1:F:562:LYS:HD3	1:F:562:LYS:HA	1.69	0.41
1:D:418:LEU:HD13	1:D:500:GLY:CA	2.50	0.41
1:B:457:GLU:CG	2:B:689:HOH:O	2.64	0.41
1:A:435:ILE:CG2	1:A:505:VAL:HG22	2.51	0.41
1:A:435:ILE:HG23	1:A:505:VAL:HG22	2.02	0.41
1:A:510:ALA:O	1:A:511:SER:C	2.59	0.41
1:B:419:PHE:CD2	2:B:679:HOH:O	2.74	0.41
1:E:549:VAL:HG11	1:E:573:ASP:HB2	2.01	0.41
1:B:523:GLU:HG3	1:B:609:LEU:CD2	2.40	0.41
1:D:457:GLU:HB3	1:D:490:SER:O	2.20	0.41
1:B:502:TYR:HA	2:B:782:HOH:O	2.20	0.41
1:E:465:ARG:HH22	1:E:503:GLU:HG2	1.85	0.41
1:C:459:ARG:HD2	2:C:825:HOH:O	2.21	0.41
1:E:424:TYR:HA	1:E:527:VAL:O	2.21	0.41
1:B:609:LEU:HD12	1:B:609:LEU:C	2.41	0.41
1:A:526:PRO:HB2	1:A:601:GLU:HB2	2.02	0.41
1:D:505:VAL:HG12	1:D:506:GLU:N	2.36	0.41
1:E:444:PRO:HB2	1:E:499:VAL:HG21	2.02	0.41
1:A:595:VAL:HG12	1:A:596:LEU:N	2.36	0.41
1:A:441:ILE:HG12	1:A:441:ILE:O	2.21	0.41
1:B:500:GLY:HA3	1:B:502:TYR:CE1	2.55	0.41
1:E:473:ALA:HB3	1:E:514:ILE:HG21	2.02	0.41
1:E:498:PHE:CD2	1:E:498:PHE:N	2.88	0.41
1:F:465:ARG:HH11	1:F:465:ARG:HG3	1.85	0.41
1:F:474:VAL:CG2	1:F:496:ILE:HD11	2.51	0.41
1:F:474:VAL:O	1:F:477:VAL:HG13	2.20	0.41
1:F:496:ILE:HD13	1:F:496:ILE:HG21	1.62	0.41
1:B:419:PHE:HA	1:B:428:ARG:HH22	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:445:ILE:HG21	2:F:701:HOH:O	2.20	0.41
1:C:523:GLU:HB2	1:C:525:ILE:HG13	2.03	0.41
1:E:467:GLN:HB2	1:E:471:ARG:NH1	2.36	0.41
1:F:597:GLU:CB	2:F:817:HOH:O	2.35	0.40
1:E:418:LEU:HD13	1:E:419:PHE:H	1.87	0.40
1:A:571:ILE:O	1:A:574:VAL:HB	2.21	0.40
1:F:614:LYS:HB2	1:F:615:GLU:H	1.47	0.40
1:A:469:ILE:HG12	2:A:758:HOH:O	2.20	0.40
1:C:563:LYS:HG2	1:C:585:GLU:CB	2.51	0.40
1:F:592:ILE:HG22	1:F:593:ASN:N	2.35	0.40
1:E:574:VAL:HG12	1:E:575:LEU:N	2.36	0.40
1:F:465:ARG:C	1:F:466:LEU:HG	2.41	0.40
1:E:532:ALA:HB2	1:E:561:LEU:HD12	2.03	0.40
1:E:481:ILE:HG23	1:E:485:THR:HB	2.03	0.40
1:B:519:ILE:HG21	1:B:596:LEU:HD21	2.03	0.40
1:A:492:MET:CE	1:A:522:ILE:HD13	2.52	0.40
1:B:556:ALA:HA	1:B:561:LEU:HD12	2.04	0.40
1:F:537:LEU:HD12	1:F:542:GLU:O	2.22	0.40
1:B:420:ILE:HG21	2:B:700:HOH:O	2.21	0.40
1:B:609:LEU:HA	1:B:612:LYS:HG3	2.02	0.40
1:E:545:PRO:HA	1:E:567:PRO:HG2	2.02	0.40
1:F:428:ARG:HD2	1:F:446:ILE:HG23	2.03	0.40
1:F:592:ILE:HG22	1:F:593:ASN:H	1.85	0.40
1:C:587:ILE:HA	1:C:588:PRO:HD2	1.96	0.40
1:A:536:SER:HB2	1:A:544:LEU:HB2	2.04	0.40
1:C:591:ARG:HB2	1:C:591:ARG:HE	1.59	0.40
1:D:463:THR:HG22	1:E:468:GLU:HB2	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	191/205 (93%)	175 (92%)	13 (7%)	3 (2%)	12	48
1	B	192/205 (94%)	146 (76%)	29 (15%)	17 (9%)	1	4
1	C	192/205 (94%)	163 (85%)	22 (12%)	7 (4%)	4	24
1	D	192/205 (94%)	163 (85%)	21 (11%)	8 (4%)	3	20
1	E	191/205 (93%)	149 (78%)	26 (14%)	16 (8%)	1	5
1	F	192/205 (94%)	165 (86%)	21 (11%)	6 (3%)	5	28
All	All	1150/1230 (94%)	961 (84%)	132 (12%)	57 (5%)	3	15

All (57) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	439	ALA
1	B	438	SER
1	B	440	GLY
1	B	528	ASP
1	B	529	GLN
1	B	571	ILE
1	B	592	ILE
1	B	606	LYS
1	B	607	ASN
1	B	614	LYS
1	C	479	ALA
1	D	489	ILE
1	D	510	ALA
1	E	437	GLU
1	E	439	ALA
1	E	601	GLU
1	F	510	ALA
1	B	505	VAL
1	B	576	LEU
1	B	610	MET
1	D	436	GLY
1	E	484	TYR
1	E	558	GLN
1	E	580	HIS
1	E	599	VAL
1	F	476	ASN
1	F	578	ALA
1	F	614	LYS
1	A	438	SER
1	B	513	SER

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Mol	Chain	Res	Type
1	C	482	LYS
1	D	487	ARG
1	E	425	GLU
1	C	476	ASN
1	C	578	ALA
1	D	509	SER
1	E	568	LYS
1	E	569	ASP
1	E	575	LEU
1	B	595	VAL
1	B	611	SER
1	C	483	LYS
1	D	557	ILE
1	D	614	LYS
1	E	472	GLU
1	E	584	ILE
1	E	611	SER
1	F	475	MET
1	B	424	TYR
1	B	584	ILE
1	C	592	ILE
1	E	524	GLY
1	F	465	ARG
1	C	524	GLY
1	D	588	PRO
1	E	427	GLY
1	A	499	VAL

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%)	130 (81%)	30 (19%)	2	10
1	B	161/168 (96%)	121 (75%)	40 (25%)	1	3
1	C	161/168 (96%)	129 (80%)	32 (20%)	1	8

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	161/168 (96%)	135 (84%)	26 (16%)	3	14
1	E	160/168 (95%)	122 (76%)	38 (24%)	1	4
1	F	161/168 (96%)	130 (81%)	31 (19%)	2	9
All	All	964/1008 (96%)	767 (80%)	197 (20%)	1	7

All (197) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	422	GLU
1	A	435	ILE
1	A	438	SER
1	A	441	ILE
1	A	446	ILE
1	A	457	GLU
1	A	465	ARG
1	A	477	VAL
1	A	480	ILE
1	A	481	ILE
1	A	485	THR
1	A	487	ARG
1	A	491	ASN
1	A	501	THR
1	A	506	GLU
1	A	539	VAL
1	A	540	LYS
1	A	542	GLU
1	A	562	LYS
1	A	568	LYS
1	A	570	ASN
1	A	574	VAL
1	A	579	GLU
1	A	580	HIS
1	A	584	ILE
1	A	597	GLU
1	A	608	ARG
1	A	610	MET
1	A	611	SER
1	A	614	LYS
1	B	417	LYS
1	B	418	LEU
1	B	419	PHE

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Mol	Chain	Res	Type
1	B	420	ILE
1	B	421	THR
1	B	422	GLU
1	B	443	LEU
1	B	449	VAL
1	B	453	MET
1	B	459	ARG
1	B	463	THR
1	B	467	GLN
1	B	475	MET
1	B	480	ILE
1	B	482	LYS
1	B	485	THR
1	B	487	ARG
1	B	489	ILE
1	B	490	SER
1	B	491	ASN
1	B	492	MET
1	B	502	TYR
1	B	505	VAL
1	B	518	VAL
1	B	539	VAL
1	B	540	LYS
1	B	551	GLN
1	B	558	GLN
1	B	563	LYS
1	B	569	ASP
1	B	571	ILE
1	B	579	GLU
1	B	588	PRO
1	B	591	ARG
1	B	592	ILE
1	B	593	ASN
1	B	604	LYS
1	B	605	LYS
1	B	608	ARG
1	B	609	LEU
1	C	417	LYS
1	C	419	PHE
1	C	428	ARG
1	C	435	ILE
1	C	437	GLU

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Mol	Chain	Res	Type
1	C	441	ILE
1	C	446	ILE
1	C	463	THR
1	C	476	ASN
1	C	477	VAL
1	C	480	ILE
1	C	482	LYS
1	C	485	THR
1	C	487	ARG
1	C	501	THR
1	C	502	TYR
1	C	509	SER
1	C	513	SER
1	C	514	ILE
1	C	539	VAL
1	C	540	LYS
1	C	542	GLU
1	C	549	VAL
1	C	571	ILE
1	C	577	ASP
1	C	585	GLU
1	C	591	ARG
1	C	593	ASN
1	C	597	GLU
1	C	608	ARG
1	C	614	LYS
1	C	615	GLU
1	D	424	TYR
1	D	428	ARG
1	D	435	ILE
1	D	441	ILE
1	D	453	MET
1	D	459	ARG
1	D	465	ARG
1	D	471	ARG
1	D	480	ILE
1	D	482	LYS
1	D	487	ARG
1	D	501	THR
1	D	503	GLU
1	D	513	SER
1	D	529	GLN

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Mol	Chain	Res	Type
1	D	542	GLU
1	D	551	GLN
1	D	565	ILE
1	D	568	LYS
1	D	583	LYS
1	D	591	ARG
1	D	597	GLU
1	D	601	GLU
1	D	604	LYS
1	D	608	ARG
1	D	611	SER
1	E	418	LEU
1	E	420	ILE
1	E	422	GLU
1	E	434	VAL
1	E	435	ILE
1	E	438	SER
1	E	446	ILE
1	E	448	GLU
1	E	459	ARG
1	E	465	ARG
1	E	466	LEU
1	E	475	MET
1	E	478	SER
1	E	482	LYS
1	E	488	ASP
1	E	490	SER
1	E	492	MET
1	E	501	THR
1	E	503	GLU
1	E	505	VAL
1	E	522	ILE
1	E	523	GLU
1	E	531	VAL
1	E	540	LYS
1	E	549	VAL
1	E	551	GLN
1	E	558	GLN
1	E	562	LYS
1	E	566	ILE
1	E	571	ILE
1	E	583	LYS

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Mol	Chain	Res	Type
1	E	584	ILE
1	E	585	GLU
1	E	600	LEU
1	E	605	LYS
1	E	608	ARG
1	E	612	LYS
1	E	614	LYS
1	F	417	LYS
1	F	418	LEU
1	F	420	ILE
1	F	435	ILE
1	F	437	GLU
1	F	438	SER
1	F	446	ILE
1	F	457	GLU
1	F	459	ARG
1	F	465	ARG
1	F	472	GLU
1	F	478	SER
1	F	482	LYS
1	F	485	THR
1	F	487	ARG
1	F	489	ILE
1	F	501	THR
1	F	502	TYR
1	F	509	SER
1	F	513	SER
1	F	539	VAL
1	F	540	LYS
1	F	562	LYS
1	F	571	ILE
1	F	579	GLU
1	F	583	LYS
1	F	591	ARG
1	F	593	ASN
1	F	605	LYS
1	F	614	LYS
1	F	615	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	551	GLN
1	B	558	GLN
1	C	476	ASN
1	C	551	GLN
1	D	551	GLN
1	D	558	GLN
1	E	497	GLN
1	E	529	GLN
1	E	607	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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%)	-0.72	1 (0%) 91 76	2, 6, 29, 44	0
1	B	196/205 (95%)	-0.34	4 (2%) 68 39	2, 15, 49, 67	0
1	C	196/205 (95%)	-0.71	1 (0%) 91 76	2, 5, 28, 48	0
1	D	196/205 (95%)	-0.72	1 (0%) 91 76	2, 5, 25, 42	0
1	E	195/205 (95%)	-0.38	2 (1%) 84 60	2, 13, 44, 61	0
1	F	196/205 (95%)	-0.67	0 100 100	2, 7, 34, 68	0
All	All	1174/1230 (95%)	-0.59	9 (0%) 87 67	2, 9, 38, 68	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	453	MET	3.9
1	B	615	GLU	3.2
1	E	417	LYS	3.1
1	C	453	MET	2.4
1	A	453	MET	2.3
1	D	437	GLU	2.3
1	B	421	THR	2.3
1	E	418	LEU	2.3
1	B	418	LEU	2.2

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 carbohydrates 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.