Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 09:11 AM GMT

PDB ID	:	3HIF
Title	:	The crystal structure of apo wild type CAP at 3.6 A resolution.
Authors	:	Steitz, T.A.; Sharma, H.; Wang, J.; Kong, J.; Yu, S.
Deposited on	:	2009-05-19
Resolution	:	3.59 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

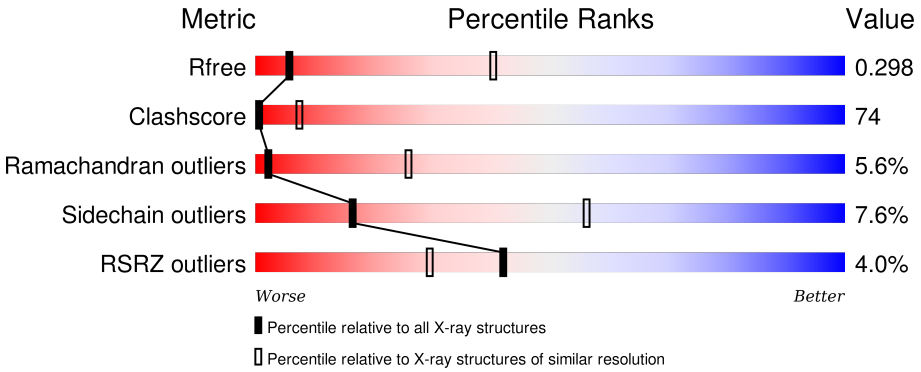
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.59 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	1408 (3.80-3.40)
Clashscore	102246	1010 (3.74-3.46)
Ramachandran outliers	100387	1007 (3.76-3.44)
Sidechain outliers	100360	1007 (3.76-3.44)
RSRZ outliers	91569	1003 (3.78-3.42)

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 <=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	210	3% 43% 39% 9% • 5%
1	B	210	45% 35% 12% • 5%
1	C	210	3% 40% 40% 11% • 5%
1	D	210	2% 53% 33% 8% • 5%
1	E	210	10% 38% 44% 10% • 5%

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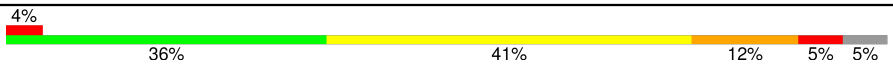
Mol	Chain	Length	Quality of chain
1	F	210	

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 9456 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 Catabolite gene activator.

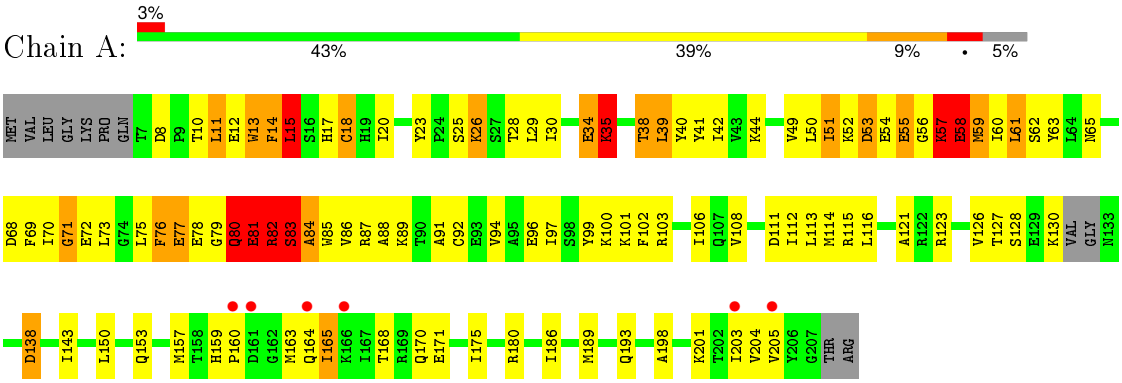
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	199	Total	C	N	O	S	0	0	0
			1576	998	275	294	9			
1	B	199	Total	C	N	O	S	0	0	0
			1576	998	275	294	9			
1	C	199	Total	C	N	O	S	0	0	0
			1576	998	275	294	9			
1	D	199	Total	C	N	O	S	0	0	0
			1576	998	275	294	9			
1	E	199	Total	C	N	O	S	0	0	0
			1576	998	275	294	9			
1	F	199	Total	C	N	O	S	0	0	0
			1576	998	275	294	9			

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 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.

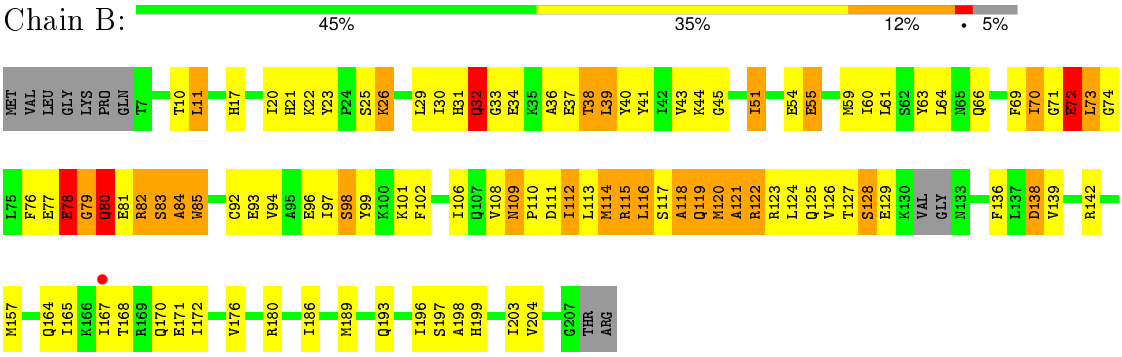
- Molecule 1: Catabolite gene activator

Chain A:



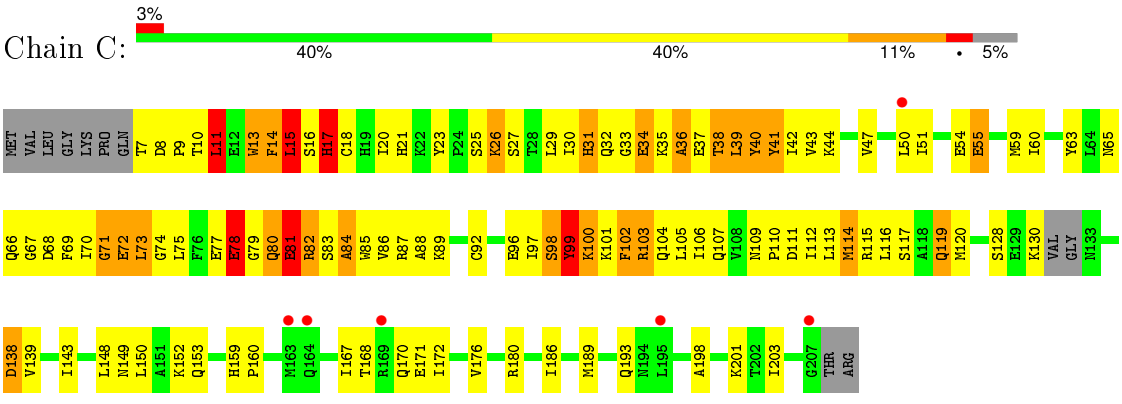
- Molecule 1: Catabolite gene activator

Chain B:



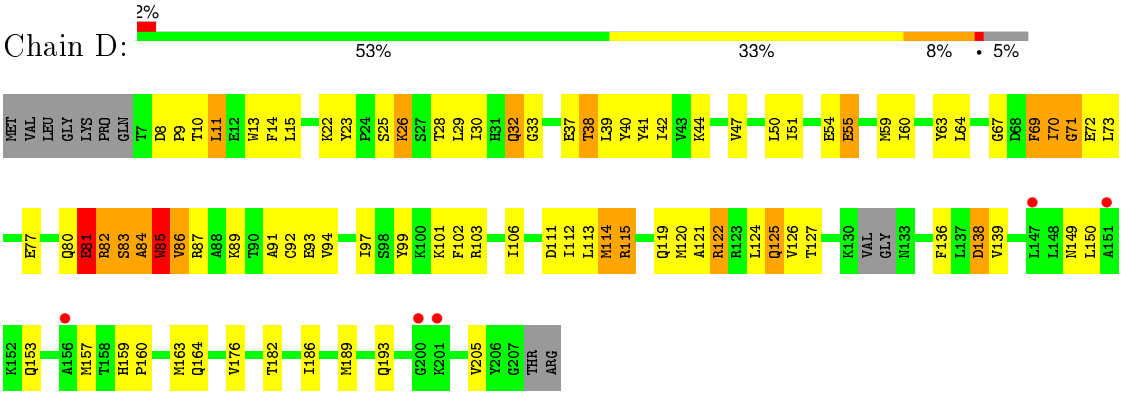
- Molecule 1: Catabolite gene activator

Chain C:



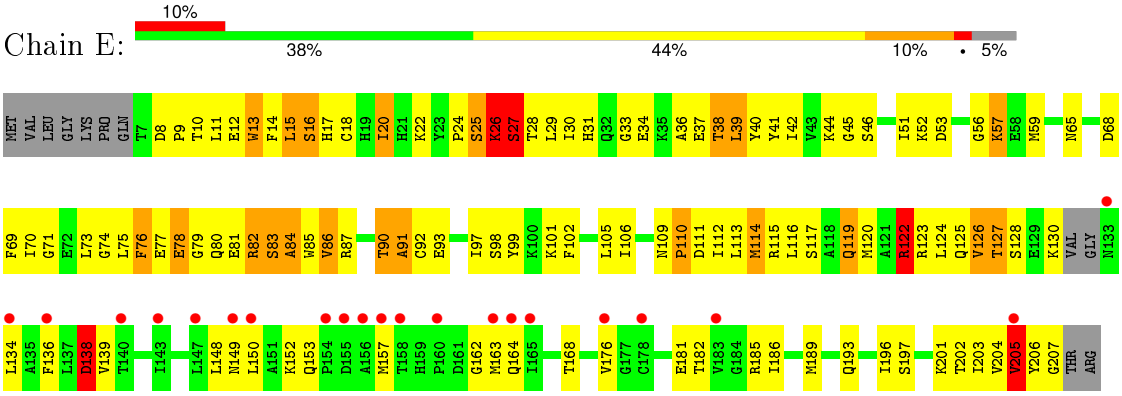
• Molecule 1: Catabolite gene activator

Chain D:



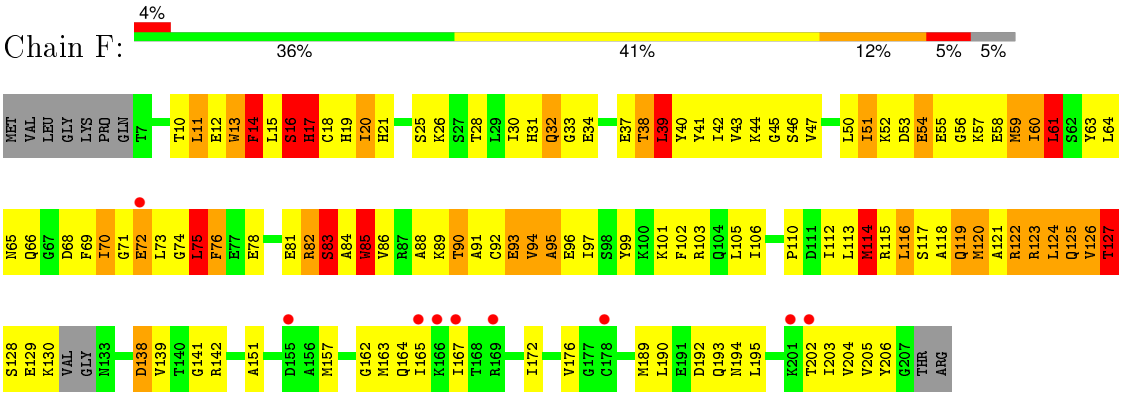
• Molecule 1: Catabolite gene activator

Chain E:



• Molecule 1: Catabolite gene activator

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	125.29Å 125.29Å 224.68Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.06 – 3.59 48.05 – 3.59	Depositor EDS
% Data completeness (in resolution range)	98.9 (48.06-3.59) 98.9 (48.05-3.59)	Depositor EDS
R_{merge}	0.46	Depositor
R_{sym}	0.53	Depositor
$< I/\sigma(I) >$ [1]	1.27 (at 3.57Å)	Xtriage
Refinement program	REFMAC 5.4.0077	Depositor
R, R_{free}	0.295 , 0.318 0.291 , 0.298	Depositor DCC
R_{free} test set	1232 reflections (5.10%)	DCC
Wilson B-factor (Å^2)	100.5	Xtriage
Anisotropy	0.139	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , -10.0	EDS
Estimated twinning fraction	0.043 for -h,-k,l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.31$	Xtriage
Outliers	1 of 24165 reflections (0.004%)	Xtriage
F_o,F_c correlation	0.83	EDS
Total number of atoms	9456	wwPDB-VP
Average B, all atoms (Å^2)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.02% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.54	3/1600 (0.2%)	1.07	19/2154 (0.9%)
1	B	0.71	3/1600 (0.2%)	0.82	11/2154 (0.5%)
1	C	0.65	3/1600 (0.2%)	1.72	23/2154 (1.1%)
1	D	0.54	3/1600 (0.2%)	0.81	13/2154 (0.6%)
1	E	0.51	2/1600 (0.1%)	1.05	16/2154 (0.7%)
1	F	0.54	3/1600 (0.2%)	1.12	28/2154 (1.3%)
All	All	0.59	17/9600 (0.2%)	1.14	110/12924 (0.9%)

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	2
1	B	0	1
1	C	1	3
1	D	0	2
1	E	0	1
1	F	0	2
All	All	1	11

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	112	ILE	CG1-CD1	20.25	2.90	1.50
1	C	78	GLU	C-N	-14.81	1.06	1.33
1	C	138	ASP	CG-OD1	11.91	1.52	1.25
1	A	138	ASP	CG-OD1	11.88	1.52	1.25
1	F	138	ASP	CG-OD1	11.88	1.52	1.25
1	D	138	ASP	CG-OD1	11.86	1.52	1.25
1	B	138	ASP	CG-OD1	11.83	1.52	1.25
1	E	138	ASP	CG-OD1	11.83	1.52	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	138	ASP	CG-OD2	11.81	1.52	1.25
1	F	138	ASP	CG-OD2	11.79	1.52	1.25
1	A	138	ASP	CG-OD2	11.77	1.52	1.25
1	D	138	ASP	CG-OD2	11.75	1.52	1.25
1	E	138	ASP	CG-OD2	11.72	1.52	1.25
1	B	138	ASP	CG-OD2	11.72	1.52	1.25
1	D	85	TRP	C-N	-9.72	1.11	1.34
1	A	58	GLU	C-N	-8.85	1.13	1.34
1	F	76	PHE	C-N	-5.30	1.21	1.34

All (110) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	82	ARG	N-CA-CB	-40.78	37.20	110.60
1	C	81	GLU	CB-CA-C	-29.48	51.45	110.40
1	C	78	GLU	C-N-CA	26.64	178.25	122.30
1	C	102	PHE	CB-CA-C	-19.82	70.76	110.40
1	E	82	ARG	CB-CA-C	-19.36	71.67	110.40
1	C	81	GLU	N-CA-C	18.05	159.73	111.00
1	C	78	GLU	O-C-N	-17.33	93.75	123.20
1	A	35	LYS	N-CA-CB	16.43	140.17	110.60
1	C	13	TRP	CB-CA-C	-16.13	78.13	110.40
1	E	83	SER	N-CA-CB	-16.10	86.36	110.50
1	A	80	GLN	CB-CA-C	-16.08	78.25	110.40
1	A	59	MET	N-CA-CB	-15.65	82.42	110.60
1	F	12	GLU	CB-CA-C	-15.31	79.78	110.40
1	C	99	TYR	CB-CA-C	-15.23	79.93	110.40
1	F	127	THR	CB-CA-C	-14.78	71.69	111.60
1	B	32	GLN	N-CA-C	14.12	149.13	111.00
1	A	58	GLU	O-C-N	-13.77	100.67	122.70
1	F	120	MET	N-CA-CB	-12.77	87.61	110.60
1	E	122	ARG	CB-CA-C	-12.73	84.94	110.40
1	A	34	GLU	N-CA-C	12.40	144.48	111.00
1	E	26	LYS	CB-CA-C	-12.26	85.88	110.40
1	E	13	TRP	CB-CA-C	-12.22	85.95	110.40
1	A	80	GLN	N-CA-C	12.19	143.91	111.00
1	D	85	TRP	N-CA-C	-12.09	78.35	111.00
1	D	85	TRP	O-C-N	-11.55	104.21	122.70
1	C	78	GLU	CA-C-N	11.45	139.10	116.20
1	E	27	SER	N-CA-C	-11.31	80.47	111.00
1	C	78	GLU	CB-CA-C	-11.07	88.25	110.40
1	F	59	MET	CB-CA-C	10.42	131.25	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	16	SER	CB-CA-C	10.41	129.89	110.10
1	F	32	GLN	N-CA-C	10.22	138.59	111.00
1	B	32	GLN	CB-CA-C	-9.88	90.64	110.40
1	F	17	HIS	N-CA-CB	-9.71	93.11	110.60
1	B	55	GLU	CB-CA-C	-9.54	91.31	110.40
1	E	126	VAL	CB-CA-C	-9.53	93.30	111.40
1	C	79	GLY	N-CA-C	9.50	136.86	113.10
1	C	11	LEU	CB-CA-C	-9.47	92.20	110.20
1	D	69	PHE	CB-CA-C	-9.28	91.84	110.40
1	A	58	GLU	CB-CA-C	-9.12	92.17	110.40
1	D	138	ASP	CB-CG-OD1	-9.02	110.18	118.30
1	E	138	ASP	CB-CG-OD1	-8.80	110.38	118.30
1	F	138	ASP	CB-CG-OD1	-8.80	110.38	118.30
1	E	127	THR	N-CA-CB	-8.71	93.75	110.30
1	F	34	GLU	CB-CA-C	-8.66	93.08	110.40
1	C	138	ASP	CB-CG-OD1	-8.61	110.55	118.30
1	D	55	GLU	CB-CA-C	-8.59	93.23	110.40
1	A	138	ASP	CB-CG-OD1	-8.58	110.58	118.30
1	B	138	ASP	CB-CG-OD1	-8.55	110.60	118.30
1	D	85	TRP	CB-CA-C	8.45	127.30	110.40
1	F	94	VAL	CB-CA-C	-8.38	95.47	111.40
1	A	81	GLU	N-CA-CB	-8.36	95.56	110.60
1	B	138	ASP	CB-CG-OD2	-8.18	110.94	118.30
1	F	73	LEU	CB-CA-C	-8.17	94.68	110.20
1	E	126	VAL	N-CA-C	8.04	132.71	111.00
1	B	98	SER	CB-CA-C	7.94	125.19	110.10
1	A	138	ASP	CB-CG-OD2	-7.91	111.18	118.30
1	D	138	ASP	CB-CG-OD2	-7.86	111.23	118.30
1	C	138	ASP	CB-CG-OD2	-7.84	111.24	118.30
1	F	119	GLN	CB-CA-C	-7.80	94.80	110.40
1	B	112	ILE	CB-CG1-CD1	-7.74	92.24	113.90
1	E	138	ASP	CB-CG-OD2	-7.67	111.40	118.30
1	D	82	ARG	N-CA-CB	-7.59	96.94	110.60
1	A	13	TRP	N-CA-CB	-7.57	96.98	110.60
1	A	52	LYS	CB-CA-C	-7.45	95.51	110.40
1	F	138	ASP	CB-CG-OD2	-7.43	111.61	118.30
1	F	76	PHE	CB-CA-C	-7.21	95.97	110.40
1	F	13	TRP	N-CA-C	-7.14	91.72	111.00
1	D	85	TRP	CA-C-N	7.14	132.91	117.20
1	C	14	PHE	N-CA-CB	-7.08	97.86	110.60
1	C	11	LEU	N-CA-C	7.06	130.06	111.00
1	C	100	LYS	CB-CA-C	-6.95	96.51	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	59	MET	N-CA-C	-6.79	92.66	111.00
1	A	58	GLU	CA-C-N	6.79	132.13	117.20
1	C	99	TYR	N-CA-C	-6.76	92.75	111.00
1	F	95	ALA	N-CA-CB	-6.69	100.73	110.10
1	F	138	ASP	OD1-CG-OD2	-6.66	110.65	123.30
1	F	119	GLN	N-CA-C	6.66	128.97	111.00
1	A	138	ASP	OD1-CG-OD2	-6.61	110.73	123.30
1	B	138	ASP	OD1-CG-OD2	-6.60	110.77	123.30
1	D	70	ILE	N-CA-CB	-6.59	95.65	110.80
1	E	138	ASP	OD1-CG-OD2	-6.58	110.79	123.30
1	C	138	ASP	OD1-CG-OD2	-6.58	110.80	123.30
1	D	138	ASP	OD1-CG-OD2	-6.53	110.90	123.30
1	E	27	SER	N-CA-CB	6.24	119.86	110.50
1	D	86	VAL	N-CA-C	-6.13	94.44	111.00
1	E	205	VAL	CB-CA-C	-6.09	99.84	111.40
1	B	109	ASN	C-N-CD	-6.08	107.21	120.60
1	B	72	GLU	N-CA-C	-6.08	94.60	111.00
1	F	127	THR	C-N-CA	6.04	136.80	121.70
1	C	31	HIS	CB-CA-C	6.02	122.44	110.40
1	F	60	ILE	N-CA-C	-5.97	94.88	111.00
1	E	13	TRP	N-CA-C	5.94	127.03	111.00
1	B	121	ALA	CB-CA-C	-5.75	101.47	110.10
1	F	73	LEU	N-CA-C	5.72	126.45	111.00
1	F	76	PHE	O-C-N	-5.65	113.65	122.70
1	C	39	LEU	CA-CB-CG	-5.52	102.60	115.30
1	A	51	ILE	CB-CA-C	5.49	122.57	111.60
1	C	119	GLN	CB-CA-C	-5.47	99.46	110.40
1	D	81	GLU	N-CA-C	-5.39	96.43	111.00
1	F	114	MET	CB-CA-C	-5.36	99.69	110.40
1	A	53	ASP	N-CA-CB	-5.32	101.02	110.60
1	E	25	SER	CB-CA-C	-5.25	100.12	110.10
1	F	12	GLU	N-CA-C	5.25	125.17	111.00
1	A	51	ILE	N-CA-C	-5.24	96.84	111.00
1	A	81	GLU	N-CA-C	-5.23	96.87	111.00
1	F	32	GLN	CB-CA-C	-5.23	99.94	110.40
1	F	82	ARG	N-CA-C	5.14	124.89	111.00
1	F	39	LEU	CA-CB-CG	-5.04	103.70	115.30
1	C	31	HIS	N-CA-C	-5.04	97.40	111.00
1	A	13	TRP	N-CA-C	-5.01	97.47	111.00

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	C	81	GLU	CA

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	138	ASP	Sidechain
1	A	58	GLU	Mainchain
1	B	138	ASP	Sidechain
1	C	138	ASP	Sidechain
1	C	78	GLU	Mainchain
1	C	99	TYR	Peptide
1	D	138	ASP	Sidechain
1	D	85	TRP	Mainchain
1	E	138	ASP	Sidechain
1	F	127	THR	Peptide
1	F	138	ASP	Sidechain

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	1576	0	1608	196	0
1	B	1576	0	1609	221	0
1	C	1576	0	1608	229	0
1	D	1576	0	1608	131	0
1	E	1576	0	1608	315	0
1	F	1576	0	1608	366	0
All	All	9456	0	9649	1412	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 74.

All (1412) 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:41:TYR:HD1	1:C:69:PHE:CE1	0.96	1.65
1:C:41:TYR:CD1	1:C:69:PHE:CE1	1.86	1.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:51:ILE:HD12	1:F:61:LEU:CG	1.29	1.62
1:E:134:LEU:HG	1:F:195:LEU:CD1	1.21	1.57
1:F:68:ASP:CA	1:F:119:GLN:HE22	1.16	1.56
1:E:134:LEU:CD2	1:F:190:LEU:HD22	1.33	1.55
1:F:51:ILE:CD1	1:F:61:LEU:CG	1.89	1.50
1:D:114:MET:CE	1:D:114:MET:HA	1.42	1.48
1:F:68:ASP:HA	1:F:119:GLN:NE2	1.29	1.47
1:F:51:ILE:CD1	1:F:61:LEU:HD12	1.46	1.45
1:E:117:SER:HA	1:E:120:MET:CE	1.47	1.44
1:E:25:SER:O	1:E:26:LYS:CG	1.65	1.44
1:F:32:GLN:NE2	1:F:85:TRP:CZ3	1.86	1.44
1:F:32:GLN:NE2	1:F:85:TRP:HZ3	1.13	1.44
1:E:39:LEU:HB2	1:E:99:TYR:CE2	1.53	1.43
1:F:51:ILE:CD1	1:F:61:LEU:CD1	1.96	1.43
1:E:84:ALA:CB	1:E:85:TRP:HA	1.31	1.43
1:F:84:ALA:CA	1:F:85:TRP:HB2	1.40	1.42
1:A:81:GLU:HA	1:A:82:ARG:CB	1.18	1.37
1:B:36:ALA:CA	1:B:82:ARG:HH22	1.36	1.36
1:C:80:GLN:O	1:C:81:GLU:HG3	1.21	1.32
1:A:56:GLY:O	1:A:57:LYS:CD	1.77	1.32
1:E:134:LEU:CG	1:F:195:LEU:HD13	1.57	1.31
1:A:81:GLU:CA	1:A:82:ARG:CB	2.08	1.31
1:A:81:GLU:CA	1:A:82:ARG:HB3	1.61	1.30
1:F:121:ALA:O	1:F:124:LEU:HB2	1.29	1.29
1:B:40:TYR:HB2	1:B:70:ILE:CG2	1.63	1.28
1:E:197:SER:OG	1:E:204:VAL:CG1	1.83	1.27
1:E:134:LEU:CG	1:F:195:LEU:CD1	2.14	1.25
1:F:53:ASP:OD2	1:F:54:GLU:HG3	1.31	1.25
1:C:17:HIS:CD2	1:C:105:LEU:HD21	1.71	1.24
1:E:182:THR:O	1:E:186:ILE:HD13	1.36	1.24
1:F:84:ALA:CB	1:F:85:TRP:HB2	1.66	1.23
1:F:116:LEU:O	1:F:116:LEU:HD23	1.33	1.23
1:C:41:TYR:CD1	1:C:69:PHE:HE1	1.36	1.22
1:F:130:LYS:HG2	1:F:189:MET:SD	1.80	1.22
1:A:56:GLY:O	1:A:57:LYS:HD3	1.05	1.22
1:E:197:SER:OG	1:E:204:VAL:HG12	1.33	1.22
1:E:205:VAL:HG12	1:E:206:TYR:N	1.38	1.22
1:C:15:LEU:HD23	1:C:15:LEU:N	1.41	1.21
1:F:51:ILE:CD1	1:F:61:LEU:CB	2.21	1.19
1:C:13:TRP:CG	1:C:13:TRP:O	1.86	1.19
1:F:68:ASP:CA	1:F:119:GLN:NE2	1.86	1.17

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:46:SER:H	1:E:90:THR:CG2	1.57	1.17
1:F:127:THR:HG22	1:F:127:THR:O	1.39	1.17
1:E:205:VAL:CG1	1:E:206:TYR:H	1.44	1.17
1:F:51:ILE:HD11	1:F:61:LEU:CB	1.74	1.16
1:F:116:LEU:C	1:F:116:LEU:HD23	1.59	1.16
1:E:84:ALA:CB	1:E:85:TRP:CA	2.22	1.16
1:E:84:ALA:HB3	1:E:85:TRP:HA	1.22	1.16
1:E:134:LEU:CD2	1:F:190:LEU:CD2	2.23	1.16
1:F:50:LEU:O	1:F:51:ILE:HG12	1.45	1.15
1:B:36:ALA:HA	1:B:82:ARG:NH2	1.58	1.15
1:C:35:LYS:O	1:C:36:ALA:O	1.65	1.15
1:E:127:THR:CG2	1:E:128:SER:H	1.60	1.15
1:F:123:ARG:CG	1:F:123:ARG:HH11	1.57	1.14
1:E:127:THR:CG2	1:E:128:SER:N	2.06	1.14
1:A:81:GLU:HA	1:A:82:ARG:HB2	1.14	1.13
1:F:84:ALA:HB1	1:F:85:TRP:CB	1.78	1.13
1:F:30:ILE:HG12	1:F:86:VAL:HB	1.31	1.13
1:D:114:MET:CA	1:D:114:MET:CE	2.27	1.12
1:D:149:ASN:O	1:D:153:GLN:HG2	1.44	1.12
1:F:11:LEU:HD21	1:F:41:TYR:HE1	1.05	1.12
1:E:25:SER:O	1:E:26:LYS:HG2	0.96	1.12
1:D:182:THR:O	1:D:186:ILE:HD13	1.45	1.12
1:C:15:LEU:CD2	1:C:15:LEU:H	1.56	1.11
1:D:114:MET:CA	1:D:114:MET:HE2	1.81	1.11
1:B:40:TYR:HD2	1:B:70:ILE:CG2	1.63	1.11
1:B:40:TYR:CD2	1:B:70:ILE:CG2	2.34	1.11
1:E:123:ARG:O	1:E:126:VAL:HG12	1.46	1.11
1:A:55:GLU:HG3	1:A:56:GLY:N	1.49	1.10
1:E:116:LEU:O	1:E:120:MET:HE2	1.51	1.10
1:D:122:ARG:CB	1:D:122:ARG:HH21	1.63	1.10
1:E:71:GLY:O	1:E:99:TYR:OH	1.67	1.10
1:D:83:SER:O	1:D:84:ALA:O	1.70	1.10
1:C:41:TYR:HD1	1:C:69:PHE:CD1	1.69	1.10
1:E:126:VAL:HG13	1:E:127:THR:N	1.62	1.10
1:E:134:LEU:HD22	1:F:190:LEU:HD22	1.13	1.09
1:A:54:GLU:O	1:A:55:GLU:HG2	1.51	1.09
1:E:46:SER:H	1:E:90:THR:HG23	1.04	1.09
1:C:14:PHE:HB3	1:C:15:LEU:CD2	1.83	1.09
1:F:30:ILE:HD11	1:F:86:VAL:CG2	1.82	1.09
1:E:25:SER:HB3	1:E:26:LYS:HD3	1.35	1.08
1:A:55:GLU:CG	1:A:56:GLY:H	1.59	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:54:GLU:O	1:C:55:GLU:HB2	1.43	1.08
1:F:51:ILE:CD1	1:F:61:LEU:HB2	1.84	1.08
1:A:50:LEU:O	1:A:51:ILE:HG23	1.50	1.08
1:F:84:ALA:CB	1:F:85:TRP:CB	2.30	1.08
1:E:29:LEU:HB2	1:E:86:VAL:HG12	1.35	1.08
1:F:51:ILE:HD13	1:F:61:LEU:HD12	1.21	1.08
1:E:134:LEU:HD21	1:F:190:LEU:HD22	1.27	1.08
1:F:127:THR:CG2	1:F:127:THR:O	1.75	1.08
1:F:51:ILE:HD11	1:F:61:LEU:HD12	1.28	1.08
1:E:127:THR:HG23	1:E:128:SER:N	1.62	1.08
1:E:37:GLU:O	1:E:38:THR:HG23	1.54	1.08
1:E:38:THR:HA	1:E:39:LEU:CB	1.83	1.08
1:F:60:ILE:HG22	1:F:61:LEU:H	0.95	1.07
1:F:60:ILE:HG22	1:F:61:LEU:N	1.68	1.07
1:E:117:SER:CA	1:E:120:MET:HE3	1.81	1.07
1:F:84:ALA:HB1	1:F:85:TRP:HB3	1.34	1.07
1:B:116:LEU:HD23	1:B:116:LEU:C	1.74	1.07
1:F:124:LEU:O	1:F:126:VAL:N	1.88	1.07
1:C:40:TYR:HB3	1:C:70:ILE:HD12	1.33	1.06
1:D:122:ARG:CG	1:D:122:ARG:HH21	1.68	1.06
1:F:84:ALA:CA	1:F:85:TRP:CB	2.30	1.06
1:E:134:LEU:HG	1:F:195:LEU:HD12	1.31	1.06
1:E:17:HIS:CD2	1:E:105:LEU:HD21	1.90	1.06
1:B:30:ILE:HG21	1:B:82:ARG:HD2	1.31	1.06
1:C:14:PHE:HB3	1:C:15:LEU:HD23	1.09	1.06
1:E:25:SER:C	1:E:26:LYS:CD	2.23	1.06
1:E:38:THR:HA	1:E:39:LEU:HB3	1.36	1.05
1:C:15:LEU:N	1:C:15:LEU:CD2	2.16	1.05
1:A:35:LYS:N	1:A:81:GLU:HB2	1.72	1.05
1:B:119:GLN:HG3	1:B:120:MET:H	1.19	1.05
1:B:64:LEU:HD12	1:B:70:ILE:HD11	1.38	1.05
1:F:84:ALA:HA	1:F:85:TRP:CB	1.85	1.04
1:C:23:TYR:CG	1:C:29:LEU:HD21	1.91	1.04
1:F:122:ARG:HH21	1:F:122:ARG:CG	1.70	1.04
1:E:127:THR:HG22	1:E:128:SER:H	1.16	1.04
1:C:68:ASP:HA	1:C:119:GLN:OE1	1.57	1.04
1:A:56:GLY:C	1:A:57:LYS:HD3	1.76	1.04
1:F:123:ARG:HG3	1:F:123:ARG:HH11	1.17	1.04
1:E:117:SER:CA	1:E:120:MET:CE	2.36	1.04
1:B:54:GLU:O	1:B:55:GLU:HB2	1.58	1.04
1:E:84:ALA:HB1	1:E:85:TRP:HA	1.04	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:30:ILE:HG21	1:B:82:ARG:CD	1.88	1.03
1:F:30:ILE:CD1	1:F:86:VAL:HG23	1.88	1.03
1:D:54:GLU:O	1:D:55:GLU:HB2	1.58	1.03
1:C:41:TYR:HD2	1:C:41:TYR:C	1.61	1.02
1:F:60:ILE:CG2	1:F:61:LEU:H	1.71	1.02
1:E:25:SER:O	1:E:26:LYS:CD	2.06	1.02
1:F:41:TYR:CG	1:F:69:PHE:CE1	2.48	1.02
1:F:41:TYR:CG	1:F:69:PHE:HE1	1.76	1.02
1:F:116:LEU:C	1:F:116:LEU:CD2	2.27	1.02
1:D:82:ARG:O	1:D:82:ARG:HG3	1.55	1.02
1:F:122:ARG:HG3	1:F:122:ARG:NH2	1.56	1.02
1:B:170:GLN:HB3	1:B:180:ARG:HD3	1.41	1.01
1:F:194:ASN:C	1:F:206:TYR:HE1	1.64	1.01
1:F:68:ASP:CB	1:F:119:GLN:NE2	2.23	1.01
1:E:130:LYS:O	1:E:185:ARG:NE	1.56	1.01
1:D:122:ARG:HB3	1:D:122:ARG:NH2	1.76	1.01
1:F:11:LEU:HD21	1:F:41:TYR:CE1	1.96	1.00
1:B:72:GLU:O	1:B:73:LEU:HB2	1.56	1.00
1:B:36:ALA:CA	1:B:82:ARG:NH2	2.18	1.00
1:F:70:ILE:O	1:F:70:ILE:HG22	1.62	1.00
1:F:51:ILE:CD1	1:F:61:LEU:HG	1.66	1.00
1:C:17:HIS:HD2	1:C:105:LEU:HD21	0.86	0.99
1:E:84:ALA:HB1	1:E:85:TRP:CA	1.91	0.99
1:C:23:TYR:CD1	1:C:29:LEU:CD2	2.45	0.99
1:F:51:ILE:HD11	1:F:61:LEU:CD1	1.74	0.99
1:C:30:ILE:CG2	1:C:31:HIS:H	1.74	0.99
1:B:51:ILE:HD13	1:B:51:ILE:H	1.28	0.99
1:A:50:LEU:CD2	1:A:60:ILE:HG13	1.92	0.99
1:C:80:GLN:C	1:C:81:GLU:HG3	1.79	0.99
1:B:77:GLU:O	1:B:80:GLN:HB2	1.62	0.99
1:E:56:GLY:O	1:E:57:LYS:HB2	1.58	0.99
1:C:41:TYR:C	1:C:41:TYR:CD2	2.29	0.99
1:D:114:MET:HA	1:D:114:MET:HE3	1.44	0.99
1:E:75:LEU:N	1:E:99:TYR:HE1	1.59	0.98
1:B:40:TYR:HB2	1:B:70:ILE:HG22	1.45	0.98
1:F:30:ILE:HD11	1:F:86:VAL:HG23	0.99	0.98
1:C:41:TYR:HB2	1:C:69:PHE:HD1	1.25	0.98
1:D:122:ARG:NH2	1:D:122:ARG:CB	2.27	0.98
1:D:86:VAL:O	1:D:87:ARG:HG3	1.63	0.97
1:C:30:ILE:HD12	1:C:86:VAL:HG23	1.46	0.97
1:F:122:ARG:HH11	1:F:123:ARG:HH21	1.12	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:194:ASN:O	1:F:206:TYR:CE1	2.18	0.97
1:C:40:TYR:HB3	1:C:70:ILE:CD1	1.92	0.97
1:C:30:ILE:HD12	1:C:86:VAL:CG2	1.93	0.97
1:C:102:PHE:O	1:C:102:PHE:CD2	2.17	0.97
1:E:39:LEU:CB	1:E:99:TYR:CE2	2.47	0.97
1:F:84:ALA:HA	1:F:85:TRP:HB2	0.99	0.96
1:F:41:TYR:HD2	1:F:42:ILE:H	1.09	0.96
1:B:36:ALA:CB	1:B:82:ARG:NH2	2.28	0.96
1:B:40:TYR:CB	1:B:70:ILE:CG2	2.44	0.96
1:C:41:TYR:CD1	1:C:69:PHE:CD1	2.49	0.95
1:F:189:MET:O	1:F:193:GLN:HG2	1.65	0.95
1:F:123:ARG:N	1:F:123:ARG:CD	2.30	0.95
1:E:25:SER:C	1:E:26:LYS:HD2	1.86	0.94
1:E:14:PHE:O	1:E:17:HIS:HB2	1.67	0.94
1:B:30:ILE:HD11	1:B:40:TYR:CE2	2.01	0.94
1:B:74:GLY:O	1:B:99:TYR:HE1	1.49	0.94
1:A:56:GLY:O	1:A:57:LYS:CG	2.13	0.94
1:C:30:ILE:HG22	1:C:31:HIS:N	1.79	0.94
1:F:53:ASP:CG	1:F:54:GLU:H	1.67	0.94
1:A:50:LEU:O	1:A:51:ILE:CG2	2.16	0.94
1:E:46:SER:N	1:E:90:THR:CG2	2.31	0.94
1:D:32:GLN:OE1	1:D:85:TRP:CE3	2.21	0.94
1:A:171:GLU:O	1:A:175:ILE:HD13	1.67	0.93
1:C:15:LEU:HD23	1:C:15:LEU:H	0.78	0.93
1:F:121:ALA:O	1:F:124:LEU:CB	2.16	0.93
1:E:25:SER:OG	1:E:26:LYS:HD2	1.68	0.93
1:E:39:LEU:HB2	1:E:99:TYR:HE2	1.11	0.93
1:B:36:ALA:CB	1:B:82:ARG:HH22	1.80	0.93
1:F:32:GLN:HG3	1:F:83:SER:HA	1.50	0.93
1:E:116:LEU:HD23	1:E:120:MET:HE2	1.50	0.93
1:B:30:ILE:CG2	1:B:82:ARG:HD2	1.98	0.93
1:D:39:LEU:HB2	1:D:99:TYR:CE2	2.03	0.93
1:A:14:PHE:CD2	1:A:112:ILE:HG21	2.03	0.93
1:E:38:THR:N	1:E:99:TYR:CD2	2.37	0.93
1:B:36:ALA:HA	1:B:82:ARG:HH22	0.78	0.93
1:C:30:ILE:CG2	1:C:31:HIS:N	2.28	0.93
1:C:14:PHE:CB	1:C:15:LEU:HD23	1.98	0.92
1:C:38:THR:O	1:C:99:TYR:CE2	2.22	0.92
1:E:126:VAL:HG13	1:E:127:THR:H	1.22	0.92
1:E:25:SER:C	1:E:26:LYS:CG	2.37	0.92
1:F:32:GLN:HE22	1:F:85:TRP:HZ3	1.15	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:81:GLU:HA	1:A:82:ARG:HB3	0.94	0.92
1:F:30:ILE:HG13	1:F:86:VAL:H	1.33	0.92
1:F:41:TYR:CD2	1:F:42:ILE:N	2.38	0.91
1:B:30:ILE:O	1:B:85:TRP:HB2	1.70	0.91
1:C:17:HIS:HD2	1:C:105:LEU:CD2	1.80	0.91
1:A:35:LYS:HA	1:A:81:GLU:CB	1.99	0.91
1:C:80:GLN:HE21	1:C:80:GLN:N	1.69	0.91
1:E:30:ILE:HG21	1:E:82:ARG:CD	2.00	0.91
1:E:164:GLN:HB2	1:E:204:VAL:HG23	1.52	0.91
1:F:122:ARG:NH1	1:F:123:ARG:HH21	1.56	0.91
1:E:116:LEU:HD23	1:E:120:MET:CE	2.01	0.91
1:A:80:GLN:HE21	1:A:80:GLN:N	1.69	0.91
1:E:120:MET:SD	1:F:120:MET:HE3	2.10	0.90
1:E:84:ALA:HB3	1:E:85:TRP:CA	1.94	0.90
1:F:164:GLN:HA	1:F:204:VAL:HA	1.53	0.90
1:F:126:VAL:HG12	1:F:193:GLN:NE2	1.85	0.90
1:B:40:TYR:HB2	1:B:70:ILE:HG21	1.50	0.90
1:D:114:MET:HE2	1:D:114:MET:HA	0.91	0.90
1:E:15:LEU:C	1:E:17:HIS:H	1.74	0.90
1:F:123:ARG:N	1:F:123:ARG:HD2	1.85	0.90
1:E:30:ILE:HG21	1:E:82:ARG:NE	1.87	0.90
1:E:30:ILE:HG21	1:E:82:ARG:HD2	1.52	0.90
1:B:40:TYR:CD2	1:B:70:ILE:HG21	2.04	0.90
1:A:58:GLU:O	1:A:59:MET:C	2.00	0.90
1:F:194:ASN:C	1:F:206:TYR:CE1	2.45	0.89
1:A:81:GLU:HG3	1:A:81:GLU:O	1.71	0.89
1:E:29:LEU:HB2	1:E:86:VAL:CG1	2.01	0.89
1:E:20:ILE:HD12	1:E:20:ILE:H	1.37	0.89
1:A:100:LYS:HD2	1:E:34:GLU:HG2	1.51	0.89
1:A:80:GLN:CA	1:A:80:GLN:HE21	1.84	0.89
1:C:80:GLN:O	1:C:81:GLU:CG	2.16	0.89
1:F:122:ARG:HG3	1:F:122:ARG:HH21	0.76	0.89
1:E:116:LEU:C	1:E:120:MET:HE2	1.93	0.89
1:E:117:SER:HA	1:E:120:MET:HE3	0.89	0.89
1:F:53:ASP:CG	1:F:54:GLU:N	2.24	0.89
1:C:98:SER:C	1:C:100:LYS:H	1.76	0.89
1:C:43:VAL:O	1:C:44:LYS:HG3	1.73	0.89
1:E:37:GLU:C	1:E:38:THR:HG23	1.91	0.88
1:E:46:SER:OG	1:E:90:THR:CG2	2.21	0.88
1:E:15:LEU:O	1:E:17:HIS:N	2.07	0.88
1:E:46:SER:OG	1:E:90:THR:HG22	1.74	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:35:LYS:CA	1:A:81:GLU:HB3	2.03	0.88
1:F:122:ARG:NH1	1:F:123:ARG:NH2	2.22	0.88
1:E:25:SER:CB	1:E:26:LYS:CD	2.52	0.88
1:A:60:ILE:HG22	1:A:61:LEU:N	1.88	0.88
1:A:82:ARG:HG3	1:A:82:ARG:O	1.73	0.88
1:C:41:TYR:CD2	1:C:42:ILE:N	2.41	0.87
1:F:32:GLN:CA	1:F:83:SER:O	2.21	0.87
1:E:25:SER:CB	1:E:26:LYS:HD3	2.05	0.87
1:B:64:LEU:HD12	1:B:70:ILE:CD1	2.05	0.87
1:F:122:ARG:HH11	1:F:123:ARG:NH2	1.71	0.87
1:E:75:LEU:HA	1:E:99:TYR:CD1	2.09	0.87
1:E:162:GLY:HA3	1:E:207:GLY:N	1.89	0.87
1:A:35:LYS:N	1:A:81:GLU:CB	2.38	0.87
1:A:35:LYS:HA	1:A:81:GLU:HB3	1.55	0.87
1:F:123:ARG:NH1	1:F:123:ARG:HG3	1.82	0.86
1:C:14:PHE:CE2	1:C:112:ILE:HG21	2.10	0.86
1:E:134:LEU:H	1:F:195:LEU:CD1	1.87	0.86
1:E:30:ILE:CG2	1:E:82:ARG:HD2	2.06	0.86
1:E:204:VAL:HG13	1:E:204:VAL:O	1.75	0.86
1:C:41:TYR:HB2	1:C:69:PHE:CD1	2.10	0.86
1:A:80:GLN:CA	1:A:80:GLN:NE2	2.35	0.86
1:A:14:PHE:CE2	1:A:112:ILE:HG21	2.11	0.86
1:E:134:LEU:CD1	1:F:195:LEU:HB3	2.06	0.86
1:D:122:ARG:HG3	1:D:122:ARG:HH21	1.39	0.86
1:F:41:TYR:CD2	1:F:69:PHE:HE1	1.94	0.85
1:B:51:ILE:HD13	1:B:51:ILE:N	1.91	0.85
1:A:35:LYS:H	1:A:81:GLU:HB2	1.39	0.85
1:E:39:LEU:HB2	1:E:99:TYR:CD2	2.11	0.85
1:A:60:ILE:CG2	1:A:61:LEU:H	1.90	0.85
1:C:23:TYR:CG	1:C:29:LEU:CD2	2.57	0.85
1:F:123:ARG:O	1:F:124:LEU:HD23	1.77	0.85
1:C:30:ILE:HG23	1:C:31:HIS:H	1.41	0.85
1:F:51:ILE:O	1:F:59:MET:HB2	1.76	0.85
1:E:134:LEU:CB	1:F:195:LEU:HD13	2.07	0.85
1:C:30:ILE:O	1:C:31:HIS:CG	2.30	0.85
1:F:41:TYR:O	1:F:94:VAL:HG13	1.76	0.84
1:F:69:PHE:O	1:F:70:ILE:HB	1.74	0.84
1:E:30:ILE:CG2	1:E:82:ARG:HE	1.89	0.84
1:E:14:PHE:CD2	1:E:105:LEU:CD1	2.60	0.84
1:A:50:LEU:HD21	1:A:60:ILE:HG13	1.57	0.84
1:F:194:ASN:O	1:F:206:TYR:CD1	2.31	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:205:VAL:HG12	1:E:206:TYR:H	0.67	0.84
1:F:164:GLN:HB2	1:F:204:VAL:HG22	1.57	0.84
1:A:53:ASP:OD1	1:A:54:GLU:N	2.11	0.83
1:A:10:THR:HG23	1:A:112:ILE:CD1	2.07	0.83
1:F:50:LEU:O	1:F:84:ALA:CB	2.27	0.83
1:C:10:THR:O	1:C:13:TRP:HB3	1.78	0.83
1:F:69:PHE:N	1:F:119:GLN:NE2	2.26	0.83
1:E:39:LEU:CB	1:E:99:TYR:HE2	1.84	0.83
1:B:44:LYS:O	1:B:92:CYS:HB2	1.78	0.83
1:F:123:ARG:HG2	1:F:123:ARG:HH11	1.44	0.83
1:B:36:ALA:HB2	1:B:82:ARG:NH2	1.92	0.82
1:E:164:GLN:HA	1:E:204:VAL:HA	1.61	0.82
1:A:10:THR:HG23	1:A:112:ILE:HD11	1.60	0.82
1:E:126:VAL:CG1	1:E:127:THR:H	1.91	0.82
1:E:46:SER:N	1:E:90:THR:HG23	1.89	0.82
1:B:116:LEU:CD2	1:B:116:LEU:C	2.47	0.82
1:A:165:ILE:HD13	1:A:203:ILE:O	1.80	0.82
1:F:69:PHE:H	1:F:119:GLN:NE2	1.77	0.82
1:C:17:HIS:CD2	1:C:105:LEU:CD2	2.58	0.82
1:F:14:PHE:CD1	1:F:14:PHE:C	2.53	0.82
1:E:204:VAL:HG22	1:E:205:VAL:O	1.80	0.82
1:A:189:MET:O	1:A:193:GLN:HG2	1.80	0.81
1:D:80:GLN:HG2	1:D:81:GLU:O	1.80	0.81
1:B:127:THR:O	1:B:127:THR:HG23	1.80	0.81
1:B:40:TYR:CB	1:B:70:ILE:HG22	2.06	0.81
1:E:20:ILE:HD12	1:E:20:ILE:N	1.95	0.81
1:A:38:THR:HG22	1:A:39:LEU:O	1.80	0.81
1:E:13:TRP:CD1	1:E:13:TRP:O	2.33	0.81
1:E:14:PHE:HD2	1:E:105:LEU:HD13	1.44	0.81
1:C:54:GLU:O	1:C:55:GLU:CB	2.28	0.81
1:E:14:PHE:CE2	1:E:105:LEU:HD12	2.14	0.81
1:E:40:TYR:CD2	1:E:70:ILE:HB	2.16	0.81
1:E:75:LEU:HA	1:E:99:TYR:CE1	2.15	0.81
1:F:51:ILE:CG1	1:F:61:LEU:HB2	2.09	0.81
1:B:30:ILE:HD11	1:B:40:TYR:CD2	2.14	0.81
1:A:82:ARG:O	1:A:82:ARG:CG	2.29	0.81
1:B:38:THR:HG22	1:B:39:LEU:O	1.80	0.81
1:B:21:HIS:ND1	1:B:23:TYR:CE2	2.48	0.81
1:E:42:ILE:HD12	1:E:68:ASP:HB2	1.63	0.81
1:E:134:LEU:HG	1:F:195:LEU:HD13	0.81	0.80
1:E:25:SER:HB3	1:E:26:LYS:CD	2.10	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:35:LYS:CA	1:A:81:GLU:CB	2.60	0.80
1:A:35:LYS:H	1:A:81:GLU:CB	1.94	0.80
1:C:40:TYR:CE1	1:C:96:GLU:OE1	2.35	0.80
1:E:30:ILE:CG2	1:E:82:ARG:NE	2.43	0.80
1:B:127:THR:O	1:B:128:SER:HB2	1.81	0.80
1:B:119:GLN:O	1:B:120:MET:C	2.19	0.80
1:E:37:GLU:O	1:E:38:THR:CG2	2.29	0.80
1:B:40:TYR:CD2	1:B:70:ILE:HG22	2.15	0.80
1:E:30:ILE:O	1:E:85:TRP:HB2	1.82	0.80
1:A:55:GLU:HG3	1:A:56:GLY:H	0.70	0.80
1:F:46:SER:H	1:F:90:THR:CG2	1.95	0.80
1:E:150:LEU:HA	1:E:153:GLN:CG	2.12	0.80
1:F:41:TYR:HD2	1:F:42:ILE:N	1.78	0.79
1:F:69:PHE:O	1:F:70:ILE:CB	2.30	0.79
1:F:195:LEU:HA	1:F:206:TYR:HD1	1.47	0.79
1:B:51:ILE:HD12	1:B:61:LEU:HG	1.63	0.79
1:F:114:MET:CE	1:F:114:MET:HA	2.12	0.79
1:E:75:LEU:CA	1:E:99:TYR:CE1	2.66	0.79
1:E:75:LEU:N	1:E:99:TYR:CE1	2.49	0.79
1:F:123:ARG:O	1:F:124:LEU:CD2	2.30	0.79
1:C:80:GLN:NE2	1:C:80:GLN:N	2.31	0.79
1:E:196:ILE:HG22	1:E:205:VAL:HA	1.63	0.79
1:E:138:ASP:HA	1:F:141:GLY:HA2	1.65	0.79
1:A:10:THR:CG2	1:A:112:ILE:CD1	2.60	0.79
1:E:162:GLY:HA3	1:E:207:GLY:H	1.47	0.79
1:B:74:GLY:O	1:B:99:TYR:CE1	2.36	0.79
1:B:77:GLU:HB3	1:B:80:GLN:HG3	1.65	0.79
1:F:52:LYS:HB3	1:F:57:LYS:O	1.82	0.79
1:F:124:LEU:O	1:F:125:GLN:C	2.22	0.79
1:E:17:HIS:HD2	1:E:105:LEU:HD21	1.46	0.78
1:B:119:GLN:HG3	1:B:120:MET:N	1.98	0.78
1:D:38:THR:HG22	1:D:39:LEU:O	1.83	0.78
1:A:62:SER:OG	1:A:63:TYR:N	2.16	0.78
1:F:162:GLY:HA3	1:F:205:VAL:O	1.83	0.78
1:F:20:ILE:N	1:F:20:ILE:HD12	1.98	0.78
1:F:32:GLN:HA	1:F:83:SER:O	1.82	0.78
1:F:41:TYR:CD2	1:F:69:PHE:CE1	2.71	0.78
1:F:125:GLN:O	1:F:129:GLU:HG3	1.83	0.78
1:A:54:GLU:O	1:A:55:GLU:CG	2.32	0.78
1:F:68:ASP:HB3	1:F:119:GLN:HE21	1.49	0.78
1:E:164:GLN:CB	1:E:204:VAL:HG23	2.14	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:197:SER:OG	1:E:204:VAL:HG11	1.81	0.78
1:B:51:ILE:HD13	1:B:59:MET:O	1.83	0.78
1:B:21:HIS:CE1	1:B:23:TYR:OH	2.36	0.78
1:C:13:TRP:O	1:C:13:TRP:CD1	2.37	0.77
1:E:134:LEU:CD2	1:F:195:LEU:HD12	2.14	0.77
1:E:40:TYR:HB2	1:E:70:ILE:HG12	1.67	0.77
1:F:19:HIS:O	1:F:95:ALA:HA	1.83	0.77
1:B:128:SER:O	1:B:129:GLU:C	2.19	0.77
1:B:85:TRP:H	1:B:85:TRP:HE3	1.32	0.77
1:A:60:ILE:HG22	1:A:61:LEU:H	1.44	0.77
1:A:10:THR:CG2	1:A:112:ILE:HD12	2.14	0.77
1:F:126:VAL:HG12	1:F:193:GLN:HE22	1.48	0.77
1:E:51:ILE:HD12	1:E:59:MET:HB3	1.65	0.77
1:F:50:LEU:O	1:F:51:ILE:CG1	2.30	0.77
1:B:115:ARG:O	1:B:118:ALA:HB3	1.85	0.77
1:C:80:GLN:CA	1:C:80:GLN:HE21	1.97	0.76
1:E:134:LEU:CG	1:F:195:LEU:HD12	1.99	0.76
1:B:39:LEU:HB2	1:B:99:TYR:CE2	2.19	0.76
1:B:30:ILE:CD1	1:B:40:TYR:CE2	2.67	0.76
1:A:80:GLN:HA	1:A:80:GLN:NE2	2.01	0.76
1:F:30:ILE:HG12	1:F:86:VAL:CB	2.13	0.76
1:F:32:GLN:HG3	1:F:83:SER:CA	2.15	0.76
1:E:40:TYR:O	1:E:69:PHE:HA	1.86	0.76
1:F:53:ASP:OD2	1:F:54:GLU:CG	2.25	0.76
1:E:69:PHE:HD2	1:E:119:GLN:HE21	1.34	0.76
1:A:11:LEU:HD22	1:A:11:LEU:O	1.85	0.76
1:E:30:ILE:CG2	1:E:82:ARG:CD	2.63	0.76
1:E:134:LEU:HD22	1:F:190:LEU:CD2	2.00	0.76
1:B:40:TYR:CB	1:B:70:ILE:HG21	2.13	0.76
1:B:115:ARG:O	1:B:118:ALA:N	2.19	0.76
1:F:195:LEU:HA	1:F:206:TYR:CD1	2.21	0.76
1:F:30:ILE:CG1	1:F:86:VAL:H	1.99	0.76
1:D:39:LEU:HB2	1:D:99:TYR:HE2	1.49	0.76
1:B:40:TYR:HB2	1:B:70:ILE:CB	2.15	0.76
1:E:14:PHE:HE2	1:E:105:LEU:HD12	1.51	0.75
1:C:83:SER:O	1:C:84:ALA:CB	2.33	0.75
1:E:150:LEU:HA	1:E:153:GLN:HG2	1.68	0.75
1:F:70:ILE:CG2	1:F:70:ILE:O	2.34	0.75
1:D:37:GLU:HA	1:D:99:TYR:CD1	2.20	0.75
1:F:130:LYS:CG	1:F:189:MET:SD	2.69	0.75
1:E:38:THR:CA	1:E:39:LEU:CB	2.63	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:56:GLY:O	1:A:57:LYS:CB	2.34	0.75
1:F:69:PHE:H	1:F:119:GLN:HE21	1.34	0.75
1:F:51:ILE:HG13	1:F:61:LEU:HB2	1.67	0.75
1:E:30:ILE:HG23	1:E:82:ARG:HE	1.49	0.75
1:F:30:ILE:CD1	1:F:86:VAL:CG2	2.56	0.75
1:B:74:GLY:C	1:B:99:TYR:HE1	1.90	0.74
1:F:204:VAL:HG12	1:F:205:VAL:N	2.01	0.74
1:F:151:ALA:HA	1:F:165:ILE:CG2	2.18	0.74
1:C:38:THR:O	1:C:99:TYR:HE2	1.68	0.74
1:B:64:LEU:CD1	1:B:70:ILE:CD1	2.65	0.74
1:E:25:SER:CB	1:E:26:LYS:HD2	2.14	0.74
1:C:8:ASP:CG	1:C:115:ARG:HH12	1.91	0.74
1:F:163:MET:O	1:F:205:VAL:N	2.20	0.74
1:E:134:LEU:N	1:F:195:LEU:CD1	2.51	0.74
1:E:164:GLN:HG3	1:E:204:VAL:HB	1.69	0.74
1:C:26:LYS:N	1:C:88:ALA:O	2.20	0.74
1:E:134:LEU:H	1:F:195:LEU:HD13	1.51	0.74
1:C:80:GLN:NE2	1:C:80:GLN:H	1.85	0.74
1:B:21:HIS:HD1	1:B:23:TYR:HE2	1.31	0.74
1:E:134:LEU:HD21	1:F:190:LEU:CD2	2.04	0.74
1:E:51:ILE:CD1	1:E:59:MET:HB3	2.16	0.74
1:E:53:ASP:OD2	1:E:59:MET:CE	2.36	0.74
1:F:38:THR:HG22	1:F:39:LEU:O	1.87	0.73
1:F:13:TRP:CE3	1:F:14:PHE:N	2.56	0.73
1:B:83:SER:O	1:B:84:ALA:HB3	1.86	0.73
1:B:40:TYR:CG	1:B:70:ILE:CG2	2.71	0.73
1:F:41:TYR:O	1:F:94:VAL:CG1	2.36	0.73
1:B:198:ALA:HA	1:B:203:ILE:HD13	1.69	0.73
1:D:63:TYR:HE1	1:D:89:LYS:HD2	1.53	0.73
1:E:134:LEU:HG	1:F:195:LEU:CG	2.16	0.73
1:C:150:LEU:HA	1:C:153:GLN:HG2	1.69	0.73
1:D:111:ASP:O	1:D:114:MET:HB2	1.88	0.73
1:D:41:TYR:HD1	1:D:69:PHE:CE1	2.06	0.73
1:F:68:ASP:C	1:F:119:GLN:NE2	2.42	0.73
1:B:40:TYR:CG	1:B:70:ILE:HG21	2.22	0.72
1:B:116:LEU:HD23	1:B:117:SER:N	2.03	0.72
1:C:69:PHE:H	1:C:119:GLN:HE22	1.35	0.72
1:E:41:TYR:HA	1:E:68:ASP:O	1.88	0.72
1:E:38:THR:CA	1:E:99:TYR:CE2	2.72	0.72
1:F:17:HIS:CD2	1:F:105:LEU:HD21	2.24	0.72
1:C:101:LYS:O	1:C:104:GLN:N	2.20	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:122:ARG:O	1:B:126:VAL:HG23	1.89	0.72
1:F:123:ARG:CD	1:F:123:ARG:H	2.02	0.72
1:D:86:VAL:O	1:D:87:ARG:CG	2.36	0.72
1:E:13:TRP:O	1:E:13:TRP:CG	2.39	0.72
1:F:122:ARG:HG2	1:F:123:ARG:N	2.02	0.71
1:F:58:GLU:C	1:F:59:MET:O	2.22	0.71
1:F:51:ILE:HD12	1:F:61:LEU:HG	0.72	0.71
1:C:13:TRP:O	1:C:13:TRP:CD2	2.43	0.71
1:A:112:ILE:HD12	1:A:112:ILE:N	2.03	0.71
1:D:106:ILE:HD12	1:D:113:LEU:HB2	1.71	0.71
1:C:8:ASP:OD1	1:C:115:ARG:NH1	2.24	0.71
1:D:70:ILE:HG22	1:D:71:GLY:N	2.02	0.71
1:D:102:PHE:CE2	1:D:106:ILE:HD11	2.25	0.71
1:A:83:SER:O	1:A:84:ALA:HB2	1.89	0.71
1:B:54:GLU:O	1:B:55:GLU:CB	2.35	0.71
1:E:134:LEU:H	1:F:195:LEU:HD11	1.55	0.71
1:C:102:PHE:O	1:C:102:PHE:HD2	1.68	0.71
1:F:51:ILE:HD11	1:F:61:LEU:CG	1.84	0.71
1:C:98:SER:O	1:C:100:LYS:N	2.20	0.71
1:E:40:TYR:HB2	1:E:70:ILE:CG1	2.20	0.70
1:A:76:PHE:O	1:A:77:GLU:HB3	1.89	0.70
1:A:60:ILE:CG2	1:A:61:LEU:N	2.47	0.70
1:B:72:GLU:O	1:B:73:LEU:CB	2.38	0.70
1:B:165:ILE:HD11	1:B:203:ILE:HB	1.72	0.70
1:F:94:VAL:HG12	1:F:95:ALA:N	2.05	0.70
1:A:83:SER:O	1:A:84:ALA:CB	2.39	0.70
1:E:28:THR:HA	1:E:87:ARG:HG3	1.73	0.70
1:F:51:ILE:HD12	1:F:61:LEU:CB	2.02	0.70
1:E:116:LEU:O	1:E:120:MET:CE	2.37	0.70
1:C:149:ASN:O	1:C:153:GLN:HG2	1.91	0.70
1:A:50:LEU:C	1:A:51:ILE:HG23	2.10	0.70
1:E:189:MET:O	1:E:193:GLN:HG2	1.92	0.70
1:F:68:ASP:HB3	1:F:119:GLN:NE2	1.99	0.70
1:F:123:ARG:HD3	1:F:123:ARG:H	1.55	0.70
1:C:30:ILE:HD12	1:C:86:VAL:HG21	1.72	0.70
1:D:112:ILE:HD12	1:D:112:ILE:N	2.06	0.70
1:F:123:ARG:C	1:F:124:LEU:HD23	2.12	0.70
1:E:134:LEU:CD1	1:F:195:LEU:CB	2.70	0.70
1:E:14:PHE:CE2	1:E:105:LEU:CD1	2.75	0.70
1:F:122:ARG:C	1:F:124:LEU:H	1.95	0.70
1:D:114:MET:CA	1:D:114:MET:HE3	2.09	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:164:GLN:HB2	1:A:204:VAL:HG22	1.74	0.70
1:A:49:VAL:O	1:A:61:LEU:HB2	1.92	0.69
1:D:70:ILE:O	1:D:72:GLU:N	2.25	0.69
1:F:63:TYR:HE1	1:F:89:LYS:HD2	1.57	0.69
1:A:97:ILE:HD11	1:A:101:LYS:HE3	1.74	0.69
1:B:38:THR:O	1:B:82:ARG:NH1	2.26	0.69
1:A:72:GLU:CD	1:A:123:ARG:HH22	1.95	0.69
1:E:25:SER:OG	1:E:26:LYS:CD	2.39	0.69
1:F:41:TYR:CD1	1:F:69:PHE:HE1	2.11	0.69
1:E:134:LEU:HD12	1:F:195:LEU:HB3	1.72	0.69
1:B:38:THR:CA	1:B:99:TYR:CE2	2.76	0.69
1:F:54:GLU:O	1:F:56:GLY:N	2.20	0.69
1:F:164:GLN:OE1	1:F:202:THR:HG21	1.92	0.69
1:C:104:GLN:O	1:C:107:GLN:N	2.26	0.69
1:C:39:LEU:O	1:C:40:TYR:HB2	1.91	0.69
1:E:17:HIS:O	1:E:97:ILE:HD12	1.93	0.69
1:C:150:LEU:HA	1:C:153:GLN:CG	2.23	0.69
1:F:63:TYR:CE1	1:F:89:LYS:HD2	2.28	0.69
1:A:8:ASP:OD1	1:A:115:ARG:NH2	2.22	0.69
1:C:80:GLN:C	1:C:81:GLU:CG	2.58	0.68
1:C:23:TYR:CB	1:C:29:LEU:HD21	2.23	0.68
1:F:50:LEU:O	1:F:84:ALA:HB2	1.92	0.68
1:C:33:GLY:O	1:C:34:GLU:O	2.12	0.68
1:C:38:THR:O	1:C:99:TYR:CD2	2.47	0.68
1:F:39:LEU:HD12	1:F:71:GLY:HA3	1.75	0.68
1:C:69:PHE:HD2	1:C:116:LEU:HA	1.59	0.68
1:C:14:PHE:O	1:C:16:SER:C	2.31	0.68
1:B:118:ALA:O	1:B:119:GLN:C	2.32	0.68
1:E:65:ASN:N	1:E:68:ASP:OD2	2.27	0.68
1:C:103:ARG:HG3	1:C:103:ARG:HH21	1.58	0.68
1:C:69:PHE:CD2	1:C:116:LEU:HA	2.28	0.68
1:E:124:LEU:O	1:E:127:THR:HG22	1.93	0.68
1:E:15:LEU:C	1:E:17:HIS:N	2.44	0.68
1:F:43:VAL:HB	1:F:93:GLU:OE2	1.94	0.68
1:E:80:GLN:HG2	1:E:81:GLU:H	1.59	0.68
1:F:58:GLU:O	1:F:59:MET:C	2.31	0.68
1:F:114:MET:HE2	1:F:114:MET:HA	1.76	0.68
1:E:53:ASP:OD2	1:E:59:MET:HE1	1.93	0.68
1:F:164:GLN:CB	1:F:204:VAL:HG22	2.24	0.68
1:E:46:SER:N	1:E:90:THR:HG21	2.06	0.68
1:B:32:GLN:NE2	1:B:85:TRP:CZ3	2.62	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:38:THR:CA	1:E:99:TYR:CD2	2.77	0.67
1:F:32:GLN:HG3	1:F:83:SER:O	1.93	0.67
1:B:83:SER:O	1:B:84:ALA:CB	2.40	0.67
1:B:120:MET:O	1:B:123:ARG:HB2	1.95	0.67
1:E:15:LEU:HD23	1:E:15:LEU:H	1.59	0.67
1:B:74:GLY:C	1:B:99:TYR:CE1	2.68	0.67
1:C:40:TYR:CB	1:C:70:ILE:HD12	2.18	0.67
1:E:120:MET:O	1:E:123:ARG:HB3	1.93	0.67
1:B:51:ILE:CD1	1:B:51:ILE:N	2.58	0.67
1:A:56:GLY:C	1:A:57:LYS:CD	2.48	0.67
1:E:46:SER:OG	1:E:90:THR:HG21	1.93	0.67
1:B:116:LEU:O	1:B:116:LEU:HD23	1.94	0.67
1:D:41:TYR:HD1	1:D:69:PHE:CD1	2.13	0.67
1:B:45:GLY:HA3	1:B:92:CYS:HB3	1.76	0.67
1:B:189:MET:O	1:B:193:GLN:HG2	1.95	0.67
1:C:20:ILE:N	1:C:20:ILE:HD12	2.09	0.67
1:C:17:HIS:O	1:C:97:ILE:HD12	1.94	0.67
1:F:51:ILE:HD13	1:F:61:LEU:CD1	1.92	0.67
1:F:20:ILE:HD12	1:F:20:ILE:H	1.60	0.67
1:D:44:LYS:O	1:D:92:CYS:HB2	1.95	0.67
1:A:30:ILE:HD11	1:A:40:TYR:CZ	2.30	0.67
1:B:32:GLN:NE2	1:B:85:TRP:CE3	2.63	0.66
1:B:40:TYR:HD2	1:B:70:ILE:HG23	1.57	0.66
1:C:23:TYR:CD1	1:C:29:LEU:HD23	2.28	0.66
1:F:28:THR:HG21	1:F:31:HIS:ND1	2.09	0.66
1:E:31:HIS:HD2	1:E:34:GLU:OE1	1.79	0.66
1:C:20:ILE:H	1:C:20:ILE:HD12	1.59	0.66
1:B:51:ILE:CG2	1:B:84:ALA:HB2	2.25	0.66
1:B:119:GLN:O	1:B:122:ARG:N	2.28	0.66
1:A:111:ASP:O	1:A:114:MET:HB2	1.95	0.66
1:A:70:ILE:O	1:A:71:GLY:C	2.34	0.66
1:F:74:GLY:O	1:F:75:LEU:C	2.32	0.66
1:D:189:MET:O	1:D:193:GLN:HG2	1.95	0.66
1:C:50:LEU:HD23	1:C:87:ARG:HD3	1.77	0.66
1:E:26:LYS:HD2	1:E:26:LYS:N	2.10	0.66
1:F:102:PHE:CE2	1:F:106:ILE:HD11	2.30	0.66
1:C:11:LEU:O	1:C:15:LEU:HG	1.95	0.66
1:A:38:THR:HA	1:A:39:LEU:HB3	1.78	0.66
1:C:16:SER:O	1:C:17:HIS:HB2	1.96	0.66
1:A:80:GLN:HA	1:A:80:GLN:HE21	1.61	0.66
1:D:112:ILE:HD12	1:D:112:ILE:H	1.60	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:50:LEU:C	1:F:51:ILE:CG1	2.64	0.66
1:E:205:VAL:HG12	1:E:206:TYR:CA	2.24	0.66
1:F:50:LEU:C	1:F:51:ILE:HG12	2.14	0.65
1:E:10:THR:O	1:E:13:TRP:HB3	1.97	0.65
1:C:114:MET:CE	1:C:114:MET:HA	2.25	0.65
1:E:90:THR:O	1:E:91:ALA:C	2.33	0.65
1:B:32:GLN:CG	1:B:32:GLN:O	2.44	0.65
1:B:119:GLN:O	1:B:123:ARG:N	2.24	0.65
1:F:114:MET:HA	1:F:114:MET:HE3	1.78	0.65
1:F:117:SER:HB3	1:F:120:MET:CE	2.27	0.65
1:B:116:LEU:CD2	1:B:117:SER:N	2.59	0.65
1:B:77:GLU:CB	1:B:80:GLN:HG3	2.25	0.65
1:A:72:GLU:H	1:A:72:GLU:CD	2.00	0.65
1:A:29:LEU:C	1:A:30:ILE:HD13	2.16	0.65
1:E:134:LEU:HD11	1:F:195:LEU:CB	2.27	0.65
1:B:41:TYR:CD1	1:B:69:PHE:CE2	2.84	0.65
1:E:164:GLN:CA	1:E:204:VAL:HG23	2.27	0.65
1:C:10:THR:HG21	1:C:111:ASP:HB3	1.77	0.65
1:E:150:LEU:O	1:E:153:GLN:HB2	1.97	0.65
1:B:111:ASP:O	1:B:114:MET:HB2	1.96	0.65
1:E:8:ASP:OD2	1:E:115:ARG:NH1	2.30	0.65
1:D:63:TYR:CE1	1:D:89:LYS:HD2	2.32	0.65
1:E:75:LEU:CA	1:E:99:TYR:HE1	2.08	0.65
1:A:55:GLU:CG	1:A:56:GLY:N	2.30	0.65
1:B:115:ARG:O	1:B:118:ALA:CB	2.45	0.64
1:D:82:ARG:O	1:D:82:ARG:CG	2.38	0.64
1:A:165:ILE:HD13	1:A:165:ILE:H	1.62	0.64
1:C:41:TYR:HD2	1:C:41:TYR:O	1.80	0.64
1:C:14:PHE:HD1	1:C:15:LEU:CD2	2.10	0.64
1:C:40:TYR:HE1	1:C:96:GLU:OE1	1.79	0.64
1:F:124:LEU:O	1:F:127:THR:N	2.30	0.64
1:F:41:TYR:CD1	1:F:69:PHE:CE1	2.86	0.64
1:E:204:VAL:CG1	1:E:204:VAL:O	2.45	0.64
1:F:53:ASP:OD2	1:F:54:GLU:N	2.29	0.64
1:F:53:ASP:CG	1:F:54:GLU:HG3	2.15	0.64
1:F:97:ILE:HD11	1:F:101:LYS:HE3	1.80	0.64
1:E:84:ALA:HB3	1:E:85:TRP:CB	2.27	0.64
1:A:75:LEU:HD13	1:A:99:TYR:CD2	2.33	0.64
1:A:50:LEU:HD22	1:A:60:ILE:HG13	1.79	0.63
1:B:120:MET:O	1:B:123:ARG:N	2.31	0.63
1:C:83:SER:O	1:C:84:ALA:HB3	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:167:ILE:HD13	1:F:172:ILE:CD1	2.28	0.63
1:E:134:LEU:N	1:F:195:LEU:HD11	2.11	0.63
1:D:41:TYR:CD1	1:D:69:PHE:CE1	2.87	0.63
1:D:70:ILE:CG2	1:D:71:GLY:N	2.60	0.63
1:F:32:GLN:HG3	1:F:83:SER:C	2.19	0.63
1:E:124:LEU:O	1:E:125:GLN:C	2.36	0.63
1:A:198:ALA:HA	1:A:203:ILE:HD13	1.79	0.63
1:C:41:TYR:CE1	1:C:69:PHE:CE1	2.75	0.63
1:C:112:ILE:HD12	1:C:112:ILE:H	1.62	0.63
1:F:13:TRP:HE3	1:F:14:PHE:H	1.46	0.63
1:F:69:PHE:N	1:F:119:GLN:HE21	1.93	0.63
1:E:164:GLN:HB2	1:E:204:VAL:CG2	2.26	0.63
1:B:21:HIS:ND1	1:B:23:TYR:HE2	1.90	0.62
1:E:150:LEU:HA	1:E:153:GLN:HG3	1.79	0.62
1:C:69:PHE:N	1:C:119:GLN:HE22	1.96	0.62
1:F:195:LEU:CA	1:F:206:TYR:CD1	2.82	0.62
1:F:11:LEU:CD2	1:F:41:TYR:HE1	1.98	0.62
1:D:150:LEU:HA	1:D:153:GLN:CG	2.29	0.62
1:D:39:LEU:HB2	1:D:99:TYR:CD2	2.34	0.62
1:A:38:THR:HA	1:A:39:LEU:CB	2.29	0.62
1:A:164:GLN:CB	1:A:204:VAL:HG22	2.30	0.62
1:E:74:GLY:HA2	1:E:77:GLU:HB2	1.80	0.62
1:C:36:ALA:O	1:C:37:GLU:HB3	1.99	0.62
1:B:32:GLN:N	1:B:85:TRP:HB3	2.13	0.62
1:E:182:THR:O	1:E:186:ILE:CD1	2.31	0.62
1:E:24:PRO:O	1:E:27:SER:HB3	2.00	0.62
1:B:38:THR:N	1:B:99:TYR:CE2	2.68	0.62
1:D:102:PHE:CZ	1:D:106:ILE:HD11	2.34	0.62
1:E:40:TYR:HD2	1:E:70:ILE:HB	1.65	0.62
1:B:127:THR:O	1:B:127:THR:CG2	2.47	0.62
1:A:39:LEU:HB2	1:A:99:TYR:CE2	2.35	0.62
1:F:54:GLU:C	1:F:56:GLY:H	2.01	0.62
1:A:14:PHE:O	1:A:15:LEU:HB2	1.98	0.62
1:E:150:LEU:CA	1:E:153:GLN:HG2	2.30	0.62
1:C:14:PHE:CD1	1:C:15:LEU:CD2	2.83	0.62
1:E:8:ASP:OD1	1:E:115:ARG:NH2	2.25	0.62
1:A:10:THR:CG2	1:A:112:ILE:HD11	2.26	0.62
1:F:82:ARG:O	1:F:84:ALA:O	2.18	0.62
1:B:40:TYR:HB2	1:B:70:ILE:HB	1.82	0.62
1:E:56:GLY:O	1:E:57:LYS:CB	2.41	0.62
1:F:114:MET:CE	1:F:114:MET:CA	2.75	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:79:GLY:O	1:A:80:GLN:HB2	2.00	0.61
1:B:70:ILE:O	1:B:70:ILE:HG22	1.99	0.61
1:F:43:VAL:O	1:F:44:LYS:CG	2.48	0.61
1:D:111:ASP:OD2	1:D:115:ARG:NH1	2.34	0.61
1:F:43:VAL:HG12	1:F:44:LYS:HG3	1.82	0.61
1:C:63:TYR:HE1	1:C:89:LYS:HD2	1.65	0.61
1:F:117:SER:HB3	1:F:120:MET:HE1	1.81	0.61
1:E:123:ARG:O	1:E:126:VAL:CG1	2.36	0.61
1:D:119:GLN:O	1:D:120:MET:C	2.37	0.61
1:F:21:HIS:O	1:F:93:GLU:HA	2.00	0.61
1:A:28:THR:HG23	1:A:86:VAL:O	2.00	0.61
1:A:53:ASP:CG	1:A:54:GLU:H	2.01	0.61
1:F:114:MET:C	1:F:116:LEU:H	2.04	0.61
1:E:37:GLU:C	1:E:38:THR:CG2	2.65	0.61
1:B:20:ILE:HD12	1:B:20:ILE:H	1.66	0.61
1:C:189:MET:O	1:C:193:GLN:HG2	2.00	0.61
1:B:38:THR:C	1:B:99:TYR:HE2	2.05	0.61
1:D:122:ARG:CZ	1:D:122:ARG:HB3	2.31	0.61
1:B:196:ILE:C	1:B:196:ILE:HD12	2.21	0.61
1:B:51:ILE:CD1	1:B:59:MET:O	2.48	0.61
1:F:32:GLN:CB	1:F:83:SER:O	2.49	0.60
1:B:31:HIS:HA	1:B:85:TRP:CD1	2.35	0.60
1:A:50:LEU:CD2	1:A:60:ILE:HA	2.30	0.60
1:E:77:GLU:O	1:E:78:GLU:C	2.37	0.60
1:C:104:GLN:O	1:C:105:LEU:C	2.39	0.60
1:A:65:ASN:N	1:A:68:ASP:OD2	2.32	0.60
1:C:14:PHE:O	1:C:17:HIS:HB2	2.01	0.60
1:F:121:ALA:O	1:F:124:LEU:N	2.34	0.60
1:A:81:GLU:O	1:A:81:GLU:CG	2.49	0.60
1:A:112:ILE:CD1	1:A:112:ILE:N	2.64	0.60
1:F:124:LEU:C	1:F:126:VAL:N	2.52	0.60
1:B:51:ILE:HD12	1:B:61:LEU:CG	2.29	0.60
1:B:170:GLN:CB	1:B:180:ARG:HD3	2.25	0.60
1:F:102:PHE:CZ	1:F:106:ILE:HD11	2.37	0.60
1:F:68:ASP:HA	1:F:119:GLN:HE22	0.44	0.60
1:F:122:ARG:O	1:F:124:LEU:N	2.30	0.60
1:A:81:GLU:CA	1:A:82:ARG:HB2	2.03	0.60
1:A:14:PHE:HE2	1:A:102:PHE:CE1	2.19	0.60
1:B:70:ILE:CG2	1:B:70:ILE:O	2.49	0.60
1:B:113:LEU:O	1:B:117:SER:HB2	2.02	0.60
1:C:37:GLU:HG3	1:C:38:THR:H	1.65	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:28:THR:CA	1:E:87:ARG:HG3	2.31	0.60
1:A:11:LEU:HB2	1:A:115:ARG:HH22	1.67	0.60
1:C:68:ASP:CA	1:C:119:GLN:OE1	2.41	0.60
1:F:204:VAL:CG1	1:F:205:VAL:N	2.65	0.60
1:B:165:ILE:CD1	1:B:203:ILE:HB	2.32	0.60
1:A:77:GLU:O	1:A:77:GLU:HG2	2.00	0.60
1:F:40:TYR:HB3	1:F:94:VAL:HG11	1.82	0.59
1:F:51:ILE:O	1:F:59:MET:CB	2.47	0.59
1:C:65:ASN:O	1:C:66:GLN:C	2.40	0.59
1:B:118:ALA:O	1:B:120:MET:N	2.35	0.59
1:E:119:GLN:OE1	1:E:119:GLN:O	2.21	0.59
1:A:126:VAL:CG1	1:A:193:GLN:HE22	2.16	0.59
1:F:164:GLN:CD	1:F:202:THR:CG2	2.71	0.59
1:F:39:LEU:HB2	1:F:99:TYR:CE2	2.37	0.59
1:E:13:TRP:CZ3	1:E:109:ASN:HB3	2.36	0.59
1:D:86:VAL:C	1:D:87:ARG:HG3	2.21	0.59
1:D:70:ILE:CG2	1:D:71:GLY:H	2.16	0.59
1:E:11:LEU:O	1:E:15:LEU:HD23	2.03	0.59
1:D:51:ILE:CD1	1:D:59:MET:HB3	2.32	0.59
1:C:14:PHE:HD1	1:C:15:LEU:HD21	1.66	0.59
1:F:204:VAL:HG12	1:F:205:VAL:H	1.66	0.59
1:D:33:GLY:O	1:D:81:GLU:HG3	2.03	0.59
1:B:108:VAL:O	1:B:109:ASN:OD1	2.21	0.59
1:C:63:TYR:CE1	1:C:89:LYS:HD2	2.37	0.59
1:C:37:GLU:HA	1:C:99:TYR:HB2	1.85	0.59
1:D:124:LEU:O	1:D:127:THR:N	2.29	0.59
1:F:14:PHE:CD1	1:F:14:PHE:O	2.56	0.59
1:D:83:SER:C	1:D:84:ALA:O	2.38	0.59
1:E:65:ASN:O	1:E:68:ASP:OD2	2.20	0.59
1:C:14:PHE:CZ	1:C:112:ILE:HG21	2.38	0.58
1:C:14:PHE:O	1:C:16:SER:N	2.36	0.58
1:E:38:THR:HA	1:E:99:TYR:CD2	2.38	0.58
1:B:38:THR:HG21	1:B:96:GLU:HB2	1.84	0.58
1:E:33:GLY:HA2	1:E:81:GLU:HG3	1.84	0.58
1:F:69:PHE:O	1:F:70:ILE:CG1	2.52	0.58
1:A:106:ILE:CG2	1:A:113:LEU:HD22	2.33	0.58
1:E:162:GLY:CA	1:E:207:GLY:H	2.14	0.58
1:D:13:TRP:CZ3	1:D:112:ILE:CD1	2.86	0.58
1:C:198:ALA:HA	1:C:203:ILE:HD13	1.84	0.58
1:E:134:LEU:N	1:F:195:LEU:HD13	2.16	0.58
1:E:120:MET:SD	1:F:120:MET:CE	2.90	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:120:MET:O	1:B:124:LEU:N	2.37	0.58
1:B:41:TYR:HD1	1:B:69:PHE:CE2	2.22	0.58
1:D:51:ILE:HD12	1:D:59:MET:HB3	1.84	0.58
1:A:17:HIS:O	1:A:18:CYS:HB3	2.03	0.58
1:E:134:LEU:HD23	1:F:190:LEU:CD2	2.31	0.58
1:F:30:ILE:CG1	1:F:86:VAL:HB	2.21	0.58
1:A:51:ILE:HG21	1:A:61:LEU:HD12	1.86	0.58
1:C:148:LEU:HD23	1:C:152:LYS:HE2	1.83	0.58
1:A:80:GLN:H	1:A:80:GLN:HE21	1.51	0.58
1:C:32:GLN:HG3	1:C:84:ALA:H	1.67	0.58
1:F:123:ARG:HD3	1:F:123:ARG:N	2.13	0.58
1:F:157:MET:HB2	1:F:164:GLN:HB3	1.84	0.58
1:F:164:GLN:CG	1:F:202:THR:CG2	2.82	0.58
1:D:42:ILE:HD11	1:D:70:ILE:HD11	1.85	0.58
1:C:14:PHE:CD2	1:C:112:ILE:HG12	2.39	0.58
1:F:51:ILE:HD11	1:F:61:LEU:HB2	1.55	0.58
1:C:50:LEU:HD13	1:C:60:ILE:HD13	1.86	0.58
1:B:197:SER:OG	1:B:204:VAL:HB	2.03	0.58
1:A:57:LYS:O	1:A:58:GLU:C	2.42	0.58
1:A:75:LEU:O	1:A:103:ARG:NH1	2.36	0.58
1:A:11:LEU:CD2	1:A:11:LEU:O	2.51	0.58
1:B:33:GLY:O	1:B:81:GLU:HG2	2.04	0.58
1:C:112:ILE:N	1:C:112:ILE:HD12	2.18	0.57
1:F:10:THR:HG22	1:F:112:ILE:HD13	1.86	0.57
1:F:122:ARG:C	1:F:124:LEU:N	2.55	0.57
1:F:58:GLU:O	1:F:59:MET:O	2.22	0.57
1:D:122:ARG:HG3	1:D:122:ARG:NH2	2.09	0.57
1:B:79:GLY:O	1:B:80:GLN:C	2.41	0.57
1:B:167:ILE:HD13	1:B:172:ILE:CD1	2.34	0.57
1:E:25:SER:O	1:E:26:LYS:HD3	1.99	0.57
1:F:117:SER:CA	1:F:120:MET:HE2	2.34	0.57
1:F:164:GLN:CD	1:F:202:THR:HG21	2.25	0.57
1:F:51:ILE:HD11	1:F:61:LEU:HB3	1.79	0.57
1:C:103:ARG:HG3	1:C:103:ARG:NH2	2.16	0.57
1:F:90:THR:OG1	1:F:91:ALA:N	2.37	0.57
1:F:167:ILE:HD13	1:F:172:ILE:HD11	1.86	0.57
1:C:40:TYR:HB3	1:C:70:ILE:HD13	1.85	0.57
1:F:14:PHE:CD2	1:F:112:ILE:HG12	2.40	0.57
1:F:47:VAL:HG12	1:F:88:ALA:HA	1.87	0.57
1:B:127:THR:O	1:B:128:SER:CB	2.52	0.57
1:B:64:LEU:CD1	1:B:70:ILE:HD12	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:186:ILE:N	1:D:186:ILE:HD12	2.19	0.57
1:A:102:PHE:CE2	1:A:106:ILE:HD11	2.40	0.57
1:C:167:ILE:HD13	1:C:172:ILE:CD1	2.35	0.57
1:D:102:PHE:O	1:D:106:ILE:HG12	2.05	0.57
1:A:11:LEU:HB2	1:A:115:ARG:NH2	2.20	0.57
1:E:204:VAL:C	1:E:205:VAL:O	2.39	0.57
1:C:114:MET:HE3	1:C:114:MET:HA	1.85	0.57
1:B:39:LEU:HD21	1:B:102:PHE:CD1	2.40	0.57
1:E:157:MET:HB2	1:E:164:GLN:HB3	1.87	0.57
1:E:202:THR:C	1:E:203:ILE:HD12	2.24	0.57
1:C:16:SER:O	1:C:17:HIS:CB	2.53	0.56
1:E:73:LEU:H	1:E:73:LEU:HD12	1.70	0.56
1:E:15:LEU:CD2	1:E:15:LEU:N	2.68	0.56
1:C:10:THR:O	1:C:13:TRP:CB	2.51	0.56
1:A:164:GLN:HA	1:A:204:VAL:HA	1.86	0.56
1:F:122:ARG:CG	1:F:122:ARG:NH2	2.41	0.56
1:E:134:LEU:HD11	1:F:195:LEU:HB2	1.85	0.56
1:B:31:HIS:HA	1:B:85:TRP:HD1	1.69	0.56
1:D:28:THR:HA	1:D:87:ARG:HG2	1.88	0.56
1:E:86:VAL:HG12	1:E:86:VAL:O	2.06	0.56
1:A:164:GLN:CG	1:A:204:VAL:HG22	2.34	0.56
1:B:20:ILE:HD12	1:B:20:ILE:N	2.20	0.56
1:B:167:ILE:HD13	1:B:172:ILE:HD13	1.87	0.56
1:E:38:THR:HA	1:E:39:LEU:HB2	1.77	0.56
1:F:32:GLN:NE2	1:F:85:TRP:CH2	2.63	0.56
1:E:53:ASP:OD2	1:E:59:MET:HE3	2.04	0.56
1:D:54:GLU:O	1:D:55:GLU:CB	2.39	0.56
1:E:20:ILE:CD1	1:E:20:ILE:H	2.13	0.56
1:F:165:ILE:N	1:F:203:ILE:O	2.38	0.56
1:D:112:ILE:CD1	1:D:112:ILE:H	2.19	0.56
1:C:21:HIS:HB2	1:C:23:TYR:CE2	2.41	0.56
1:C:78:GLU:HG2	1:C:103:ARG:HH12	1.71	0.56
1:F:123:ARG:NH1	1:F:123:ARG:CG	2.30	0.56
1:E:38:THR:HA	1:E:99:TYR:CE2	2.41	0.56
1:E:197:SER:HG	1:E:204:VAL:CG1	2.13	0.56
1:B:112:ILE:HG23	1:B:113:LEU:H	1.70	0.56
1:A:163:MET:O	1:A:205:VAL:N	2.34	0.56
1:E:22:LYS:HG2	1:E:93:GLU:HG2	1.86	0.56
1:F:39:LEU:HD12	1:F:71:GLY:CA	2.36	0.56
1:E:14:PHE:CE1	1:E:18:CYS:SG	2.99	0.56
1:F:165:ILE:HD11	1:F:203:ILE:HB	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:124:LEU:CD2	1:E:127:THR:HG21	2.36	0.56
1:E:15:LEU:HD23	1:E:15:LEU:N	2.20	0.56
1:C:41:TYR:CE2	1:C:42:ILE:O	2.60	0.55
1:B:36:ALA:CB	1:B:82:ARG:CZ	2.84	0.55
1:E:15:LEU:O	1:E:18:CYS:N	2.36	0.55
1:A:8:ASP:OD1	1:A:11:LEU:HB2	2.05	0.55
1:F:110:PRO:O	1:F:113:LEU:N	2.38	0.55
1:C:35:LYS:C	1:C:36:ALA:O	2.44	0.55
1:F:39:LEU:HB2	1:F:99:TYR:CD2	2.42	0.55
1:C:170:GLN:NE2	1:C:171:GLU:HG3	2.22	0.55
1:F:42:ILE:HG22	1:F:66:GLN:HA	1.88	0.55
1:D:114:MET:HE3	1:D:114:MET:N	2.22	0.55
1:B:120:MET:O	1:B:123:ARG:CA	2.54	0.55
1:A:168:THR:HG22	1:A:201:LYS:HG3	1.88	0.55
1:E:205:VAL:HG12	1:E:206:TYR:O	2.07	0.55
1:A:49:VAL:O	1:A:61:LEU:CB	2.55	0.55
1:C:30:ILE:CD1	1:C:86:VAL:CG2	2.78	0.55
1:D:38:THR:HG23	1:D:97:ILE:O	2.07	0.55
1:A:13:TRP:HZ2	1:A:108:VAL:HG11	1.71	0.55
1:E:37:GLU:O	1:E:38:THR:CB	2.54	0.55
1:B:37:GLU:C	1:B:99:TYR:CD2	2.80	0.55
1:B:38:THR:C	1:B:99:TYR:CE2	2.80	0.55
1:F:204:VAL:CG1	1:F:205:VAL:H	2.20	0.55
1:A:30:ILE:CD1	1:A:40:TYR:CZ	2.90	0.55
1:E:18:CYS:SG	1:E:97:ILE:HB	2.47	0.55
1:B:40:TYR:CG	1:B:70:ILE:HG22	2.39	0.55
1:E:186:ILE:HD12	1:E:186:ILE:N	2.22	0.55
1:A:72:GLU:HG2	1:A:73:LEU:HD12	1.87	0.54
1:B:82:ARG:O	1:B:84:ALA:N	2.40	0.54
1:A:55:GLU:OE1	1:A:57:LYS:HE3	2.06	0.54
1:C:44:LYS:O	1:C:92:CYS:HB2	2.06	0.54
1:C:69:PHE:H	1:C:119:GLN:NE2	2.05	0.54
1:C:17:HIS:O	1:C:97:ILE:CD1	2.55	0.54
1:D:30:ILE:HD12	1:D:86:VAL:HG21	1.89	0.54
1:A:51:ILE:CG2	1:A:61:LEU:HD12	2.37	0.54
1:A:157:MET:HB2	1:A:164:GLN:HB3	1.89	0.54
1:A:97:ILE:HD11	1:A:101:LYS:CE	2.37	0.54
1:E:69:PHE:H	1:E:119:GLN:NE2	2.05	0.54
1:E:39:LEU:N	1:E:99:TYR:HE2	2.06	0.54
1:B:41:TYR:CE1	1:B:69:PHE:CE2	2.96	0.54
1:D:77:GLU:OE1	1:D:80:GLN:OE1	2.26	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:117:SER:HA	1:E:120:MET:HE1	1.72	0.54
1:F:46:SER:N	1:F:90:THR:CG2	2.68	0.54
1:E:138:ASP:HA	1:F:141:GLY:CA	2.37	0.54
1:C:167:ILE:HD13	1:C:172:ILE:HD13	1.90	0.54
1:D:22:LYS:HG2	1:D:93:GLU:HG2	1.90	0.54
1:F:33:GLY:O	1:F:81:GLU:HG3	2.07	0.54
1:A:18:CYS:HB2	1:A:96:GLU:O	2.08	0.54
1:E:16:SER:O	1:E:17:HIS:ND1	2.41	0.54
1:B:85:TRP:HE3	1:B:85:TRP:N	2.02	0.54
1:D:149:ASN:O	1:D:153:GLN:CG	2.36	0.54
1:B:170:GLN:HA	1:B:180:ARG:HG2	1.89	0.54
1:A:70:ILE:HG22	1:A:71:GLY:N	2.23	0.54
1:A:25:SER:O	1:A:26:LYS:HB2	2.07	0.53
1:D:30:ILE:HG21	1:D:82:ARG:HD2	1.90	0.53
1:D:13:TRP:CZ3	1:D:112:ILE:HD13	2.43	0.53
1:F:43:VAL:CG1	1:F:93:GLU:OE2	2.56	0.53
1:E:77:GLU:OE1	1:E:80:GLN:CD	2.46	0.53
1:C:21:HIS:HB2	1:C:23:TYR:OH	2.08	0.53
1:F:37:GLU:HA	1:F:99:TYR:CD1	2.44	0.53
1:B:38:THR:HA	1:B:39:LEU:HB3	1.89	0.53
1:A:50:LEU:HD23	1:A:60:ILE:HA	1.91	0.53
1:F:20:ILE:N	1:F:20:ILE:CD1	2.69	0.53
1:C:32:GLN:HE21	1:C:84:ALA:HA	1.73	0.53
1:A:53:ASP:CG	1:A:54:GLU:N	2.58	0.53
1:D:38:THR:HA	1:D:39:LEU:HB3	1.91	0.53
1:A:10:THR:HG21	1:A:111:ASP:OD2	2.09	0.53
1:E:114:MET:CE	1:E:114:MET:HA	2.38	0.53
1:F:32:GLN:CG	1:F:83:SER:O	2.57	0.53
1:A:82:ARG:O	1:A:82:ARG:CD	2.57	0.53
1:A:106:ILE:HD12	1:A:113:LEU:HB2	1.90	0.53
1:C:41:TYR:CB	1:C:69:PHE:CD1	2.86	0.53
1:F:46:SER:H	1:F:90:THR:HG23	1.71	0.53
1:D:83:SER:O	1:D:84:ALA:C	2.41	0.53
1:E:44:LYS:O	1:E:92:CYS:HB2	2.09	0.53
1:E:38:THR:C	1:E:99:TYR:CE2	2.83	0.53
1:F:75:LEU:HD13	1:F:103:ARG:CZ	2.39	0.52
1:D:182:THR:O	1:D:186:ILE:CD1	2.38	0.52
1:C:30:ILE:O	1:C:31:HIS:ND1	2.42	0.52
1:E:14:PHE:CD2	1:E:112:ILE:HD13	2.44	0.52
1:D:32:GLN:OE1	1:D:85:TRP:HE3	1.90	0.52
1:B:114:MET:HA	1:B:114:MET:CE	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:13:TRP:CE3	1:F:14:PHE:CA	2.93	0.52
1:A:75:LEU:N	1:A:99:TYR:CZ	2.77	0.52
1:A:17:HIS:O	1:A:18:CYS:CB	2.57	0.52
1:B:22:LYS:HG2	1:B:93:GLU:HG2	1.90	0.52
1:F:25:SER:O	1:F:26:LYS:HB2	2.10	0.52
1:F:71:GLY:O	1:F:72:GLU:HB3	2.09	0.52
1:C:70:ILE:O	1:C:71:GLY:C	2.48	0.52
1:F:41:TYR:CD2	1:F:41:TYR:C	2.82	0.52
1:C:50:LEU:CD1	1:C:60:ILE:HD13	2.40	0.52
1:E:111:ASP:O	1:E:114:MET:HB2	2.09	0.52
1:A:150:LEU:HA	1:A:153:GLN:HG2	1.92	0.52
1:E:83:SER:O	1:E:84:ALA:O	2.26	0.52
1:E:39:LEU:CA	1:E:99:TYR:HE2	2.23	0.52
1:B:30:ILE:CD1	1:B:40:TYR:HE2	2.20	0.52
1:D:13:TRP:CE3	1:D:112:ILE:HD11	2.45	0.52
1:D:14:PHE:HB2	1:D:112:ILE:HG12	1.91	0.52
1:E:134:LEU:HG	1:F:195:LEU:CB	2.40	0.52
1:F:114:MET:C	1:F:116:LEU:N	2.63	0.52
1:E:30:ILE:HG22	1:E:82:ARG:HD2	1.90	0.52
1:C:80:GLN:HE21	1:C:81:GLU:N	2.08	0.52
1:E:38:THR:N	1:E:99:TYR:CE2	2.75	0.52
1:C:30:ILE:O	1:C:31:HIS:CD2	2.63	0.52
1:A:42:ILE:HD12	1:A:68:ASP:HB2	1.92	0.52
1:E:181:GLU:HG2	1:F:53:ASP:OD1	2.11	0.51
1:B:120:MET:CA	1:B:123:ARG:HB2	2.39	0.51
1:A:106:ILE:HG21	1:A:113:LEU:HD22	1.92	0.51
1:F:65:ASN:CG	1:F:66:GLN:H	2.13	0.51
1:F:38:THR:HG23	1:F:97:ILE:O	2.10	0.51
1:E:8:ASP:HB3	1:E:11:LEU:HB2	1.92	0.51
1:B:38:THR:HA	1:B:39:LEU:CB	2.40	0.51
1:A:114:MET:HE2	1:B:76:PHE:HE1	1.75	0.51
1:D:29:LEU:HD21	1:D:94:VAL:HG21	1.91	0.51
1:F:117:SER:HA	1:F:120:MET:HE2	1.92	0.51
1:A:15:LEU:CD1	1:A:20:ILE:HD11	2.40	0.51
1:B:73:LEU:O	1:B:80:GLN:NE2	2.43	0.51
1:E:38:THR:CA	1:E:99:TYR:HE2	2.23	0.51
1:D:97:ILE:HD11	1:D:101:LYS:HG2	1.92	0.51
1:F:75:LEU:CD1	1:F:103:ARG:NE	2.74	0.51
1:B:125:GLN:O	1:B:129:GLU:OE2	2.29	0.51
1:B:30:ILE:HG21	1:B:82:ARG:HD3	1.87	0.51
1:C:37:GLU:O	1:C:38:THR:O	2.29	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:121:ALA:O	1:F:122:ARG:C	2.49	0.51
1:B:39:LEU:HB2	1:B:99:TYR:HE2	1.75	0.51
1:E:205:VAL:CG1	1:E:206:TYR:N	2.14	0.51
1:A:112:ILE:CD1	1:A:112:ILE:H	2.24	0.51
1:C:98:SER:C	1:C:100:LYS:N	2.42	0.51
1:F:15:LEU:C	1:F:17:HIS:N	2.62	0.51
1:E:8:ASP:CG	1:E:115:ARG:HH12	2.14	0.51
1:E:38:THR:HG22	1:E:98:SER:HA	1.93	0.51
1:D:136:PHE:CE1	1:D:186:ILE:HD11	2.46	0.51
1:A:10:THR:HG21	1:A:111:ASP:HB3	1.93	0.51
1:E:150:LEU:O	1:E:153:GLN:CB	2.59	0.51
1:A:62:SER:HG	1:A:63:TYR:H	1.57	0.51
1:F:167:ILE:HD13	1:F:172:ILE:HD13	1.93	0.51
1:F:122:ARG:CG	1:F:123:ARG:N	2.72	0.51
1:B:36:ALA:HB1	1:B:82:ARG:NH1	2.26	0.51
1:E:168:THR:HG22	1:E:201:LYS:HG3	1.93	0.51
1:C:75:LEU:HA	1:C:99:TYR:CE1	2.45	0.50
1:C:30:ILE:CD1	1:C:86:VAL:HG21	2.39	0.50
1:D:50:LEU:CD1	1:D:60:ILE:HG12	2.41	0.50
1:C:14:PHE:C	1:C:16:SER:N	2.64	0.50
1:B:116:LEU:O	1:B:117:SER:C	2.48	0.50
1:E:52:LYS:HA	1:E:57:LYS:O	2.11	0.50
1:F:41:TYR:C	1:F:94:VAL:HG13	2.31	0.50
1:C:21:HIS:HB2	1:C:23:TYR:CZ	2.46	0.50
1:C:39:LEU:O	1:C:40:TYR:O	2.30	0.50
1:B:40:TYR:HD2	1:B:70:ILE:HG22	1.54	0.50
1:B:112:ILE:CD1	1:B:112:ILE:CG1	2.90	0.50
1:C:14:PHE:CE2	1:C:112:ILE:HG12	2.47	0.50
1:B:39:LEU:HB2	1:B:99:TYR:CD2	2.46	0.50
1:E:204:VAL:O	1:E:205:VAL:O	2.30	0.50
1:C:50:LEU:CD2	1:C:87:ARG:HD3	2.39	0.50
1:C:25:SER:C	1:C:27:SER:H	2.14	0.50
1:F:68:ASP:CA	1:F:119:GLN:HE21	2.09	0.50
1:C:114:MET:HE3	1:D:113:LEU:HD21	1.92	0.50
1:C:72:GLU:O	1:C:74:GLY:N	2.43	0.50
1:E:30:ILE:HD11	1:E:40:TYR:CE2	2.47	0.50
1:D:69:PHE:HD2	1:D:119:GLN:OE1	1.95	0.50
1:E:203:ILE:HD12	1:E:203:ILE:N	2.27	0.50
1:E:148:LEU:HD23	1:E:152:LYS:HE2	1.94	0.50
1:F:126:VAL:C	1:F:128:SER:H	2.15	0.50
1:F:74:GLY:O	1:F:75:LEU:O	2.29	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:116:LEU:HD21	1:B:120:MET:CE	2.41	0.50
1:B:79:GLY:O	1:B:80:GLN:O	2.30	0.50
1:D:32:GLN:OE1	1:D:85:TRP:CZ3	2.62	0.50
1:B:109:ASN:C	1:B:111:ASP:H	2.16	0.50
1:A:76:PHE:HE1	1:B:114:MET:CE	2.24	0.50
1:A:164:GLN:HG3	1:A:204:VAL:HG22	1.93	0.50
1:E:38:THR:C	1:E:99:TYR:HE2	2.14	0.50
1:E:65:ASN:O	1:E:68:ASP:CG	2.49	0.50
1:E:42:ILE:N	1:E:68:ASP:O	2.39	0.50
1:F:45:GLY:HA3	1:F:92:CYS:HB3	1.94	0.50
1:A:29:LEU:HD21	1:A:94:VAL:HG21	1.94	0.50
1:C:101:LYS:O	1:C:104:GLN:HB2	2.12	0.49
1:F:60:ILE:CG2	1:F:61:LEU:N	2.40	0.49
1:F:75:LEU:HD13	1:F:103:ARG:NH1	2.27	0.49
1:B:21:HIS:CE1	1:B:23:TYR:CE2	3.00	0.49
1:D:139:VAL:HG13	1:D:176:VAL:HG11	1.93	0.49
1:F:13:TRP:O	1:F:15:LEU:N	2.45	0.49
1:F:54:GLU:C	1:F:56:GLY:N	2.62	0.49
1:E:46:SER:CA	1:E:90:THR:CG2	2.90	0.49
1:D:124:LEU:O	1:D:125:GLN:C	2.49	0.49
1:C:40:TYR:HB2	1:C:70:ILE:HB	1.93	0.49
1:C:33:GLY:O	1:C:81:GLU:O	2.29	0.49
1:B:168:THR:OG1	1:B:170:GLN:HG3	2.12	0.49
1:B:78:GLU:O	1:B:80:GLN:N	2.36	0.49
1:D:14:PHE:CD2	1:D:112:ILE:HG21	2.48	0.49
1:F:43:VAL:CB	1:F:93:GLU:OE2	2.58	0.49
1:A:82:ARG:O	1:A:83:SER:O	2.30	0.49
1:D:150:LEU:HA	1:D:153:GLN:HG3	1.94	0.49
1:C:30:ILE:HB	1:C:86:VAL:HB	1.94	0.49
1:A:25:SER:HB2	1:A:89:LYS:O	2.13	0.49
1:A:41:TYR:HD1	1:A:69:PHE:CE1	2.30	0.49
1:F:47:VAL:HA	1:F:89:LYS:H	1.78	0.49
1:F:117:SER:CB	1:F:120:MET:CE	2.90	0.49
1:D:70:ILE:HG22	1:D:71:GLY:H	1.75	0.49
1:F:32:GLN:HB2	1:F:85:TRP:CE3	2.48	0.49
1:E:127:THR:HG22	1:E:128:SER:N	1.94	0.49
1:B:39:LEU:N	1:B:99:TYR:HE2	2.11	0.49
1:E:163:MET:O	1:E:205:VAL:N	2.46	0.49
1:B:43:VAL:O	1:B:66:GLN:HG3	2.12	0.49
1:C:112:ILE:CD1	1:C:112:ILE:H	2.25	0.49
1:E:149:ASN:O	1:E:153:GLN:HG2	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:112:ILE:CD1	1:D:112:ILE:N	2.74	0.49
1:E:76:PHE:HE2	1:F:114:MET:HE2	1.78	0.49
1:C:10:THR:HG21	1:C:111:ASP:CB	2.43	0.49
1:B:120:MET:O	1:B:123:ARG:CB	2.58	0.49
1:C:8:ASP:OD1	1:C:115:ARG:NH2	2.46	0.49
1:D:150:LEU:HA	1:D:153:GLN:HG2	1.95	0.48
1:A:14:PHE:HE2	1:A:102:PHE:HE1	1.59	0.48
1:F:126:VAL:HG13	1:F:192:ASP:HB3	1.95	0.48
1:F:38:THR:HG21	1:F:96:GLU:HB2	1.94	0.48
1:A:60:ILE:HG23	1:A:61:LEU:H	1.75	0.48
1:B:124:LEU:C	1:B:126:VAL:H	2.17	0.48
1:D:10:THR:HG23	1:D:112:ILE:CD1	2.44	0.48
1:F:19:HIS:O	1:F:96:GLU:N	2.45	0.48
1:B:82:ARG:O	1:B:83:SER:C	2.51	0.48
1:E:139:VAL:HG13	1:E:176:VAL:HG11	1.96	0.48
1:C:37:GLU:HA	1:C:99:TYR:CG	2.47	0.48
1:F:114:MET:HE3	1:F:114:MET:CA	2.40	0.48
1:A:8:ASP:OD2	1:A:115:ARG:NH1	2.41	0.48
1:F:151:ALA:HA	1:F:165:ILE:HG23	1.95	0.48
1:D:51:ILE:C	1:D:51:ILE:HD12	2.33	0.48
1:F:38:THR:HA	1:F:39:LEU:CB	2.43	0.48
1:B:51:ILE:HG22	1:B:84:ALA:HB2	1.95	0.48
1:D:86:VAL:HG12	1:D:87:ARG:N	2.27	0.48
1:F:44:LYS:O	1:F:92:CYS:HB2	2.13	0.48
1:E:136:PHE:CE1	1:E:186:ILE:HD11	2.48	0.48
1:B:120:MET:HA	1:B:123:ARG:HB2	1.95	0.48
1:F:43:VAL:O	1:F:44:LYS:HG3	2.13	0.48
1:F:114:MET:HE2	1:F:114:MET:CA	2.43	0.48
1:A:121:ALA:HB1	1:B:73:LEU:HG	1.95	0.48
1:F:28:THR:CG2	1:F:31:HIS:CE1	2.96	0.48
1:C:75:LEU:O	1:C:103:ARG:NH1	2.47	0.48
1:F:94:VAL:HG12	1:F:95:ALA:H	1.74	0.48
1:D:119:GLN:O	1:D:121:ALA:N	2.47	0.48
1:A:76:PHE:N	1:A:76:PHE:CD2	2.80	0.48
1:F:15:LEU:O	1:F:16:SER:C	2.51	0.48
1:C:80:GLN:HE21	1:C:81:GLU:H	1.61	0.48
1:E:197:SER:HG	1:E:204:VAL:HG11	1.76	0.48
1:A:75:LEU:CD1	1:A:99:TYR:CD2	2.96	0.48
1:E:38:THR:CA	1:E:39:LEU:HB3	2.26	0.47
1:C:150:LEU:HD23	1:C:153:GLN:HG3	1.96	0.47
1:C:106:ILE:HD13	1:C:113:LEU:HD22	1.94	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:97:ILE:CD1	1:A:101:LYS:HE3	2.42	0.47
1:A:29:LEU:O	1:A:30:ILE:HD13	2.14	0.47
1:A:40:TYR:HB2	1:A:70:ILE:CG1	2.44	0.47
1:F:13:TRP:CZ3	1:F:14:PHE:HB2	2.49	0.47
1:E:53:ASP:CG	1:E:59:MET:CE	2.83	0.47
1:A:50:LEU:HD22	1:A:60:ILE:HA	1.95	0.47
1:A:39:LEU:HB2	1:A:99:TYR:HE2	1.79	0.47
1:F:43:VAL:O	1:F:44:LYS:HG2	2.12	0.47
1:B:29:LEU:HD21	1:B:94:VAL:HG21	1.94	0.47
1:C:69:PHE:CE2	1:C:116:LEU:HB2	2.49	0.47
1:D:136:PHE:HE1	1:D:186:ILE:HD11	1.78	0.47
1:C:23:TYR:CD1	1:C:29:LEU:HD22	2.42	0.47
1:A:23:TYR:O	1:A:91:ALA:HA	2.13	0.47
1:F:15:LEU:O	1:F:17:HIS:N	2.47	0.47
1:F:30:ILE:CG1	1:F:86:VAL:CB	2.88	0.47
1:B:117:SER:O	1:B:118:ALA:O	2.33	0.47
1:C:102:PHE:O	1:C:102:PHE:CG	2.21	0.47
1:A:106:ILE:HG23	1:A:113:LEU:HD22	1.96	0.47
1:D:70:ILE:O	1:D:71:GLY:C	2.53	0.47
1:D:73:LEU:HD12	1:D:73:LEU:H	1.78	0.47
1:C:72:GLU:C	1:C:74:GLY:N	2.67	0.47
1:F:94:VAL:CG1	1:F:95:ALA:N	2.76	0.47
1:B:82:ARG:HH21	1:B:82:ARG:CG	2.28	0.47
1:A:55:GLU:HG3	1:A:56:GLY:O	2.14	0.47
1:B:112:ILE:HG23	1:B:113:LEU:N	2.29	0.47
1:D:38:THR:HA	1:D:39:LEU:CB	2.44	0.47
1:F:32:GLN:HB2	1:F:85:TRP:CZ3	2.49	0.47
1:F:39:LEU:HA	1:F:39:LEU:HD12	1.46	0.47
1:A:81:GLU:CB	1:A:82:ARG:HB3	2.41	0.47
1:D:11:LEU:O	1:D:15:LEU:HG	2.15	0.47
1:A:78:GLU:OE2	1:A:78:GLU:HA	2.15	0.47
1:E:117:SER:N	1:E:120:MET:CE	2.78	0.47
1:E:205:VAL:O	1:E:206:TYR:CD2	2.67	0.47
1:F:43:VAL:HG12	1:F:93:GLU:OE2	2.15	0.47
1:A:102:PHE:CZ	1:A:106:ILE:HD11	2.50	0.47
1:E:45:GLY:HA3	1:E:92:CYS:HB3	1.97	0.47
1:C:168:THR:HG22	1:C:201:LYS:HG3	1.96	0.47
1:D:23:TYR:O	1:D:91:ALA:HA	2.15	0.47
1:F:189:MET:HG3	1:F:193:GLN:HE21	1.80	0.47
1:E:136:PHE:HE1	1:E:186:ILE:HD11	1.80	0.47
1:C:30:ILE:HB	1:C:86:VAL:N	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:25:SER:O	1:D:26:LYS:HB2	2.15	0.47
1:D:13:TRP:HZ3	1:D:112:ILE:HD13	1.81	0.46
1:A:97:ILE:HD11	1:A:101:LYS:HG2	1.97	0.46
1:F:28:THR:HG21	1:F:31:HIS:CE1	2.50	0.46
1:C:37:GLU:O	1:C:38:THR:OG1	2.29	0.46
1:C:37:GLU:CG	1:C:38:THR:N	2.78	0.46
1:F:124:LEU:O	1:F:126:VAL:CA	2.60	0.46
1:F:117:SER:HB3	1:F:120:MET:HE2	1.98	0.46
1:B:36:ALA:HB1	1:B:82:ARG:HH12	1.80	0.46
1:B:69:PHE:N	1:B:69:PHE:CD2	2.83	0.46
1:A:30:ILE:HD12	1:A:40:TYR:OH	2.15	0.46
1:E:124:LEU:HD22	1:E:127:THR:HG21	1.97	0.46
1:C:111:ASP:O	1:C:114:MET:HB2	2.16	0.46
1:E:114:MET:HE3	1:E:114:MET:HA	1.97	0.46
1:C:40:TYR:C	1:C:70:ILE:HD12	2.36	0.46
1:B:122:ARG:O	1:B:126:VAL:CG2	2.59	0.46
1:D:99:TYR:O	1:D:103:ARG:HG3	2.16	0.46
1:E:36:ALA:C	1:E:37:GLU:HG3	2.36	0.46
1:A:13:TRP:O	1:A:15:LEU:N	2.48	0.46
1:E:162:GLY:CA	1:E:207:GLY:N	2.69	0.46
1:C:20:ILE:CD1	1:C:20:ILE:H	2.28	0.46
1:A:170:GLN:HB3	1:A:180:ARG:HH21	1.79	0.46
1:E:126:VAL:CG1	1:E:127:THR:N	2.37	0.46
1:B:64:LEU:HD13	1:B:70:ILE:CD1	2.45	0.46
1:B:119:GLN:CG	1:B:120:MET:H	2.06	0.46
1:E:122:ARG:HA	1:E:125:GLN:HB2	1.97	0.46
1:C:67:GLY:O	1:C:119:GLN:OE1	2.34	0.46
1:F:70:ILE:HA	1:F:71:GLY:O	2.15	0.46
1:B:165:ILE:C	1:B:165:ILE:HD12	2.36	0.46
1:A:76:PHE:HE1	1:B:114:MET:HE1	1.80	0.46
1:A:102:PHE:O	1:A:106:ILE:HG12	2.16	0.46
1:F:97:ILE:CD1	1:F:101:LYS:HE3	2.44	0.46
1:E:42:ILE:CD1	1:E:68:ASP:HB2	2.38	0.46
1:E:150:LEU:C	1:E:153:GLN:HG2	2.35	0.46
1:D:30:ILE:CG2	1:D:82:ARG:HD2	2.46	0.45
1:A:175:ILE:N	1:A:175:ILE:HD12	2.31	0.45
1:C:7:THR:O	1:C:9:PRO:HD3	2.16	0.45
1:D:64:LEU:HD13	1:D:70:ILE:HG12	1.98	0.45
1:A:76:PHE:CE1	1:B:114:MET:HE1	2.51	0.45
1:B:142:ARG:HD2	1:B:176:VAL:HG13	1.98	0.45
1:F:126:VAL:CG1	1:F:193:GLN:NE2	2.69	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:195:LEU:N	1:F:206:TYR:CE1	2.84	0.45
1:E:38:THR:N	1:E:99:TYR:HD2	2.04	0.45
1:B:39:LEU:HD21	1:B:102:PHE:CG	2.51	0.45
1:B:82:ARG:HH21	1:B:82:ARG:HG3	1.81	0.45
1:B:106:ILE:HD13	1:B:113:LEU:HD22	1.98	0.45
1:C:14:PHE:CD1	1:C:15:LEU:HD21	2.47	0.45
1:C:39:LEU:HD13	1:C:99:TYR:CE2	2.51	0.45
1:A:80:GLN:O	1:A:82:ARG:HA	2.17	0.45
1:B:40:TYR:O	1:B:70:ILE:N	2.49	0.45
1:F:164:GLN:CG	1:F:202:THR:HG23	2.46	0.45
1:B:196:ILE:HD12	1:B:197:SER:N	2.31	0.45
1:A:44:LYS:O	1:A:92:CYS:HB2	2.16	0.45
1:C:39:LEU:HA	1:C:39:LEU:HD12	1.30	0.45
1:E:73:LEU:HD23	1:F:125:GLN:HG3	1.98	0.45
1:D:122:ARG:NH2	1:D:122:ARG:CG	2.40	0.45
1:D:82:ARG:O	1:D:83:SER:C	2.55	0.45
1:A:8:ASP:CG	1:A:11:LEU:HB2	2.37	0.45
1:E:12:GLU:OE1	1:E:12:GLU:HA	2.17	0.45
1:C:16:SER:O	1:C:16:SER:OG	2.28	0.45
1:C:18:CYS:HB3	1:C:97:ILE:HB	1.98	0.45
1:E:51:ILE:HD11	1:E:59:MET:HB3	1.93	0.45
1:C:170:GLN:HB3	1:C:180:ARG:HH21	1.81	0.45
1:C:139:VAL:HG13	1:C:176:VAL:HG11	1.99	0.45
1:C:69:PHE:CD2	1:C:116:LEU:CB	3.00	0.45
1:F:18:CYS:HB3	1:F:97:ILE:HB	1.99	0.45
1:F:97:ILE:HD11	1:F:101:LYS:CE	2.44	0.45
1:F:117:SER:CB	1:F:120:MET:HE1	2.46	0.45
1:E:38:THR:O	1:E:82:ARG:NH1	2.48	0.45
1:A:128:SER:O	1:B:61:LEU:HD22	2.17	0.45
1:B:64:LEU:CD1	1:B:70:ILE:HD11	2.22	0.45
1:B:10:THR:HG21	1:B:111:ASP:HB3	1.98	0.45
1:D:50:LEU:HD11	1:D:60:ILE:HG12	1.99	0.45
1:E:181:GLU:HG2	1:F:54:GLU:OE1	2.17	0.45
1:B:25:SER:O	1:B:26:LYS:HB2	2.17	0.45
1:A:143:ILE:HD12	1:A:186:ILE:HD12	1.99	0.45
1:E:10:THR:HG22	1:E:112:ILE:HG12	1.98	0.45
1:B:97:ILE:O	1:B:98:SER:C	2.54	0.45
1:D:70:ILE:C	1:D:72:GLU:N	2.70	0.45
1:F:139:VAL:HG13	1:F:176:VAL:HG11	1.98	0.45
1:C:69:PHE:O	1:C:72:GLU:OE1	2.35	0.44
1:F:123:ARG:O	1:F:124:LEU:HD22	2.14	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:127:THR:HG23	1:E:128:SER:CA	2.40	0.44
1:E:14:PHE:CZ	1:E:97:ILE:HG21	2.52	0.44
1:A:15:LEU:HD11	1:A:20:ILE:CD1	2.46	0.44
1:E:31:HIS:CD2	1:E:34:GLU:OE1	2.65	0.44
1:C:69:PHE:HB2	1:C:119:GLN:HE22	1.82	0.44
1:E:123:ARG:O	1:E:126:VAL:N	2.49	0.44
1:B:78:GLU:C	1:B:80:GLN:H	2.19	0.44
1:A:35:LYS:CA	1:A:81:GLU:HB2	2.34	0.44
1:D:119:GLN:O	1:D:122:ARG:N	2.50	0.44
1:F:164:GLN:OE1	1:F:202:THR:CG2	2.61	0.44
1:C:51:ILE:C	1:C:51:ILE:HD12	2.37	0.44
1:A:126:VAL:HG13	1:A:193:GLN:HE22	1.81	0.44
1:F:165:ILE:HD12	1:F:165:ILE:C	2.38	0.44
1:F:21:HIS:O	1:F:93:GLU:CA	2.64	0.44
1:E:36:ALA:O	1:E:37:GLU:HG3	2.16	0.44
1:F:164:GLN:HG2	1:F:202:THR:HG23	1.99	0.44
1:E:117:SER:N	1:E:120:MET:HE2	2.32	0.44
1:A:8:ASP:OD1	1:A:11:LEU:CB	2.65	0.44
1:B:10:THR:O	1:B:11:LEU:C	2.56	0.44
1:C:41:TYR:CG	1:C:69:PHE:CE1	2.82	0.44
1:F:13:TRP:CE3	1:F:14:PHE:HB2	2.52	0.44
1:F:19:HIS:O	1:F:95:ALA:CA	2.60	0.44
1:E:124:LEU:HD23	1:E:127:THR:HG21	1.99	0.44
1:E:164:GLN:HG3	1:E:204:VAL:CB	2.43	0.44
1:A:39:LEU:HA	1:A:39:LEU:HD12	1.71	0.44
1:B:51:ILE:CG2	1:B:84:ALA:CB	2.95	0.43
1:F:53:ASP:C	1:F:53:ASP:OD2	2.56	0.43
1:E:186:ILE:CD1	1:E:186:ILE:N	2.81	0.43
1:D:38:THR:HB	1:D:40:TYR:CE2	2.53	0.43
1:A:15:LEU:HD11	1:A:20:ILE:HD11	2.00	0.43
1:C:14:PHE:HE2	1:C:112:ILE:HG21	1.77	0.43
1:C:37:GLU:HG3	1:C:38:THR:N	2.30	0.43
1:A:40:TYR:HB3	1:A:94:VAL:CG1	2.48	0.43
1:C:69:PHE:CD2	1:C:116:LEU:CA	3.00	0.43
1:C:72:GLU:O	1:C:73:LEU:C	2.56	0.43
1:F:124:LEU:O	1:F:126:VAL:C	2.56	0.43
1:F:195:LEU:C	1:F:206:TYR:CD1	2.91	0.43
1:E:127:THR:HA	1:E:130:LYS:HE2	2.00	0.43
1:A:34:GLU:HB2	1:A:82:ARG:HG2	1.99	0.43
1:B:32:GLN:HG3	1:B:32:GLN:O	2.15	0.43
1:B:64:LEU:HD13	1:B:70:ILE:HD12	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:150:LEU:O	1:E:153:GLN:CG	2.66	0.43
1:C:85:TRP:H	1:C:85:TRP:HE3	1.67	0.43
1:C:117:SER:HA	1:C:120:MET:HE2	1.99	0.43
1:C:14:PHE:CB	1:C:15:LEU:CD2	2.73	0.43
1:F:41:TYR:CD2	1:F:69:PHE:CD1	3.06	0.43
1:E:14:PHE:HB2	1:E:112:ILE:CD1	2.48	0.43
1:C:8:ASP:HA	1:C:9:PRO:HD3	1.77	0.43
1:C:18:CYS:SG	1:C:97:ILE:HB	2.59	0.43
1:C:80:GLN:NE2	1:C:81:GLU:H	2.15	0.43
1:A:50:LEU:HD21	1:A:60:ILE:CG1	2.40	0.43
1:C:23:TYR:CE1	1:C:29:LEU:HD22	2.53	0.43
1:E:75:LEU:HA	1:E:99:TYR:HD1	1.74	0.43
1:B:21:HIS:ND1	1:B:23:TYR:CZ	2.85	0.43
1:F:39:LEU:HA	1:F:71:GLY:HA2	2.01	0.43
1:F:82:ARG:O	1:F:83:SER:C	2.57	0.43
1:C:83:SER:O	1:C:84:ALA:HB2	2.14	0.43
1:A:30:ILE:HD13	1:A:30:ILE:N	2.34	0.43
1:F:118:ALA:O	1:F:122:ARG:HB3	2.18	0.43
1:D:163:MET:O	1:D:205:VAL:N	2.47	0.43
1:C:42:ILE:HD12	1:C:68:ASP:O	2.18	0.43
1:F:117:SER:CB	1:F:120:MET:HE2	2.49	0.43
1:E:97:ILE:HD11	1:E:101:LYS:HG2	2.01	0.43
1:A:14:PHE:HB2	1:A:112:ILE:HG12	1.99	0.43
1:F:165:ILE:CD1	1:F:203:ILE:HB	2.49	0.43
1:B:136:PHE:CE1	1:B:186:ILE:HD11	2.54	0.43
1:E:106:ILE:HD13	1:E:113:LEU:HD22	1.99	0.43
1:F:11:LEU:O	1:F:15:LEU:HG	2.19	0.43
1:E:10:THR:CG2	1:E:112:ILE:HG12	2.48	0.43
1:E:37:GLU:O	1:E:38:THR:OG1	2.29	0.43
1:A:80:GLN:OE1	1:B:125:GLN:NE2	2.46	0.43
1:D:69:PHE:HB2	1:D:119:GLN:OE1	2.19	0.43
1:D:39:LEU:HD12	1:D:39:LEU:HA	1.74	0.43
1:D:33:GLY:C	1:D:81:GLU:HG3	2.39	0.43
1:F:43:VAL:O	1:F:43:VAL:HG12	2.18	0.43
1:E:123:ARG:HB3	1:E:124:LEU:H	1.67	0.42
1:B:38:THR:CA	1:B:99:TYR:HE2	2.26	0.42
1:E:28:THR:HA	1:E:87:ARG:HA	2.01	0.42
1:A:165:ILE:HD12	1:A:205:VAL:HG23	2.00	0.42
1:D:47:VAL:HG22	1:D:64:LEU:HB2	2.01	0.42
1:E:44:LYS:HG2	1:E:45:GLY:N	2.34	0.42
1:F:14:PHE:HD1	1:F:14:PHE:C	2.12	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:109:ASN:HA	1:E:110:PRO:HD2	1.92	0.42
1:E:14:PHE:HB2	1:E:112:ILE:HD13	2.01	0.42
1:A:35:LYS:HA	1:A:81:GLU:HB2	1.91	0.42
1:D:186:ILE:N	1:D:186:ILE:CD1	2.81	0.42
1:B:69:PHE:HD2	1:B:69:PHE:N	2.17	0.42
1:B:77:GLU:O	1:B:78:GLU:C	2.58	0.42
1:A:143:ILE:HD12	1:A:186:ILE:CD1	2.50	0.42
1:E:39:LEU:HD12	1:E:39:LEU:HA	1.74	0.42
1:B:51:ILE:CD1	1:B:61:LEU:HD21	2.50	0.42
1:A:56:GLY:O	1:A:57:LYS:HB2	2.15	0.42
1:C:51:ILE:HD12	1:C:59:MET:HB3	2.00	0.42
1:C:159:HIS:CG	1:C:160:PRO:HD2	2.54	0.42
1:A:127:THR:HA	1:A:130:LYS:HE2	2.02	0.42
1:C:36:ALA:O	1:C:37:GLU:CB	2.66	0.42
1:C:78:GLU:HG3	1:C:78:GLU:H	1.56	0.42
1:F:40:TYR:CD2	1:F:40:TYR:N	2.87	0.42
1:F:39:LEU:HA	1:F:71:GLY:CA	2.49	0.42
1:B:85:TRP:CE3	1:B:85:TRP:N	2.80	0.42
1:F:42:ILE:CG2	1:F:66:GLN:HA	2.49	0.42
1:B:124:LEU:C	1:B:126:VAL:N	2.71	0.42
1:A:10:THR:CG2	1:A:111:ASP:HB3	2.49	0.42
1:D:13:TRP:HZ3	1:D:112:ILE:CD1	2.30	0.42
1:D:124:LEU:O	1:D:126:VAL:N	2.52	0.42
1:F:50:LEU:HB2	1:F:85:TRP:CD1	2.55	0.42
1:F:83:SER:HB2	1:F:84:ALA:H	1.62	0.42
1:F:116:LEU:CD2	1:F:117:SER:N	2.79	0.42
1:B:38:THR:N	1:B:99:TYR:CD2	2.87	0.42
1:D:69:PHE:CD2	1:D:119:GLN:OE1	2.72	0.42
1:C:143:ILE:HD12	1:C:186:ILE:CD1	2.50	0.42
1:B:17:HIS:O	1:B:101:LYS:NZ	2.52	0.42
1:C:14:PHE:CE2	1:C:112:ILE:CG2	2.95	0.42
1:E:39:LEU:HD21	1:E:102:PHE:CD1	2.55	0.42
1:E:14:PHE:CD2	1:E:105:LEU:HD13	2.25	0.42
1:C:109:ASN:O	1:C:111:ASP:N	2.52	0.42
1:C:128:SER:C	1:C:130:LYS:H	2.22	0.42
1:E:76:PHE:CD1	1:E:76:PHE:N	2.87	0.42
1:B:36:ALA:HB2	1:B:82:ARG:CZ	2.47	0.42
1:B:119:GLN:O	1:B:121:ALA:N	2.52	0.42
1:C:18:CYS:CB	1:C:97:ILE:HB	2.50	0.42
1:F:70:ILE:HA	1:F:71:GLY:C	2.39	0.42
1:E:14:PHE:HZ	1:E:97:ILE:HG21	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:38:THR:CA	1:E:99:TYR:HD2	2.31	0.42
1:B:36:ALA:O	1:B:37:GLU:HG3	2.20	0.42
1:B:69:PHE:CE1	1:B:116:LEU:HB2	2.54	0.42
1:D:37:GLU:CA	1:D:99:TYR:CD1	2.99	0.42
1:A:14:PHE:CE2	1:A:102:PHE:HE1	2.37	0.42
1:A:159:HIS:CG	1:A:160:PRO:HD2	2.55	0.42
1:F:50:LEU:O	1:F:84:ALA:HB1	2.15	0.42
1:C:23:TYR:CE1	1:C:29:LEU:CD2	3.00	0.42
1:B:168:THR:OG1	1:B:171:GLU:HG3	2.20	0.42
1:A:14:PHE:HD1	1:A:14:PHE:O	2.02	0.42
1:A:69:PHE:CE2	1:A:116:LEU:HA	2.54	0.42
1:D:159:HIS:CG	1:D:160:PRO:HD2	2.55	0.42
1:C:101:LYS:C	1:C:103:ARG:H	2.19	0.41
1:E:134:LEU:CG	1:F:195:LEU:CB	2.98	0.41
1:E:51:ILE:CG2	1:E:84:ALA:O	2.68	0.41
1:B:120:MET:C	1:B:123:ARG:HB2	2.41	0.41
1:B:21:HIS:CE1	1:B:23:TYR:CZ	3.07	0.41
1:C:150:LEU:CA	1:C:153:GLN:HG2	2.44	0.41
1:B:157:MET:HB2	1:B:164:GLN:HB3	2.02	0.41
1:E:17:HIS:CD2	1:E:105:LEU:CD2	2.82	0.41
1:A:76:PHE:O	1:A:77:GLU:CB	2.62	0.41
1:C:41:TYR:CG	1:C:69:PHE:CD1	3.04	0.41
1:F:15:LEU:HD23	1:F:15:LEU:HA	1.91	0.41
1:F:26:LYS:N	1:F:88:ALA:O	2.30	0.41
1:E:53:ASP:CG	1:E:59:MET:HE1	2.40	0.41
1:B:36:ALA:C	1:B:37:GLU:HG3	2.40	0.41
1:E:31:HIS:HB2	1:E:34:GLU:HG3	2.02	0.41
1:A:165:ILE:N	1:A:165:ILE:HD13	2.33	0.41
1:D:157:MET:HB2	1:D:164:GLN:HB3	2.01	0.41
1:C:14:PHE:O	1:C:17:HIS:N	2.54	0.41
1:F:195:LEU:N	1:F:206:TYR:HE1	2.12	0.41
1:F:54:GLU:O	1:F:55:GLU:HB3	2.20	0.41
1:D:86:VAL:CG1	1:D:87:ARG:N	2.84	0.41
1:C:102:PHE:CE2	1:C:106:ILE:HD11	2.55	0.41
1:F:106:ILE:O	1:F:110:PRO:HG3	2.20	0.41
1:F:124:LEU:HD23	1:F:124:LEU:N	2.31	0.41
1:F:46:SER:HB3	1:F:65:ASN:HA	2.03	0.41
1:B:51:ILE:CD1	1:B:61:LEU:CD2	2.98	0.41
1:A:23:TYR:CE1	1:A:29:LEU:HG	2.56	0.41
1:C:167:ILE:HD13	1:C:172:ILE:HD11	2.03	0.41
1:C:37:GLU:C	1:C:38:THR:O	2.58	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:32:GLN:CG	1:F:83:SER:HA	2.36	0.41
1:E:8:ASP:HA	1:E:9:PRO:HD2	1.89	0.41
1:C:109:ASN:C	1:C:111:ASP:H	2.24	0.41
1:B:71:GLY:C	1:B:72:GLU:O	2.54	0.41
1:C:43:VAL:C	1:C:44:LYS:HG3	2.39	0.41
1:F:13:TRP:O	1:F:14:PHE:C	2.58	0.41
1:E:28:THR:HG22	1:E:29:LEU:N	2.36	0.41
1:C:74:GLY:C	1:C:99:TYR:HE1	2.24	0.41
1:B:32:GLN:O	1:B:32:GLN:HG2	2.20	0.41
1:B:70:ILE:HD12	1:B:70:ILE:HA	1.75	0.41
1:B:114:MET:HE3	1:B:114:MET:HA	2.03	0.41
1:E:77:GLU:OE1	1:E:80:GLN:OE1	2.39	0.41
1:B:167:ILE:HD13	1:B:172:ILE:HD11	2.03	0.41
1:C:167:ILE:CD1	1:C:172:ILE:HD13	2.51	0.41
1:B:139:VAL:HG13	1:B:176:VAL:HG11	2.03	0.41
1:E:38:THR:HG22	1:E:97:ILE:O	2.20	0.41
1:B:38:THR:HA	1:B:99:TYR:CD2	2.55	0.41
1:B:82:ARG:CG	1:B:82:ARG:NH2	2.82	0.41
1:E:164:GLN:HA	1:E:204:VAL:HG23	1.99	0.41
1:C:30:ILE:HG22	1:C:31:HIS:H	1.49	0.41
1:D:33:GLY:HA2	1:D:81:GLU:CG	2.50	0.41
1:D:10:THR:HG23	1:D:112:ILE:HD12	2.03	0.41
1:F:115:ARG:O	1:F:115:ARG:HG2	2.20	0.41
1:D:8:ASP:HA	1:D:9:PRO:HD2	1.73	0.41
1:C:35:LYS:O	1:C:36:ALA:C	2.45	0.41
1:F:38:THR:HA	1:F:39:LEU:HB3	2.02	0.41
1:F:65:ASN:CG	1:F:66:GLN:N	2.75	0.41
1:F:41:TYR:CB	1:F:69:PHE:CE1	3.03	0.41
1:B:31:HIS:CD2	1:B:34:GLU:OE1	2.74	0.41
1:D:30:ILE:HD12	1:D:86:VAL:CG2	2.51	0.41
1:B:168:THR:HG1	1:B:170:GLN:HG3	1.85	0.41
1:A:40:TYR:CD2	1:A:40:TYR:N	2.89	0.41
1:D:11:LEU:HD23	1:D:11:LEU:HA	1.83	0.41
1:F:11:LEU:HD22	1:F:15:LEU:HG	2.03	0.40
1:F:127:THR:HA	1:F:130:LYS:HE2	2.03	0.40
1:F:38:THR:O	1:F:82:ARG:NH1	2.33	0.40
1:E:14:PHE:O	1:E:17:HIS:CB	2.53	0.40
1:E:46:SER:CB	1:E:90:THR:CG2	2.99	0.40
1:D:82:ARG:O	1:D:84:ALA:N	2.53	0.40
1:C:47:VAL:HG12	1:C:88:ALA:HA	2.03	0.40
1:F:46:SER:HB2	1:F:64:LEU:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:32:GLN:C	1:C:34:GLU:H	2.24	0.40
1:E:205:VAL:HG12	1:E:206:TYR:C	2.41	0.40
1:C:143:ILE:HD12	1:C:186:ILE:HD12	2.03	0.40
1:F:119:GLN:O	1:F:123:ARG:HD3	2.21	0.40
1:F:195:LEU:CA	1:F:206:TYR:CE1	3.05	0.40
1:A:87:ARG:HG2	1:A:88:ALA:N	2.36	0.40
1:C:112:ILE:CD1	1:C:112:ILE:N	2.85	0.40
1:F:13:TRP:CD2	1:F:14:PHE:N	2.88	0.40
1:F:47:VAL:CG2	1:F:64:LEU:HB2	2.52	0.40
1:F:74:GLY:HA3	1:F:99:TYR:CE1	2.57	0.40
1:D:41:TYR:OH	1:D:67:GLY:HA2	2.21	0.40
1:C:21:HIS:CB	1:C:23:TYR:CZ	3.05	0.40
1:D:10:THR:CG2	1:D:112:ILE:HD12	2.51	0.40
1:B:60:ILE:HD13	1:B:63:TYR:OH	2.21	0.40
1:F:142:ARG:HD2	1:F:176:VAL:HG13	2.04	0.40
1:C:51:ILE:HD11	1:C:59:MET:SD	2.62	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	195/210 (93%)	163 (84%)	21 (11%)	11 (6%)	2 26
1	B	195/210 (93%)	164 (84%)	18 (9%)	13 (7%)	1 21
1	C	195/210 (93%)	154 (79%)	29 (15%)	12 (6%)	2 24
1	D	195/210 (93%)	173 (89%)	18 (9%)	4 (2%)	9 52
1	E	195/210 (93%)	159 (82%)	25 (13%)	11 (6%)	2 26
1	F	195/210 (93%)	149 (76%)	32 (16%)	14 (7%)	1 19
All	All	1170/1260 (93%)	962 (82%)	143 (12%)	65 (6%)	2 26

All (65) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	14	PHE
1	A	15	LEU
1	A	35	LYS
1	A	57	LYS
1	A	82	ARG
1	A	83	SER
1	A	84	ALA
1	B	110	PRO
1	B	118	ALA
1	B	119	GLN
1	B	128	SER
1	C	17	HIS
1	C	34	GLU
1	C	36	ALA
1	C	38	THR
1	C	84	ALA
1	D	84	ALA
1	E	16	SER
1	E	84	ALA
1	E	205	VAL
1	F	70	ILE
1	F	75	LEU
1	F	83	SER
1	F	85	TRP
1	F	125	GLN
1	A	18	CYS
1	A	71	GLY
1	B	78	GLU
1	B	80	GLN
1	B	83	SER
1	B	84	ALA
1	B	120	MET
1	C	11	LEU
1	C	15	LEU
1	C	55	GLU
1	C	71	GLY
1	C	73	LEU
1	D	71	GLY
1	E	39	LEU
1	E	57	LYS
1	E	79	GLY
1	F	76	PHE

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Mol	Chain	Res	Type
1	A	39	LEU
1	E	78	GLU
1	E	91	ALA
1	E	122	ARG
1	F	14	PHE
1	F	16	SER
1	F	39	LEU
1	F	61	LEU
1	C	40	TYR
1	C	110	PRO
1	D	83	SER
1	F	72	GLU
1	F	78	GLU
1	F	126	VAL
1	A	55	GLU
1	B	115	ARG
1	D	125	GLN
1	E	38	THR
1	F	51	ILE
1	B	32	GLN
1	B	39	LEU
1	B	79	GLY
1	E	110	PRO

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	172/181 (95%)	157 (91%)	15 (9%)	13 51
1	B	172/181 (95%)	156 (91%)	16 (9%)	11 48
1	C	172/181 (95%)	159 (92%)	13 (8%)	16 56
1	D	172/181 (95%)	164 (95%)	8 (5%)	32 72
1	E	172/181 (95%)	163 (95%)	9 (5%)	29 69
1	F	172/181 (95%)	155 (90%)	17 (10%)	10 44

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1032/1086 (95%)	954 (92%)	78 (8%)	16 56

All (78) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	LEU
1	A	12	GLU
1	A	15	LEU
1	A	26	LYS
1	A	38	THR
1	A	57	LYS
1	A	61	LEU
1	A	76	PHE
1	A	77	GLU
1	A	80	GLN
1	A	81	GLU
1	A	82	ARG
1	A	83	SER
1	A	85	TRP
1	A	165	ILE
1	B	11	LEU
1	B	26	LYS
1	B	32	GLN
1	B	38	THR
1	B	51	ILE
1	B	70	ILE
1	B	72	GLU
1	B	73	LEU
1	B	78	GLU
1	B	80	GLN
1	B	82	ARG
1	B	85	TRP
1	B	114	MET
1	B	116	LEU
1	B	122	ARG
1	B	199	HIS
1	C	11	LEU
1	C	15	LEU
1	C	17	HIS
1	C	26	LYS
1	C	41	TYR
1	C	72	GLU

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Mol	Chain	Res	Type
1	C	77	GLU
1	C	80	GLN
1	C	81	GLU
1	C	82	ARG
1	C	98	SER
1	C	103	ARG
1	C	114	MET
1	D	11	LEU
1	D	26	LYS
1	D	32	GLN
1	D	38	THR
1	D	81	GLU
1	D	114	MET
1	D	115	ARG
1	D	122	ARG
1	E	15	LEU
1	E	20	ILE
1	E	26	LYS
1	E	27	SER
1	E	76	PHE
1	E	86	VAL
1	E	90	THR
1	E	114	MET
1	E	119	GLN
1	F	11	LEU
1	F	14	PHE
1	F	17	HIS
1	F	20	ILE
1	F	38	THR
1	F	54	GLU
1	F	61	LEU
1	F	75	LEU
1	F	83	SER
1	F	85	TRP
1	F	90	THR
1	F	93	GLU
1	F	114	MET
1	F	116	LEU
1	F	122	ARG
1	F	123	ARG
1	F	124	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (49) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	31	HIS
1	A	66	GLN
1	A	80	GLN
1	A	149	ASN
1	A	164	GLN
1	A	174	GLN
1	A	193	GLN
1	B	32	GLN
1	B	66	GLN
1	B	80	GLN
1	B	125	GLN
1	B	149	ASN
1	B	153	GLN
1	B	174	GLN
1	C	17	HIS
1	C	32	GLN
1	C	66	GLN
1	C	80	GLN
1	C	104	GLN
1	C	119	GLN
1	C	149	ASN
1	C	153	GLN
1	C	174	GLN
1	D	31	HIS
1	D	66	GLN
1	D	104	GLN
1	D	149	ASN
1	D	153	GLN
1	D	164	GLN
1	D	174	GLN
1	E	31	HIS
1	E	32	GLN
1	E	66	GLN
1	E	80	GLN
1	E	104	GLN
1	E	119	GLN
1	E	149	ASN
1	E	153	GLN
1	E	174	GLN
1	F	17	HIS
1	F	21	HIS
1	F	32	GLN

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Mol	Chain	Res	Type
1	F	104	GLN
1	F	119	GLN
1	F	125	GLN
1	F	149	ASN
1	F	153	GLN
1	F	174	GLN
1	F	193	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

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	199/210 (94%)	0.21	6 (3%) 54 38	2, 12, 68, 68	0
1	B	199/210 (94%)	0.09	1 (0%) 91 86	2, 11, 68, 68	0
1	C	199/210 (94%)	0.17	6 (3%) 54 38	2, 13, 67, 67	0
1	D	199/210 (94%)	0.25	5 (2%) 61 46	2, 12, 68, 68	0
1	E	199/210 (94%)	0.50	21 (10%) 8 6	2, 10, 67, 67	0
1	F	199/210 (94%)	0.27	9 (4%) 37 26	2, 13, 68, 68	0
All	All	1194/1260 (94%)	0.25	48 (4%) 42 29	2, 12, 67, 68	0

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	157	MET	5.7
1	E	134	LEU	4.4
1	E	140	THR	4.2
1	F	166	LYS	4.0
1	E	150	LEU	3.9
1	E	165	ILE	3.8
1	F	165	ILE	3.7
1	E	158	THR	3.7
1	C	164	GLN	3.4
1	A	203	ILE	3.0
1	D	200	GLY	3.0
1	F	201	LYS	3.0
1	E	133	ASN	2.9
1	F	178	CYS	2.9
1	F	202	THR	2.7
1	E	164	GLN	2.6
1	E	154	PRO	2.6
1	E	205	VAL	2.6
1	F	72	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	163	MET	2.6
1	E	178	CYS	2.6
1	F	155	ASP	2.6
1	A	164	GLN	2.5
1	D	151	ALA	2.4
1	E	183	VAL	2.4
1	C	169	ARG	2.4
1	D	156	ALA	2.4
1	A	166	LYS	2.3
1	E	136	PHE	2.3
1	F	167	ILE	2.3
1	A	161	ASP	2.3
1	A	160	PRO	2.2
1	E	147	LEU	2.2
1	E	149	ASN	2.2
1	C	50	LEU	2.2
1	E	160	PRO	2.2
1	E	155	ASP	2.2
1	D	147	LEU	2.2
1	A	205	VAL	2.2
1	E	163	MET	2.1
1	C	207	GLY	2.1
1	C	195	LEU	2.1
1	B	167	ILE	2.1
1	E	143	ILE	2.1
1	E	176	VAL	2.0
1	F	169	ARG	2.0
1	D	201	LYS	2.0
1	E	156	ALA	2.0

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

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

6.3 Carbohydrates (i)

There are no 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.