



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:19 PM UTC

PDB ID : 4EO2 / pdb_00004eo2
Title : Structure of the bacteriophage C1 tail knob protein, gp12
Authors : Aksyuk, A.A.; Rossmann, M.G.
Deposited on : 2012-04-13
Resolution : 3.01 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Xtrriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

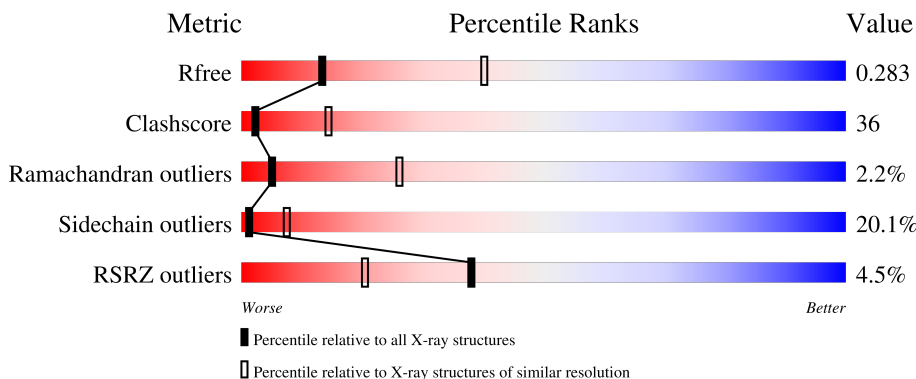
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.01 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}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	583	 5% 37% 32% 13% • 16%
1	B	583	 6% 38% 31% 13% • 16%
1	C	583	 2% 37% 32% 13% • 16%
1	D	583	 3% 35% 35% 13% • 16%
1	E	583	 3% 35% 34% 13% • 16%

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Mol	Chain	Length	Quality of chain
1	F	583	 <p>A horizontal bar chart representing the quality of chain. The bar is divided into five segments: a small red segment (4%), a green segment (34%), a yellow segment (37%), an orange segment (12%), and a grey segment (16%).</p>

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 23688 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 Major tail protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	488	3948	2504	665	761	18	0	0	0
1	B	488	3948	2504	665	761	18	0	0	0
1	C	488	3948	2504	665	761	18	0	0	0
1	D	488	3948	2504	665	761	18	0	0	0
1	E	488	3948	2504	665	761	18	0	0	0
1	F	488	3948	2504	665	761	18	0	0	0

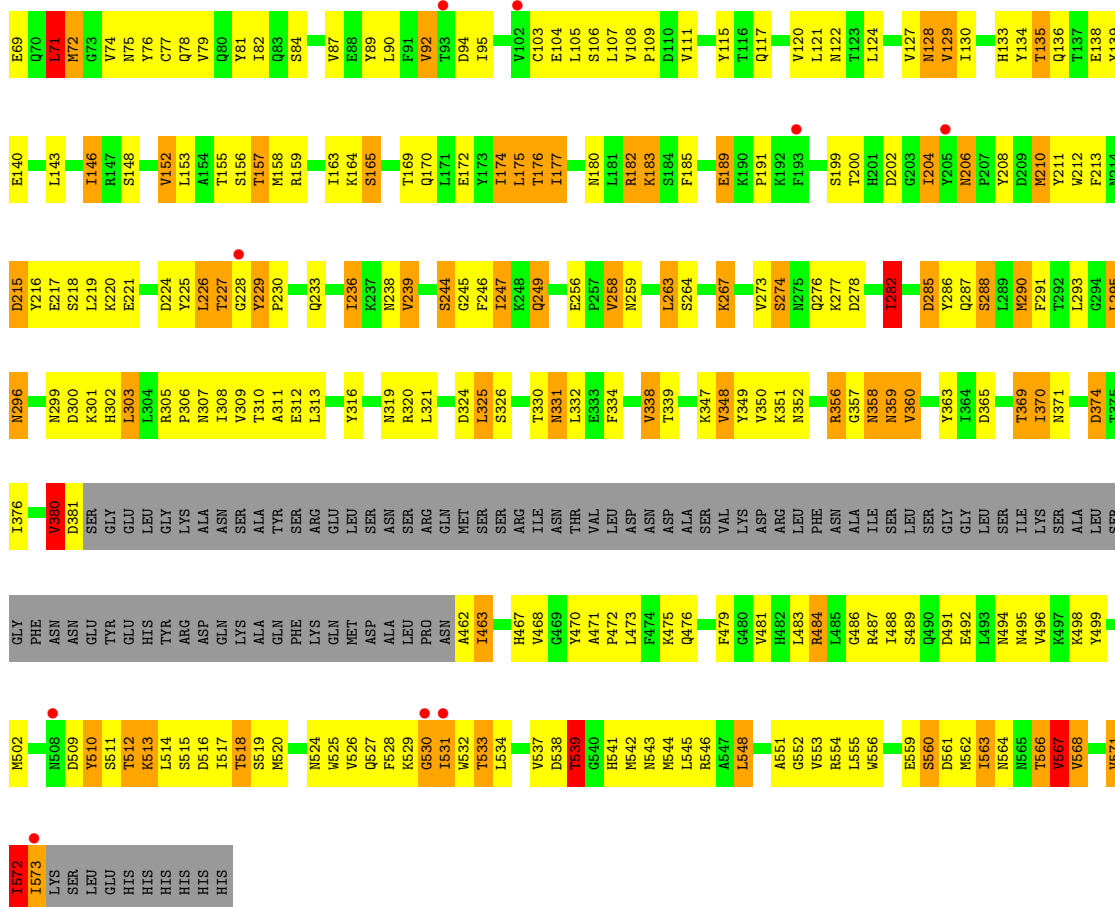
There are 54 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	575	SER	-	expression tag	UNP Q7Y3F0
A	576	LEU	-	expression tag	UNP Q7Y3F0
A	577	GLU	-	expression tag	UNP Q7Y3F0
A	578	HIS	-	expression tag	UNP Q7Y3F0
A	579	HIS	-	expression tag	UNP Q7Y3F0
A	580	HIS	-	expression tag	UNP Q7Y3F0
A	581	HIS	-	expression tag	UNP Q7Y3F0
A	582	HIS	-	expression tag	UNP Q7Y3F0
A	583	HIS	-	expression tag	UNP Q7Y3F0
B	575	SER	-	expression tag	UNP Q7Y3F0
B	576	LEU	-	expression tag	UNP Q7Y3F0
B	577	GLU	-	expression tag	UNP Q7Y3F0
B	578	HIS	-	expression tag	UNP Q7Y3F0
B	579	HIS	-	expression tag	UNP Q7Y3F0
B	580	HIS	-	expression tag	UNP Q7Y3F0
B	581	HIS	-	expression tag	UNP Q7Y3F0
B	582	HIS	-	expression tag	UNP Q7Y3F0

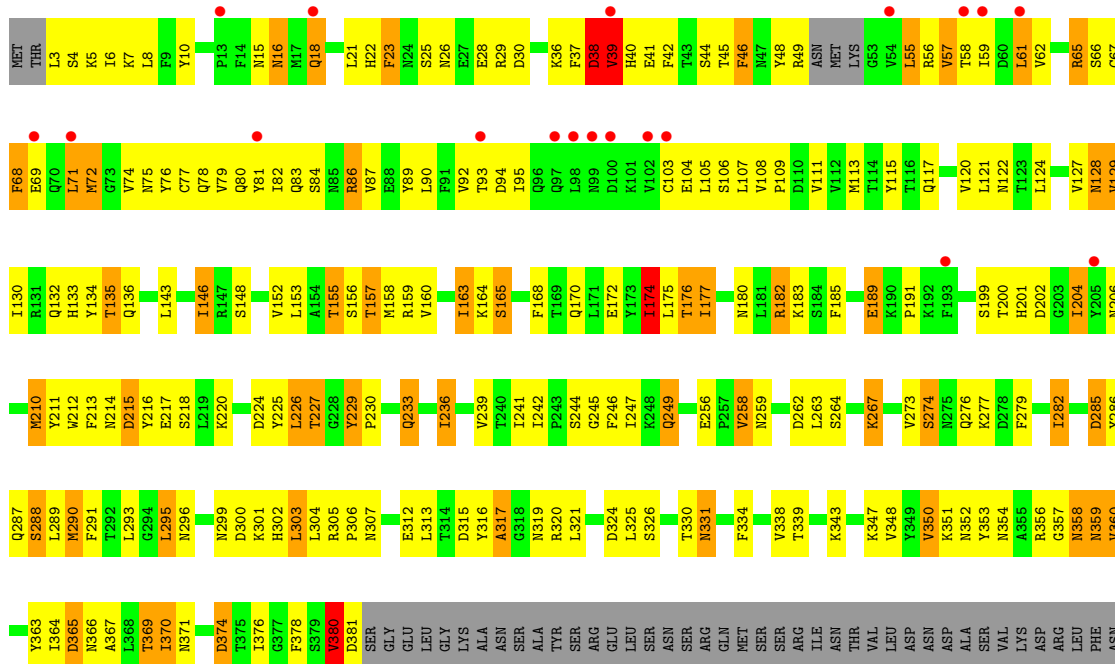
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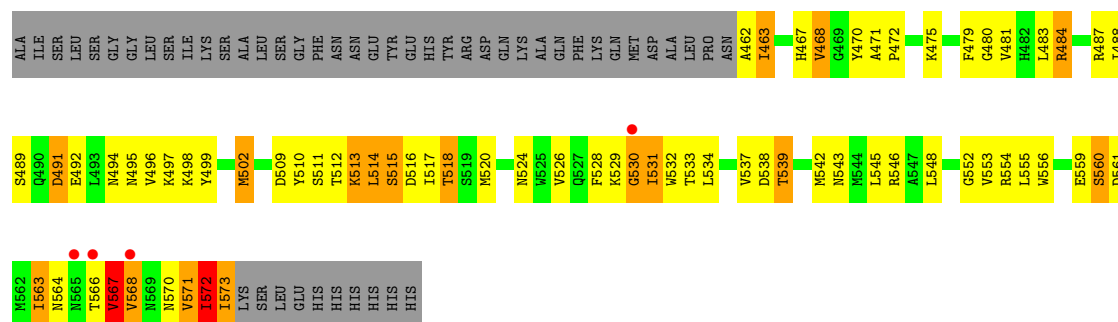
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Chain	Residue	Modelled	Actual	Comment	Reference
B	583	HIS	-	expression tag	UNP Q7Y3F0
C	575	SER	-	expression tag	UNP Q7Y3F0
C	576	LEU	-	expression tag	UNP Q7Y3F0
C	577	GLU	-	expression tag	UNP Q7Y3F0
C	578	HIS	-	expression tag	UNP Q7Y3F0
C	579	HIS	-	expression tag	UNP Q7Y3F0
C	580	HIS	-	expression tag	UNP Q7Y3F0
C	581	HIS	-	expression tag	UNP Q7Y3F0
C	582	HIS	-	expression tag	UNP Q7Y3F0
C	583	HIS	-	expression tag	UNP Q7Y3F0
D	575	SER	-	expression tag	UNP Q7Y3F0
D	576	LEU	-	expression tag	UNP Q7Y3F0
D	577	GLU	-	expression tag	UNP Q7Y3F0
D	578	HIS	-	expression tag	UNP Q7Y3F0
D	579	HIS	-	expression tag	UNP Q7Y3F0
D	580	HIS	-	expression tag	UNP Q7Y3F0
D	581	HIS	-	expression tag	UNP Q7Y3F0
D	582	HIS	-	expression tag	UNP Q7Y3F0
D	583	HIS	-	expression tag	UNP Q7Y3F0
E	575	SER	-	expression tag	UNP Q7Y3F0
E	576	LEU	-	expression tag	UNP Q7Y3F0
E	577	GLU	-	expression tag	UNP Q7Y3F0
E	578	HIS	-	expression tag	UNP Q7Y3F0
E	579	HIS	-	expression tag	UNP Q7Y3F0
E	580	HIS	-	expression tag	UNP Q7Y3F0
E	581	HIS	-	expression tag	UNP Q7Y3F0
E	582	HIS	-	expression tag	UNP Q7Y3F0
E	583	HIS	-	expression tag	UNP Q7Y3F0
F	575	SER	-	expression tag	UNP Q7Y3F0
F	576	LEU	-	expression tag	UNP Q7Y3F0
F	577	GLU	-	expression tag	UNP Q7Y3F0
F	578	HIS	-	expression tag	UNP Q7Y3F0
F	579	HIS	-	expression tag	UNP Q7Y3F0
F	580	HIS	-	expression tag	UNP Q7Y3F0
F	581	HIS	-	expression tag	UNP Q7Y3F0
F	582	HIS	-	expression tag	UNP Q7Y3F0
F	583	HIS	-	expression tag	UNP Q7Y3F0



• Molecule 1: Major tail protein





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	205.61Å 209.64Å 102.97Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.01 50.00 – 3.01	Depositor EDS
% Data completeness (in resolution range)	98.0 (50.00-3.01) 98.0 (50.00-3.01)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.21 (at 3.01Å)	Xtrriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.238 , 0.282 0.238 , 0.283	Depositor DCC
R_{free} test set	4404 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	75.3	Xtrriage
Anisotropy	0.837	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 105.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	0.000 for k,h,-l	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	23688	wwPDB-VP
Average B, all atoms (Å ²)	108.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.10% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality i

5.1 Standard geometry i

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	1.16	13/4030 (0.3%)	1.30	36/5464 (0.7%)
1	B	1.15	15/4030 (0.4%)	1.28	26/5464 (0.5%)
1	C	1.04	6/4030 (0.1%)	1.20	29/5464 (0.5%)
1	D	0.98	2/4030 (0.0%)	1.20	26/5464 (0.5%)
1	E	1.07	9/4030 (0.2%)	1.22	23/5464 (0.4%)
1	F	1.11	9/4030 (0.2%)	1.25	24/5464 (0.4%)
All	All	1.09	54/24180 (0.2%)	1.24	164/32784 (0.5%)

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	3
1	C	0	2
1	D	0	3
1	E	0	3
1	F	0	2
All	All	0	15

All (54) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	299	ASN	CG-ND2	-10.94	1.10	1.33
1	E	551	ALA	CA-CB	-8.42	1.40	1.53
1	E	152	VAL	CA-CB	-8.22	1.46	1.55
1	B	299	ASN	CG-OD1	-8.16	1.08	1.23
1	C	299	ASN	CG-ND2	-8.09	1.16	1.33
1	C	557	HIS	CA-C	7.55	1.62	1.52
1	D	367	ALA	CA-CB	-6.81	1.42	1.53
1	A	152	VAL	CA-CB	-6.80	1.48	1.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	308	ILE	CA-CB	-6.78	1.47	1.55
1	A	146	ILE	CA-CB	6.61	1.64	1.54
1	C	152	VAL	CA-CB	-6.47	1.48	1.55
1	E	57	VAL	CA-CB	6.43	1.61	1.53
1	B	162	ALA	CA-CB	-6.29	1.42	1.53
1	A	551	ALA	CA-CB	-6.25	1.45	1.54
1	F	317	ALA	CA-CB	-5.92	1.45	1.53
1	A	367	ALA	CA-CB	-5.83	1.44	1.53
1	F	160	VAL	CA-CB	-5.76	1.47	1.54
1	E	247	ILE	CA-CB	-5.72	1.47	1.54
1	B	247	ILE	CA-C	-5.70	1.45	1.52
1	B	367	ALA	CA-CB	-5.68	1.44	1.53
1	C	57	VAL	CA-CB	5.67	1.60	1.53
1	B	57	VAL	CA-CB	5.65	1.60	1.53
1	C	92	VAL	CA-CB	5.60	1.59	1.53
1	A	467	HIS	CA-C	-5.59	1.45	1.52
1	B	467	HIS	CA-C	-5.58	1.45	1.52
1	F	367	ALA	CA-CB	-5.46	1.44	1.53
1	A	241	ILE	CA-CB	-5.45	1.47	1.54
1	B	291	PHE	N-CA	-5.45	1.39	1.46
1	D	163	ILE	CA-CB	-5.41	1.47	1.54
1	F	201	HIS	CA-C	-5.37	1.46	1.52
1	B	175	LEU	CA-C	-5.36	1.46	1.52
1	A	183	LYS	CA-C	5.34	1.59	1.52
1	B	571	VAL	CA-CB	-5.33	1.50	1.55
1	F	93	THR	CA-CB	5.32	1.62	1.53
1	F	273	VAL	CA-C	-5.31	1.48	1.52
1	F	241	ILE	CA-CB	-5.30	1.48	1.54
1	A	242	ILE	CA-CB	-5.29	1.50	1.55
1	B	290	MET	SD-CE	-5.29	1.66	1.79
1	E	473	LEU	CA-C	-5.28	1.46	1.52
1	A	375	THR	CA-CB	-5.27	1.44	1.53
1	F	183	LYS	CA-C	5.27	1.59	1.52
1	A	299	ASN	CG-ND2	-5.26	1.22	1.33
1	A	38	ASP	CA-C	5.24	1.59	1.52
1	B	92	VAL	CA-CB	5.19	1.59	1.53
1	E	332	LEU	CA-C	-5.17	1.47	1.53
1	F	242	ILE	CA-CB	-5.13	1.50	1.55
1	B	355	ALA	CA-C	-5.09	1.46	1.52
1	E	92	VAL	CA-CB	5.06	1.59	1.53
1	C	201	HIS	CA-C	-5.04	1.46	1.52
1	B	368	LEU	CA-C	-5.04	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	273	VAL	CA-CB	-5.02	1.48	1.54
1	B	247	ILE	CA-CB	-5.02	1.48	1.54
1	A	162	ALA	CA-CB	-5.01	1.45	1.53
1	A	314	THR	CA-CB	-5.00	1.45	1.53

All (164) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	511	SER	N-CA-C	9.52	122.92	111.02
1	A	511	SER	N-CA-C	8.74	121.94	111.02
1	B	511	SER	N-CA-C	8.61	120.98	110.91
1	A	246	PHE	N-CA-C	-8.39	103.06	113.38
1	E	511	SER	N-CA-C	8.07	121.11	111.02
1	D	511	SER	N-CA-C	7.91	120.91	111.02
1	A	519	SER	N-CA-C	7.91	119.53	111.07
1	E	290	MET	N-CA-C	-7.88	102.68	111.82
1	C	511	SER	N-CA-C	7.34	120.20	111.02
1	B	331	ASN	N-CA-C	7.28	121.43	109.06
1	C	59	ILE	N-CA-C	7.00	118.13	107.77
1	D	290	MET	N-CA-C	-7.00	103.73	111.36
1	A	241	ILE	CB-CA-C	-6.99	101.41	110.98
1	F	163	ILE	N-CA-C	6.92	118.09	108.12
1	C	246	PHE	N-CA-C	-6.81	105.00	113.38
1	F	290	MET	N-CA-C	-6.79	103.96	111.36
1	A	72	MET	N-CA-C	6.78	121.69	112.68
1	B	321	LEU	CA-C-N	6.76	127.77	120.13
1	B	321	LEU	C-N-CA	6.76	127.77	120.13
1	F	84	SER	N-CA-C	-6.74	105.09	113.38
1	C	84	SER	N-CA-C	-6.72	105.11	113.38
1	E	331	ASN	N-CA-C	6.71	120.23	108.75
1	D	519	SER	N-CA-C	6.70	118.24	111.07
1	B	84	SER	N-CA-C	-6.70	105.14	113.38
1	D	370	ILE	CB-CA-C	-6.67	101.78	110.84
1	C	38	ASP	N-CA-C	6.66	123.14	114.75
1	E	59	ILE	N-CA-C	6.58	117.36	107.75
1	B	59	ILE	N-CA-C	6.53	117.44	107.77
1	E	211	TYR	N-CA-C	6.52	119.04	108.41
1	F	380	VAL	N-CA-C	6.51	118.53	108.44
1	B	72	MET	N-CA-C	6.48	121.30	112.68
1	D	246	PHE	N-CA-C	-6.43	105.43	113.28
1	A	380	VAL	N-CA-C	6.43	118.41	108.44
1	E	510	TYR	N-CA-C	-6.43	101.17	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	246	PHE	N-CA-C	-6.39	105.52	113.38
1	B	244	SER	N-CA-C	6.38	118.79	110.43
1	B	183	LYS	N-CA-C	6.34	117.81	108.86
1	B	246	PHE	N-CA-C	-6.33	105.60	113.38
1	B	38	ASP	N-CA-C	6.32	122.71	114.75
1	F	331	ASN	N-CA-C	6.21	119.65	108.48
1	D	211	TYR	N-CA-C	6.19	118.49	108.41
1	A	84	SER	N-CA-C	-6.19	105.77	113.38
1	D	38	ASP	N-CA-C	6.17	122.53	114.75
1	D	72	MET	N-CA-C	6.17	120.88	112.68
1	A	59	ILE	N-CA-C	6.15	116.88	107.77
1	C	72	MET	N-CA-C	6.13	120.83	112.68
1	A	238	ASN	CA-C-N	-6.12	115.59	123.19
1	A	238	ASN	C-N-CA	-6.12	115.59	123.19
1	F	370	ILE	CB-CA-C	-6.12	102.60	110.98
1	D	331	ASN	N-CA-C	6.10	119.45	108.48
1	C	331	ASN	N-CA-C	6.09	119.17	108.75
1	D	380	VAL	N-CA-C	6.09	117.88	108.44
1	B	463	ILE	CB-CA-C	-6.07	103.97	111.08
1	E	84	SER	N-CA-C	-6.04	105.96	113.38
1	E	183	LYS	N-CA-C	6.02	116.22	108.34
1	A	12	THR	CA-C-N	6.01	125.69	119.56
1	A	12	THR	C-N-CA	6.01	125.69	119.56
1	D	84	SER	N-CA-C	-6.00	106.00	113.38
1	B	290	MET	N-CA-C	-5.96	104.78	111.28
1	A	38	ASP	N-CA-C	5.96	122.26	114.75
1	B	510	TYR	N-CA-C	-5.93	101.87	110.24
1	E	380	VAL	N-CA-C	5.91	117.60	108.44
1	D	282	ILE	N-CA-C	-5.89	105.97	113.22
1	E	28	GLU	N-CA-C	-5.88	104.77	111.07
1	F	515	SER	N-CA-C	-5.84	102.26	110.50
1	B	163	ILE	N-CA-C	5.84	116.41	107.77
1	C	290	MET	N-CA-C	-5.83	104.93	111.28
1	E	38	ASP	N-CA-C	5.81	122.07	114.75
1	A	316	TYR	N-CA-C	-5.79	105.51	113.56
1	F	72	MET	N-CA-C	5.75	120.33	112.04
1	F	262	ASP	N-CA-C	-5.74	104.99	112.23
1	B	241	ILE	CB-CA-C	-5.74	103.12	110.98
1	D	59	ILE	N-CA-C	5.73	116.25	107.77
1	D	172	GLU	N-CA-C	-5.72	100.61	109.24
1	D	174	ILE	N-CA-CB	5.71	119.07	111.64
1	C	209	ASP	N-CA-C	-5.71	100.38	109.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	370	ILE	CB-CA-C	-5.70	102.64	110.96
1	A	363	TYR	CB-CA-C	-5.69	110.00	116.54
1	A	281	ALA	N-CA-C	-5.69	105.22	111.82
1	C	346	ILE	CB-CA-C	-5.67	102.68	110.96
1	C	510	TYR	N-CA-C	-5.65	102.28	110.24
1	F	366	ASN	N-CA-C	5.63	117.61	108.26
1	C	515	SER	N-CA-C	-5.61	102.59	110.50
1	B	496	VAL	CB-CA-C	-5.61	104.68	112.02
1	B	380	VAL	N-CA-C	5.60	117.12	108.44
1	C	163	ILE	N-CA-C	5.60	116.19	108.12
1	C	183	LYS	N-CA-C	5.60	116.75	108.86
1	A	368	LEU	CB-CA-C	-5.59	101.11	110.29
1	C	380	VAL	N-CA-C	5.58	117.09	108.44
1	E	72	MET	N-CA-C	5.57	120.09	112.68
1	A	183	LYS	N-CA-C	5.54	116.67	108.86
1	A	366	ASN	N-CA-C	5.53	117.44	108.26
1	B	39	VAL	N-CA-C	5.53	120.83	109.34
1	D	142	ASN	N-CA-C	-5.51	106.22	113.17
1	A	209	ASP	N-CA-C	-5.51	100.70	109.96
1	D	346	ILE	CB-CA-C	-5.49	102.94	110.96
1	B	296	ASN	CA-C-N	5.49	125.10	119.56
1	B	296	ASN	C-N-CA	5.49	125.10	119.56
1	A	290	MET	N-CA-C	-5.47	105.32	111.28
1	E	496	VAL	CB-CA-C	-5.46	104.87	112.02
1	C	363	TYR	CB-CA-C	-5.43	110.33	116.63
1	C	370	ILE	CB-CA-C	-5.42	103.04	110.96
1	D	365	ASP	N-CA-C	-5.42	106.50	113.01
1	D	262	ASP	N-CA-C	-5.42	105.41	112.23
1	D	244	SER	N-CA-C	5.41	117.52	110.43
1	E	238	ASN	CA-C-N	-5.40	115.61	123.06
1	E	238	ASN	C-N-CA	-5.40	115.61	123.06
1	F	38	ASP	N-CA-C	5.39	121.55	114.75
1	F	246	PHE	N-CA-C	-5.39	106.71	113.28
1	F	86	ARG	N-CA-C	-5.38	102.09	110.42
1	C	519	SER	N-CA-C	5.36	116.81	110.97
1	D	241	ILE	CB-CA-C	-5.35	103.65	110.98
1	C	238	ASN	CA-C-N	-5.35	115.68	123.06
1	C	238	ASN	C-N-CA	-5.35	115.68	123.06
1	B	209	ASP	N-CA-C	-5.33	101.01	109.96
1	C	172	GLU	N-CA-C	-5.30	101.24	109.24
1	D	366	ASN	N-CA-C	5.28	117.03	108.26
1	C	241	ILE	CB-CA-C	-5.26	103.77	110.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	241	ILE	CB-CA-C	-5.26	103.78	110.98
1	C	28	GLU	N-CA-C	-5.23	105.58	111.28
1	E	296	ASN	CA-C-N	5.21	124.87	119.56
1	E	296	ASN	C-N-CA	5.21	124.87	119.56
1	A	282	ILE	CA-CB-CG2	5.20	119.34	110.50
1	A	364	ILE	N-CA-C	-5.20	107.68	112.83
1	E	282	ILE	N-CA-C	-5.20	106.83	113.22
1	F	174	ILE	N-CA-CB	5.19	118.39	111.64
1	F	204	ILE	N-CA-C	5.19	115.45	107.77
1	A	118	GLY	N-CA-C	5.19	120.55	111.78
1	B	112	VAL	CB-CA-C	-5.17	105.35	111.81
1	A	206	ASN	CA-C-N	-5.16	114.46	120.04
1	A	206	ASN	C-N-CA	-5.16	114.46	120.04
1	B	502	MET	N-CA-C	5.16	118.73	112.23
1	C	39	VAL	N-CA-C	5.15	120.06	109.34
1	E	206	ASN	CA-C-N	-5.14	114.48	120.04
1	E	206	ASN	C-N-CA	-5.14	114.48	120.04
1	A	163	ILE	N-CA-C	5.14	115.52	108.12
1	F	214	ASN	N-CA-C	-5.14	107.01	113.28
1	A	39	VAL	N-CA-C	5.14	120.02	109.34
1	C	296	ASN	CA-C-N	5.13	124.79	119.56
1	C	296	ASN	C-N-CA	5.13	124.79	119.56
1	A	335	ASP	N-CA-CB	5.13	118.39	110.60
1	D	39	VAL	N-CA-C	5.13	120.01	109.34
1	F	365	ASP	N-CA-C	-5.12	106.30	112.54
1	E	39	VAL	N-CA-C	5.12	119.98	109.34
1	F	211	TYR	N-CA-C	5.12	116.75	108.41
1	B	566	THR	CB-CA-C	-5.11	101.12	109.56
1	C	463	ILE	CB-CA-C	-5.11	105.10	111.08
1	F	39	VAL	N-CA-C	5.11	119.97	109.34
1	A	314	THR	N-CA-C	5.10	116.82	108.76
1	A	245	GLY	CA-C-N	-5.05	113.52	122.26
1	A	245	GLY	C-N-CA	-5.05	113.52	122.26
1	F	343	LYS	N-CA-C	-5.05	101.41	109.23
1	F	502	MET	N-CA-C	5.05	118.59	112.23
1	B	169	THR	N-CA-C	-5.05	108.15	114.56
1	D	209	ASP	N-CA-C	-5.05	101.48	109.96
1	F	183	LYS	N-CA-C	5.05	115.98	108.86
1	C	245	GLY	CA-C-N	-5.04	113.54	122.26
1	C	245	GLY	C-N-CA	-5.04	113.54	122.26
1	D	282	ILE	CB-CA-C	5.04	120.06	110.94
1	A	346	ILE	CA-C-N	-5.03	115.73	123.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	346	ILE	C-N-CA	-5.03	115.73	123.07
1	A	275	ASN	N-CA-C	-5.02	102.85	110.28
1	D	163	ILE	N-CA-C	5.01	115.34	108.12
1	A	365	ASP	N-CA-C	-5.00	107.01	113.01

There are no chirality outliers.

All (15) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	356	ARG	Peptide
1	A	71	LEU	Peptide
1	B	183	LYS	Peptide
1	B	356	ARG	Peptide
1	B	71	LEU	Peptide
1	C	356	ARG	Peptide
1	C	71	LEU	Peptide
1	D	183	LYS	Peptide
1	D	356	ARG	Peptide
1	D	71	LEU	Peptide
1	E	183	LYS	Peptide
1	E	356	ARG	Peptide
1	E	71	LEU	Peptide
1	F	356	ARG	Peptide
1	F	71	LEU	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3948	0	3832	280	3
1	B	3948	0	3832	281	3
1	C	3948	0	3832	303	1
1	D	3948	0	3832	303	0
1	E	3948	0	3832	285	0
1	F	3948	0	3832	294	1
All	All	23688	0	22992	1682	4

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 36.

All (1682) 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:A:573:ILE:O	1:A:573:ILE:HG22	1.66	0.93
1:F:573:ILE:O	1:F:573:ILE:HG22	1.70	0.91
1:D:158:MET:O	1:D:159:ARG:HD3	1.70	0.91
1:E:573:ILE:HG22	1:E:573:ILE:O	1.71	0.91
1:A:290:MET:HE3	1:A:295:LEU:HB3	1.52	0.90
1:C:299:ASN:N	1:C:299:ASN:HD22	1.63	0.89
1:B:573:ILE:HG22	1:B:573:ILE:O	1.72	0.88
1:E:285:ASP:OD1	1:E:288:SER:OG	1.90	0.88
1:A:290:MET:HE3	1:A:295:LEU:CB	2.03	0.88
1:D:573:ILE:HG22	1:D:573:ILE:O	1.73	0.87
1:A:573:ILE:O	1:A:573:ILE:CG2	2.23	0.86
1:C:285:ASP:OD1	1:C:288:SER:OG	1.93	0.86
1:C:573:ILE:HG22	1:C:573:ILE:O	1.75	0.85
1:D:285:ASP:OD1	1:D:288:SER:OG	1.92	0.85
1:F:215:ASP:OD1	1:F:216:TYR:N	2.10	0.85
1:C:542:MET:CE	1:C:545:LEU:HD23	2.08	0.83
1:B:215:ASP:OD1	1:B:216:TYR:N	2.12	0.82
1:F:285:ASP:OD1	1:F:288:SER:OG	1.97	0.82
1:D:157:THR:HG23	1:D:157:THR:O	1.79	0.81
1:F:573:ILE:O	1:F:573:ILE:CG2	2.27	0.81
1:B:572:ILE:O	1:B:572:ILE:HG22	1.81	0.81
1:D:572:ILE:HG22	1:D:572:ILE:O	1.81	0.81
1:B:26:ASN:OD1	1:B:29:ARG:NH2	2.15	0.80
1:D:215:ASP:OD1	1:D:216:TYR:N	2.13	0.80
1:C:158:MET:O	1:C:159:ARG:HD3	1.82	0.80
1:D:573:ILE:O	1:D:573:ILE:CG2	2.31	0.79
1:A:3:LEU:HD21	1:B:68:PHE:CE2	2.18	0.79
1:C:572:ILE:HG22	1:C:572:ILE:O	1.83	0.79
1:F:26:ASN:OD1	1:F:29:ARG:NH2	2.16	0.79
1:A:572:ILE:HG22	1:A:572:ILE:O	1.81	0.78
1:E:26:ASN:OD1	1:E:29:ARG:NH2	2.16	0.78
1:A:285:ASP:OD1	1:A:288:SER:OG	2.02	0.78
1:E:572:ILE:O	1:E:572:ILE:HG22	1.84	0.77
1:C:215:ASP:OD1	1:C:216:TYR:N	2.16	0.77
1:E:215:ASP:OD1	1:E:216:TYR:N	2.17	0.77
1:A:3:LEU:N	1:A:44:SER:O	2.18	0.77
1:A:37:PHE:CZ	1:A:40:HIS:O	2.39	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:573:ILE:O	1:B:573:ILE:CG2	2.33	0.76
1:A:313:LEU:HB2	1:A:321:LEU:HB3	1.68	0.76
1:F:572:ILE:HG22	1:F:572:ILE:O	1.86	0.76
1:C:573:ILE:O	1:C:573:ILE:CG2	2.34	0.76
1:B:75:ASN:O	1:B:92:VAL:N	2.18	0.76
1:E:516:ASP:OD2	1:E:518:THR:N	2.19	0.76
1:F:78:GLN:HG2	1:F:79:VAL:N	2.00	0.76
1:E:37:PHE:CZ	1:E:40:HIS:O	2.39	0.75
1:C:312:GLU:OE2	1:C:484:ARG:NH1	2.19	0.75
1:D:516:ASP:OD2	1:D:518:THR:N	2.19	0.75
1:F:542:MET:CE	1:F:545:LEU:HD23	2.17	0.75
1:F:158:MET:O	1:F:159:ARG:HD3	1.87	0.75
1:A:233:GLN:NE2	1:A:380:VAL:HG13	2.02	0.75
1:C:298:ILE:C	1:C:299:ASN:HD22	1.94	0.75
1:B:164:LYS:O	1:B:282:ILE:HD11	1.87	0.74
1:E:189:GLU:C	1:E:191:PRO:HD3	2.13	0.74
1:A:215:ASP:OD1	1:A:216:TYR:N	2.21	0.74
1:A:158:MET:O	1:A:159:ARG:HD3	1.88	0.74
1:E:158:MET:O	1:E:159:ARG:HD3	1.87	0.73
1:B:115:TYR:CE1	1:B:537:VAL:HG13	2.24	0.73
1:A:26:ASN:OD1	1:A:29:ARG:NH2	2.22	0.73
1:A:157:THR:CG2	1:A:489:SER:H	2.01	0.73
1:D:26:ASN:OD1	1:D:29:ARG:NH2	2.21	0.73
1:B:285:ASP:OD1	1:B:288:SER:OG	2.06	0.73
1:D:157:THR:CG2	1:D:489:SER:H	2.01	0.73
1:B:59:ILE:O	1:B:59:ILE:HG23	1.87	0.73
1:B:157:THR:O	1:B:157:THR:HG23	1.88	0.73
1:D:542:MET:O	1:D:545:LEU:N	2.22	0.73
1:C:189:GLU:C	1:C:191:PRO:HD3	2.14	0.72
1:A:164:LYS:O	1:A:282:ILE:HD11	1.89	0.72
1:A:75:ASN:O	1:A:92:VAL:N	2.23	0.72
1:F:529:LYS:O	1:F:530:GLY:O	2.08	0.72
1:C:164:LYS:O	1:C:282:ILE:HD11	1.89	0.72
1:C:290:MET:HE3	1:C:295:LEU:CB	2.20	0.72
1:C:542:MET:HE2	1:C:542:MET:HA	1.71	0.72
1:F:46:PHE:CB	1:F:57:VAL:HG23	2.20	0.72
1:F:146:ILE:HD12	1:F:146:ILE:O	1.90	0.72
1:E:573:ILE:O	1:E:573:ILE:CG2	2.38	0.72
1:F:516:ASP:OD2	1:F:518:THR:N	2.20	0.72
1:D:127:VAL:HG21	1:D:528:PHE:CD1	2.24	0.71
1:D:233:GLN:NE2	1:D:380:VAL:HG13	2.06	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:37:PHE:CZ	1:B:40:HIS:O	2.42	0.71
1:C:146:ILE:HD12	1:C:146:ILE:O	1.89	0.71
1:A:542:MET:O	1:A:545:LEU:N	2.23	0.71
1:D:37:PHE:CZ	1:D:40:HIS:O	2.43	0.71
1:F:127:VAL:HG21	1:F:528:PHE:CD1	2.26	0.71
1:B:502:MET:HG2	1:B:567:VAL:HG11	1.72	0.71
1:E:233:GLN:NE2	1:E:380:VAL:HG13	2.06	0.71
1:B:516:ASP:OD2	1:B:518:THR:N	2.18	0.71
1:C:26:ASN:OD1	1:C:29:ARG:NH2	2.24	0.71
1:C:516:ASP:OD2	1:C:518:THR:N	2.20	0.70
1:E:157:THR:HG23	1:E:157:THR:O	1.90	0.70
1:A:59:ILE:HG23	1:A:59:ILE:O	1.91	0.70
1:B:164:LYS:C	1:B:282:ILE:CD1	2.64	0.70
1:A:127:VAL:HG21	1:A:528:PHE:CD1	2.25	0.70
1:F:189:GLU:C	1:F:191:PRO:HD3	2.16	0.70
1:B:233:GLN:NE2	1:B:380:VAL:HG13	2.07	0.70
1:A:516:ASP:OD2	1:A:518:THR:N	2.20	0.70
1:B:29:ARG:HD3	1:B:89:TYR:CE2	2.27	0.70
1:C:3:LEU:N	1:C:44:SER:O	2.24	0.70
1:F:157:THR:HG23	1:F:157:THR:O	1.90	0.70
1:A:542:MET:CE	1:A:545:LEU:HD23	2.22	0.70
1:F:206:ASN:OD1	1:F:210:MET:HE3	1.92	0.70
1:D:124:LEU:HD22	1:D:532:TRP:HB2	1.73	0.70
1:E:347:LYS:HE2	1:E:369:THR:CG2	2.22	0.69
1:E:164:LYS:O	1:E:282:ILE:HD11	1.92	0.69
1:B:542:MET:HE2	1:B:542:MET:HA	1.74	0.69
1:C:299:ASN:N	1:C:299:ASN:ND2	2.26	0.69
1:E:189:GLU:O	1:E:191:PRO:HD3	1.92	0.69
1:C:189:GLU:O	1:C:191:PRO:HD3	1.91	0.69
1:D:164:LYS:O	1:D:282:ILE:HD11	1.93	0.69
1:A:146:ILE:HD12	1:A:146:ILE:O	1.92	0.69
1:B:146:ILE:HD12	1:B:146:ILE:O	1.92	0.69
1:E:542:MET:CE	1:E:545:LEU:HD23	2.23	0.69
1:C:290:MET:HE3	1:C:295:LEU:HB3	1.73	0.69
1:F:37:PHE:CZ	1:F:40:HIS:O	2.46	0.69
1:F:157:THR:CG2	1:F:489:SER:H	2.06	0.69
1:D:224:ASP:O	1:D:227:THR:OG1	2.10	0.68
1:E:157:THR:CG2	1:E:489:SER:H	2.06	0.68
1:B:26:ASN:HB3	1:B:29:ARG:CZ	2.24	0.68
1:E:127:VAL:HG21	1:E:528:PHE:CD1	2.28	0.68
1:E:542:MET:HE2	1:E:542:MET:HA	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:164:LYS:C	1:C:282:ILE:CD1	2.67	0.68
1:B:42:PHE:CE1	1:B:59:ILE:HD12	2.27	0.68
1:C:42:PHE:CE1	1:C:59:ILE:HD12	2.28	0.68
1:C:233:GLN:NE2	1:C:380:VAL:HG13	2.09	0.68
1:F:542:MET:O	1:F:545:LEU:N	2.27	0.68
1:C:347:LYS:HE2	1:C:369:THR:HG22	1.73	0.68
1:A:542:MET:HA	1:A:542:MET:HE2	1.76	0.68
1:C:374:ASP:OD1	1:C:374:ASP:N	2.25	0.68
1:A:563:ILE:N	1:A:563:ILE:HD13	2.09	0.68
1:B:127:VAL:HG21	1:B:528:PHE:CD1	2.28	0.67
1:B:189:GLU:C	1:B:191:PRO:HD3	2.18	0.67
1:F:124:LEU:HD22	1:F:532:TRP:HB2	1.76	0.67
1:A:78:GLN:HG2	1:A:79:VAL:N	2.07	0.67
1:E:347:LYS:HE2	1:E:369:THR:HG22	1.77	0.67
1:F:542:MET:HA	1:F:542:MET:HE2	1.77	0.67
1:A:135:THR:O	1:A:136:GLN:C	2.38	0.67
1:A:470:TYR:CG	1:A:479:PHE:CE1	2.82	0.67
1:B:158:MET:O	1:B:159:ARG:HD3	1.94	0.67
1:D:120:VAL:HG23	1:D:121:LEU:N	2.08	0.67
1:D:180:ASN:OD1	1:D:182:ARG:HG2	1.95	0.67
1:A:180:ASN:OD1	1:A:182:ARG:HG2	1.94	0.67
1:B:111:VAL:HB	1:B:545:LEU:HD13	1.77	0.67
1:C:127:VAL:HG21	1:C:528:PHE:CD1	2.30	0.67
1:D:312:GLU:OE2	1:D:484:ARG:NH1	2.28	0.67
1:D:290:MET:HE3	1:D:295:LEU:CB	2.25	0.67
1:C:542:MET:HE2	1:C:545:LEU:HD23	1.75	0.66
1:A:177:ILE:HD13	1:A:177:ILE:O	1.95	0.66
1:A:286:TYR:N	1:A:331:ASN:OD1	2.28	0.66
1:B:177:ILE:HG22	1:B:236:ILE:HG23	1.78	0.66
1:F:92:VAL:HG23	1:F:92:VAL:O	1.94	0.66
1:C:30:ASP:OD2	1:C:89:TYR:OH	2.11	0.66
1:B:189:GLU:O	1:B:191:PRO:HD3	1.95	0.66
1:E:312:GLU:OE2	1:E:484:ARG:NH1	2.29	0.66
1:B:258:VAL:HG13	1:B:259:ASN:H	1.59	0.66
1:C:180:ASN:OD1	1:C:182:ARG:HG2	1.96	0.66
1:D:542:MET:HA	1:D:542:MET:HE2	1.77	0.66
1:B:470:TYR:CG	1:B:479:PHE:CE1	2.83	0.66
1:C:37:PHE:CZ	1:C:40:HIS:O	2.49	0.66
1:D:78:GLN:HG2	1:D:79:VAL:N	2.11	0.66
1:E:146:ILE:O	1:E:146:ILE:HD12	1.96	0.66
1:B:312:GLU:OE2	1:B:484:ARG:NH1	2.28	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:164:LYS:C	1:E:282:ILE:CD1	2.69	0.66
1:A:374:ASP:N	1:A:374:ASP:OD1	2.29	0.66
1:C:347:LYS:HE2	1:C:369:THR:CG2	2.25	0.66
1:E:470:TYR:CG	1:E:479:PHE:CE1	2.83	0.65
1:C:124:LEU:HD22	1:C:532:TRP:HB2	1.78	0.65
1:D:566:THR:O	1:D:567:VAL:C	2.39	0.65
1:A:42:PHE:CE1	1:A:59:ILE:HD12	2.32	0.65
1:D:542:MET:CE	1:D:545:LEU:HD23	2.27	0.65
1:F:135:THR:O	1:F:136:GLN:C	2.39	0.65
1:A:174:ILE:HG12	1:A:176:THR:HG22	1.77	0.65
1:C:29:ARG:HD3	1:C:89:TYR:CE2	2.32	0.65
1:E:75:ASN:O	1:E:92:VAL:N	2.30	0.65
1:A:164:LYS:C	1:A:282:ILE:CD1	2.70	0.65
1:B:542:MET:O	1:B:545:LEU:N	2.29	0.65
1:C:566:THR:O	1:C:567:VAL:C	2.40	0.65
1:A:258:VAL:HG13	1:A:259:ASN:H	1.62	0.65
1:B:133:HIS:HB3	1:B:520:MET:CE	2.27	0.65
1:D:146:ILE:HD12	1:D:146:ILE:O	1.97	0.65
1:B:128:ASN:C	1:B:128:ASN:ND2	2.54	0.65
1:F:180:ASN:OD1	1:F:182:ARG:HG2	1.96	0.65
1:A:15:ASN:CG	1:F:546:ARG:NH2	2.56	0.64
1:C:463:ILE:O	1:C:463:ILE:CD1	2.45	0.64
1:F:542:MET:HE2	1:F:545:LEU:HD23	1.79	0.64
1:C:224:ASP:O	1:C:227:THR:OG1	2.14	0.64
1:E:59:ILE:HG23	1:E:59:ILE:O	1.98	0.64
1:F:233:GLN:NE2	1:F:380:VAL:HG13	2.13	0.64
1:A:57:VAL:CG1	1:A:57:VAL:O	2.45	0.64
1:A:124:LEU:HD22	1:A:532:TRP:HB2	1.79	0.64
1:E:78:GLN:HG2	1:E:79:VAL:N	2.13	0.64
1:A:128:ASN:C	1:A:128:ASN:ND2	2.55	0.64
1:B:463:ILE:O	1:B:463:ILE:CD1	2.46	0.64
1:E:172:GLU:OE1	1:E:212:TRP:HH2	1.80	0.64
1:F:566:THR:O	1:F:567:VAL:C	2.41	0.64
1:A:157:THR:HG23	1:A:157:THR:O	1.98	0.64
1:C:40:HIS:CE1	1:C:42:PHE:HB3	2.33	0.64
1:D:215:ASP:OD1	1:D:215:ASP:C	2.41	0.64
1:D:563:ILE:HD13	1:D:563:ILE:N	2.13	0.64
1:A:359:ASN:O	1:A:360:VAL:C	2.41	0.64
1:C:563:ILE:N	1:C:563:ILE:HD13	2.13	0.64
1:B:78:GLN:HG2	1:B:79:VAL:N	2.12	0.64
1:B:566:THR:O	1:B:567:VAL:C	2.39	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:542:MET:O	1:C:545:LEU:N	2.31	0.64
1:F:206:ASN:OD1	1:F:210:MET:CE	2.46	0.64
1:C:135:THR:O	1:C:136:GLN:C	2.38	0.63
1:C:172:GLU:OE1	1:C:212:TRP:HH2	1.80	0.63
1:F:164:LYS:C	1:F:282:ILE:CD1	2.71	0.63
1:E:124:LEU:HD22	1:E:532:TRP:HB2	1.79	0.63
1:F:172:GLU:OE1	1:F:212:TRP:HH2	1.80	0.63
1:A:206:ASN:OD1	1:A:210:MET:HE3	1.97	0.63
1:E:29:ARG:HD2	1:E:30:ASP:OD2	1.99	0.63
1:B:37:PHE:CD1	1:B:38:ASP:N	2.65	0.63
1:D:164:LYS:C	1:D:282:ILE:CD1	2.72	0.63
1:D:172:GLU:OE1	1:D:212:TRP:HH2	1.80	0.63
1:B:174:ILE:HG12	1:B:176:THR:HG22	1.78	0.63
1:C:78:GLN:HG2	1:C:79:VAL:N	2.14	0.63
1:F:120:VAL:HG23	1:F:121:LEU:N	2.13	0.63
1:F:215:ASP:OD1	1:F:215:ASP:C	2.42	0.63
1:A:106:SER:O	1:A:107:LEU:HD12	1.99	0.63
1:B:172:GLU:OE1	1:B:212:TRP:HH2	1.82	0.63
1:D:42:PHE:CE1	1:D:59:ILE:HD12	2.33	0.63
1:D:546:ARG:NH2	1:E:15:ASN:CG	2.57	0.63
1:E:206:ASN:OD1	1:E:210:MET:HE3	1.99	0.63
1:F:312:GLU:OE2	1:F:484:ARG:NH1	2.32	0.63
1:D:157:THR:O	1:D:157:THR:CG2	2.47	0.63
1:D:380:VAL:HG12	1:D:381:ASP:N	2.14	0.63
1:D:46:PHE:CB	1:D:57:VAL:HG23	2.29	0.62
1:B:18:GLN:NE2	1:B:552:GLY:O	2.32	0.62
1:F:258:VAL:HG13	1:F:259:ASN:H	1.64	0.62
1:F:233:GLN:O	1:F:236:ILE:HG13	2.00	0.62
1:E:563:ILE:HD13	1:E:563:ILE:N	2.14	0.62
1:B:120:VAL:HG23	1:B:121:LEU:N	2.13	0.62
1:E:534:LEU:HB2	1:E:542:MET:CE	2.30	0.62
1:B:46:PHE:CD2	1:B:46:PHE:O	2.53	0.62
1:B:224:ASP:O	1:B:227:THR:OG1	2.17	0.62
1:F:313:LEU:HB2	1:F:321:LEU:HB3	1.82	0.62
1:B:347:LYS:HE2	1:B:369:THR:CG2	2.29	0.62
1:C:157:THR:CG2	1:C:489:SER:H	2.12	0.62
1:F:133:HIS:HB3	1:F:520:MET:HE3	1.81	0.62
1:F:189:GLU:O	1:F:191:PRO:HD3	2.00	0.62
1:C:286:TYR:N	1:C:331:ASN:OD1	2.33	0.62
1:D:75:ASN:O	1:D:92:VAL:N	2.31	0.62
1:E:356:ARG:NH2	1:F:487:ARG:O	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:46:PHE:HB3	1:F:57:VAL:HG23	1.82	0.62
1:B:40:HIS:CE1	1:B:42:PHE:HB3	2.35	0.62
1:F:75:ASN:O	1:F:92:VAL:N	2.33	0.62
1:A:120:VAL:HG23	1:A:121:LEU:N	2.15	0.62
1:A:215:ASP:OD1	1:A:215:ASP:C	2.43	0.62
1:B:491:ASP:O	1:B:492:GLU:C	2.39	0.62
1:E:380:VAL:HG12	1:E:381:ASP:N	2.15	0.62
1:F:177:ILE:HD13	1:F:177:ILE:O	1.99	0.62
1:F:351:LYS:O	1:F:352:ASN:HB2	1.99	0.62
1:C:215:ASP:OD1	1:C:215:ASP:C	2.44	0.61
1:E:40:HIS:CE1	1:E:42:PHE:HB3	2.34	0.61
1:E:29:ARG:HD3	1:E:89:TYR:CE2	2.34	0.61
1:D:134:TYR:O	1:D:572:ILE:HD13	1.99	0.61
1:C:5:LYS:NZ	1:C:41:GLU:OE2	2.33	0.61
1:D:135:THR:O	1:D:136:GLN:C	2.42	0.61
1:F:290:MET:HE3	1:F:295:LEU:HB2	1.81	0.61
1:A:312:GLU:OE2	1:A:484:ARG:NH1	2.34	0.61
1:B:26:ASN:HB3	1:B:29:ARG:NH2	2.14	0.61
1:B:182:ARG:CZ	1:B:267:LYS:HE2	2.30	0.61
1:E:42:PHE:CE1	1:E:59:ILE:HD12	2.36	0.61
1:A:29:ARG:HD3	1:A:89:TYR:CE2	2.36	0.61
1:A:40:HIS:CE1	1:A:42:PHE:HB3	2.35	0.61
1:A:224:ASP:O	1:A:227:THR:OG1	2.18	0.61
1:B:124:LEU:HD22	1:B:532:TRP:HB2	1.81	0.61
1:B:37:PHE:HZ	1:B:40:HIS:O	1.82	0.61
1:B:180:ASN:OD1	1:B:182:ARG:HG2	2.00	0.61
1:E:8:LEU:O	1:E:37:PHE:CZ	2.54	0.61
1:E:463:ILE:O	1:E:463:ILE:CD1	2.49	0.61
1:F:3:LEU:N	1:F:44:SER:O	2.33	0.61
1:F:164:LYS:O	1:F:282:ILE:HD11	2.01	0.61
1:A:174:ILE:HD13	1:A:174:ILE:O	2.01	0.61
1:E:120:VAL:HG23	1:E:121:LEU:N	2.15	0.61
1:F:217:GLU:O	1:F:220:LYS:N	2.33	0.61
1:F:224:ASP:O	1:F:227:THR:OG1	2.19	0.61
1:C:542:MET:HE1	1:C:545:LEU:HD23	1.83	0.60
1:A:182:ARG:CZ	1:A:267:LYS:HE2	2.31	0.60
1:B:75:ASN:N	1:B:75:ASN:OD1	2.34	0.60
1:B:313:LEU:HB2	1:B:321:LEU:HB3	1.82	0.60
1:B:380:VAL:HG12	1:B:381:ASP:N	2.16	0.60
1:C:470:TYR:CG	1:C:479:PHE:CE1	2.89	0.60
1:C:37:PHE:CD1	1:C:38:ASP:N	2.68	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:46:PHE:CB	1:E:57:VAL:HG23	2.31	0.60
1:E:206:ASN:OD1	1:E:210:MET:CE	2.48	0.60
1:D:374:ASP:OD1	1:D:374:ASP:N	2.35	0.60
1:F:90:LEU:HD22	1:F:107:LEU:HD23	1.83	0.60
1:A:8:LEU:O	1:A:37:PHE:CZ	2.54	0.60
1:B:157:THR:CG2	1:B:489:SER:H	2.13	0.60
1:D:174:ILE:HG12	1:D:176:THR:HG22	1.82	0.60
1:D:189:GLU:C	1:D:191:PRO:HD3	2.26	0.60
1:F:290:MET:HE3	1:F:295:LEU:CB	2.31	0.60
1:B:542:MET:CE	1:B:545:LEU:HD23	2.32	0.60
1:E:566:THR:O	1:E:567:VAL:C	2.43	0.60
1:A:463:ILE:CD1	1:A:463:ILE:O	2.50	0.60
1:F:347:LYS:HE2	1:F:369:THR:CG2	2.32	0.60
1:A:111:VAL:HB	1:A:545:LEU:HD13	1.83	0.59
1:B:133:HIS:HB3	1:B:520:MET:HE3	1.83	0.59
1:C:510:TYR:HB3	1:D:502:MET:HE2	1.84	0.59
1:C:546:ARG:NH2	1:D:15:ASN:CG	2.60	0.59
1:D:40:HIS:CE1	1:D:42:PHE:HB3	2.37	0.59
1:D:233:GLN:O	1:D:236:ILE:HG13	2.02	0.59
1:D:560:SER:O	1:D:564:ASN:ND2	2.34	0.59
1:E:128:ASN:C	1:E:128:ASN:ND2	2.58	0.59
1:C:546:ARG:NH2	1:D:15:ASN:OD1	2.35	0.59
1:E:174:ILE:HG12	1:E:176:THR:HG22	1.83	0.59
1:E:182:ARG:NH2	1:E:267:LYS:HE2	2.17	0.59
1:E:542:MET:HE2	1:E:545:LEU:HD23	1.84	0.59
1:F:563:ILE:HD13	1:F:563:ILE:N	2.17	0.59
1:B:79:VAL:HG11	1:B:81:TYR:CE2	2.37	0.59
1:E:79:VAL:HG11	1:E:81:TYR:CE2	2.37	0.59
1:F:470:TYR:CG	1:F:479:PHE:CE1	2.91	0.59
1:D:206:ASN:OD1	1:D:210:MET:HE3	2.02	0.59
1:F:347:LYS:HE2	1:F:369:THR:HG22	1.85	0.59
1:B:563:ILE:HD13	1:B:563:ILE:N	2.17	0.59
1:D:189:GLU:O	1:D:191:PRO:HD3	2.03	0.59
1:E:182:ARG:CZ	1:E:267:LYS:HE2	2.31	0.59
1:F:463:ILE:CD1	1:F:463:ILE:O	2.51	0.59
1:A:566:THR:O	1:A:567:VAL:C	2.46	0.59
1:C:206:ASN:OD1	1:C:210:MET:CE	2.50	0.59
1:A:359:ASN:C	1:A:360:VAL:O	2.41	0.59
1:B:6:ILE:CG2	1:B:7:LYS:N	2.65	0.59
1:A:177:ILE:CG2	1:A:236:ILE:HG12	2.32	0.59
1:A:542:MET:HE2	1:A:545:LEU:HD23	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:290:MET:HE3	1:D:295:LEU:HB2	1.85	0.59
1:E:502:MET:HG2	1:E:567:VAL:HG11	1.84	0.59
1:D:3:LEU:N	1:D:44:SER:O	2.36	0.59
1:D:258:VAL:HG13	1:D:259:ASN:H	1.68	0.59
1:D:470:TYR:CG	1:D:479:PHE:CE1	2.91	0.59
1:E:282:ILE:HG23	1:E:334:PHE:CD2	2.37	0.59
1:A:189:GLU:C	1:A:191:PRO:HD3	2.27	0.59
1:B:174:ILE:HD13	1:B:174:ILE:O	2.02	0.59
1:B:347:LYS:HE2	1:B:369:THR:HG22	1.84	0.59
1:C:18:GLN:NE2	1:C:552:GLY:O	2.34	0.59
1:C:258:VAL:HG13	1:C:259:ASN:H	1.68	0.59
1:E:5:LYS:NZ	1:E:41:GLU:OE2	2.35	0.59
1:E:135:THR:O	1:E:136:GLN:C	2.46	0.59
1:B:44:SER:OG	1:B:45:THR:N	2.36	0.58
1:B:67:CYS:O	1:B:68:PHE:HB2	2.03	0.58
1:B:291:PHE:C	1:B:291:PHE:CD2	2.80	0.58
1:F:380:VAL:HG12	1:F:381:ASP:N	2.18	0.58
1:F:563:ILE:O	1:F:564:ASN:ND2	2.36	0.58
1:A:18:GLN:NE2	1:A:552:GLY:O	2.34	0.58
1:C:120:VAL:HG23	1:C:121:LEU:N	2.17	0.58
1:C:128:ASN:C	1:C:128:ASN:ND2	2.62	0.58
1:D:256:GLU:O	1:D:264:SER:HA	2.04	0.58
1:E:75:ASN:HA	1:E:92:VAL:HG22	1.85	0.58
1:F:40:HIS:CE1	1:F:42:PHE:HB3	2.38	0.58
1:F:566:THR:O	1:F:568:VAL:N	2.35	0.58
1:C:29:ARG:HD2	1:C:30:ASP:OD2	2.03	0.58
1:C:380:VAL:HG12	1:C:381:ASP:N	2.19	0.58
1:E:258:VAL:HG13	1:E:259:ASN:H	1.67	0.58
1:F:286:TYR:N	1:F:331:ASN:OD1	2.36	0.58
1:F:302:HIS:CD2	1:F:303:LEU:HD13	2.38	0.58
1:C:174:ILE:HG12	1:C:176:THR:HG22	1.85	0.58
1:D:5:LYS:NZ	1:D:41:GLU:OE2	2.36	0.58
1:D:299:ASN:N	1:D:299:ASN:ND2	2.51	0.58
1:E:172:GLU:HB3	1:E:212:TRP:CH2	2.38	0.58
1:B:5:LYS:NZ	1:B:41:GLU:OE2	2.37	0.58
1:F:41:GLU:HG2	1:F:41:GLU:O	2.03	0.58
1:C:67:CYS:O	1:C:68:PHE:HB2	2.04	0.58
1:D:174:ILE:HD13	1:D:174:ILE:O	2.04	0.58
1:E:529:LYS:O	1:E:530:GLY:O	2.22	0.58
1:F:29:ARG:HD3	1:F:89:TYR:CE2	2.39	0.58
1:C:313:LEU:HB2	1:C:321:LEU:HB3	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:57:VAL:CG1	1:D:57:VAL:O	2.51	0.58
1:E:229:TYR:N	1:E:229:TYR:CD2	2.71	0.58
1:B:529:LYS:O	1:B:530:GLY:O	2.21	0.58
1:F:30:ASP:OD2	1:F:89:TYR:OH	2.20	0.58
1:F:516:ASP:OD2	1:F:518:THR:HG22	2.03	0.58
1:A:290:MET:HE3	1:A:295:LEU:HB2	1.86	0.57
1:D:90:LEU:HA	1:D:109:PRO:HA	1.84	0.57
1:F:306:PRO:HD3	1:F:326:SER:HB3	1.85	0.57
1:B:563:ILE:O	1:B:564:ASN:ND2	2.37	0.57
1:C:157:THR:HG23	1:C:157:THR:O	2.03	0.57
1:A:177:ILE:HG22	1:A:236:ILE:HG23	1.86	0.57
1:E:258:VAL:HG22	1:E:259:ASN:N	2.18	0.57
1:E:491:ASP:O	1:E:492:GLU:C	2.47	0.57
1:D:463:ILE:O	1:D:463:ILE:CD1	2.53	0.57
1:E:286:TYR:N	1:E:331:ASN:OD1	2.37	0.57
1:A:358:ASN:CG	1:A:358:ASN:O	2.47	0.57
1:B:259:ASN:O	1:B:260:GLY:C	2.46	0.57
1:C:298:ILE:HB	1:C:299:ASN:ND2	2.19	0.57
1:D:8:LEU:O	1:D:37:PHE:CZ	2.58	0.57
1:A:380:VAL:HG12	1:A:381:ASP:N	2.19	0.57
1:C:206:ASN:OD1	1:C:210:MET:HE3	2.05	0.57
1:E:542:MET:O	1:E:545:LEU:N	2.35	0.57
1:F:42:PHE:CE1	1:F:59:ILE:HD12	2.40	0.57
1:F:59:ILE:HG23	1:F:59:ILE:O	2.05	0.57
1:F:177:ILE:HG22	1:F:236:ILE:HG23	1.87	0.57
1:E:215:ASP:OD1	1:E:215:ASP:C	2.46	0.57
1:F:182:ARG:CZ	1:F:267:LYS:HE2	2.35	0.57
1:F:359:ASN:O	1:F:360:VAL:C	2.45	0.57
1:A:542:MET:O	1:A:543:ASN:C	2.48	0.57
1:B:164:LYS:C	1:B:282:ILE:HD11	2.29	0.57
1:C:305:ARG:HB2	1:C:306:PRO:HD2	1.86	0.57
1:D:358:ASN:CG	1:D:358:ASN:O	2.48	0.57
1:D:502:MET:HG2	1:D:567:VAL:HG11	1.87	0.57
1:B:290:MET:HE3	1:B:295:LEU:CB	2.35	0.57
1:B:374:ASP:OD1	1:B:374:ASP:N	2.38	0.57
1:D:46:PHE:HB3	1:D:57:VAL:HG23	1.87	0.57
1:D:67:CYS:O	1:D:68:PHE:HB2	2.05	0.57
1:E:233:GLN:O	1:E:236:ILE:HG13	2.05	0.57
1:E:539:THR:CG2	1:F:94:ASP:HA	2.34	0.57
1:F:67:CYS:O	1:F:68:PHE:HB2	2.04	0.57
1:F:359:ASN:C	1:F:360:VAL:O	2.48	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:37:PHE:HZ	1:A:40:HIS:O	1.88	0.57
1:C:152:VAL:HG21	1:C:307:ASN:HD21	1.70	0.57
1:D:37:PHE:CD1	1:D:38:ASP:N	2.73	0.57
1:A:67:CYS:O	1:A:68:PHE:HB2	2.05	0.56
1:B:59:ILE:O	1:B:59:ILE:CG2	2.51	0.56
1:B:135:THR:O	1:B:136:GLN:C	2.44	0.56
1:B:356:ARG:NH2	1:C:487:ARG:O	2.38	0.56
1:D:339:THR:HG21	1:E:472:PRO:HB3	1.87	0.56
1:D:510:TYR:HB3	1:E:502:MET:HE2	1.86	0.56
1:E:553:VAL:HG12	1:E:555:LEU:HD12	1.87	0.56
1:A:46:PHE:CB	1:A:57:VAL:HG23	2.36	0.56
1:C:172:GLU:CD	1:C:212:TRP:CZ2	2.83	0.56
1:D:18:GLN:NE2	1:D:552:GLY:O	2.39	0.56
1:D:471:ALA:HB3	1:D:472:PRO:HD3	1.86	0.56
1:E:111:VAL:HB	1:E:545:LEU:HD13	1.87	0.56
1:E:224:ASP:O	1:E:227:THR:OG1	2.21	0.56
1:E:290:MET:HE3	1:E:295:LEU:CB	2.35	0.56
1:B:134:TYR:O	1:B:572:ILE:HD13	2.05	0.56
1:B:229:TYR:CD2	1:B:229:TYR:N	2.73	0.56
1:D:59:ILE:HG23	1:D:59:ILE:O	2.03	0.56
1:D:313:LEU:HB2	1:D:321:LEU:HB3	1.87	0.56
1:E:46:PHE:O	1:E:46:PHE:CD2	2.58	0.56
1:F:18:GLN:NE2	1:F:552:GLY:O	2.38	0.56
1:F:133:HIS:HB3	1:F:520:MET:CE	2.35	0.56
1:C:148:SER:CB	1:D:156:SER:O	2.54	0.56
1:D:128:ASN:C	1:D:128:ASN:ND2	2.64	0.56
1:D:286:TYR:N	1:D:331:ASN:OD1	2.38	0.56
1:A:133:HIS:HB3	1:A:520:MET:CE	2.35	0.56
1:E:305:ARG:HB2	1:E:306:PRO:HD2	1.86	0.56
1:B:324:ASP:OD1	1:B:324:ASP:C	2.48	0.56
1:D:148:SER:CB	1:E:156:SER:O	2.53	0.56
1:F:44:SER:OG	1:F:45:THR:N	2.37	0.56
1:A:90:LEU:HD22	1:A:107:LEU:HD23	1.88	0.56
1:B:233:GLN:O	1:B:236:ILE:HG13	2.06	0.56
1:D:90:LEU:HD22	1:D:107:LEU:HD23	1.86	0.56
1:B:286:TYR:CE1	1:B:301:LYS:HE3	2.41	0.56
1:D:542:MET:O	1:D:543:ASN:C	2.48	0.56
1:E:46:PHE:HB3	1:E:57:VAL:HG23	1.87	0.56
1:E:180:ASN:OD1	1:E:182:ARG:HG2	2.06	0.56
1:F:502:MET:HG2	1:F:567:VAL:HG11	1.88	0.56
1:A:79:VAL:HG11	1:A:81:TYR:CE2	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:502:MET:O	1:B:554:ARG:NH1	2.36	0.56
1:C:6:ILE:CG2	1:C:7:LYS:N	2.69	0.56
1:D:175:LEU:CD1	1:D:177:ILE:HG23	2.36	0.56
1:D:351:LYS:HG2	1:D:352:ASN:OD1	2.06	0.56
1:E:37:PHE:HZ	1:E:40:HIS:O	1.87	0.56
1:F:5:LYS:NZ	1:F:41:GLU:OE2	2.38	0.56
1:F:134:TYR:O	1:F:572:ILE:HD13	2.05	0.56
1:A:172:GLU:OE1	1:A:212:TRP:HH2	1.89	0.56
1:B:45:THR:HG23	1:B:45:THR:O	2.05	0.56
1:C:8:LEU:O	1:C:37:PHE:CZ	2.59	0.56
1:C:42:PHE:CE1	1:C:59:ILE:CD1	2.89	0.56
1:E:3:LEU:N	1:E:44:SER:O	2.39	0.56
1:E:67:CYS:SG	1:E:68:PHE:N	2.79	0.56
1:F:305:ARG:HB2	1:F:306:PRO:HD2	1.87	0.56
1:A:134:TYR:O	1:A:572:ILE:HD13	2.06	0.55
1:A:177:ILE:HG21	1:A:236:ILE:HG12	1.87	0.55
1:B:46:PHE:CB	1:B:57:VAL:HG23	2.36	0.55
1:C:59:ILE:HG23	1:C:59:ILE:O	2.05	0.55
1:C:258:VAL:HG22	1:C:259:ASN:N	2.20	0.55
1:D:542:MET:HE2	1:D:545:LEU:HD23	1.88	0.55
1:A:502:MET:HG2	1:A:567:VAL:HG11	1.87	0.55
1:B:215:ASP:OD1	1:B:215:ASP:C	2.48	0.55
1:D:566:THR:O	1:D:568:VAL:N	2.40	0.55
1:E:324:ASP:OD1	1:E:324:ASP:C	2.49	0.55
1:F:491:ASP:O	1:F:492:GLU:C	2.47	0.55
1:C:133:HIS:HB3	1:C:520:MET:CE	2.36	0.55
1:F:175:LEU:CD1	1:F:177:ILE:HG23	2.36	0.55
1:E:174:ILE:HD13	1:E:174:ILE:O	2.05	0.55
1:F:217:GLU:O	1:F:218:SER:C	2.48	0.55
1:F:358:ASN:CG	1:F:358:ASN:O	2.50	0.55
1:F:374:ASP:OD1	1:F:374:ASP:N	2.32	0.55
1:A:206:ASN:OD1	1:A:210:MET:CE	2.55	0.55
1:B:8:LEU:O	1:B:37:PHE:CZ	2.60	0.55
1:B:57:VAL:O	1:B:57:VAL:CG1	2.55	0.55
1:C:174:ILE:O	1:C:174:ILE:HD13	2.06	0.55
1:D:534:LEU:HB2	1:D:542:MET:CE	2.36	0.55
1:E:471:ALA:HB3	1:E:472:PRO:HD3	1.89	0.55
1:F:75:ASN:HA	1:F:92:VAL:HG22	1.89	0.55
1:F:157:THR:O	1:F:157:THR:CG2	2.54	0.55
1:F:172:GLU:CD	1:F:212:TRP:CH2	2.85	0.55
1:F:177:ILE:CG2	1:F:236:ILE:HG12	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:156:SER:O	1:F:148:SER:CB	2.55	0.55
1:A:510:TYR:HB3	1:B:502:MET:HE2	1.88	0.55
1:C:559:GLU:O	1:C:560:SER:C	2.50	0.55
1:C:566:THR:O	1:C:568:VAL:N	2.40	0.55
1:D:12:THR:HG21	1:D:76:TYR:HB2	1.89	0.55
1:A:537:VAL:O	1:A:538:ASP:C	2.48	0.55
1:B:566:THR:O	1:B:568:VAL:N	2.39	0.55
1:C:545:LEU:O	1:C:546:ARG:C	2.50	0.55
1:D:79:VAL:HG11	1:D:81:TYR:CE2	2.42	0.55
1:E:164:LYS:C	1:E:282:ILE:HD11	2.31	0.55
1:E:563:ILE:O	1:E:564:ASN:ND2	2.40	0.55
1:A:175:LEU:CD1	1:A:177:ILE:HG23	2.37	0.55
1:C:471:ALA:HB3	1:C:472:PRO:HD3	1.89	0.55
1:F:534:LEU:HB2	1:F:542:MET:CE	2.37	0.55
1:A:15:ASN:OD1	1:F:546:ARG:NH2	2.40	0.54
1:A:305:ARG:HB2	1:A:306:PRO:HD2	1.88	0.54
1:B:90:LEU:HA	1:B:109:PRO:HA	1.88	0.54
1:E:296:ASN:O	1:E:300:ASP:HB2	2.06	0.54
1:F:172:GLU:CD	1:F:212:TRP:CZ2	2.85	0.54
1:A:133:HIS:HB3	1:A:520:MET:HE3	1.89	0.54
1:A:189:GLU:O	1:A:191:PRO:HD3	2.08	0.54
1:A:256:GLU:O	1:A:264:SER:HA	2.07	0.54
1:C:134:TYR:O	1:C:572:ILE:HD13	2.07	0.54
1:C:518:THR:HG23	1:C:518:THR:O	2.06	0.54
1:C:534:LEU:HB2	1:C:542:MET:SD	2.47	0.54
1:E:256:GLU:O	1:E:264:SER:HA	2.07	0.54
1:F:26:ASN:O	1:F:29:ARG:HB3	2.06	0.54
1:A:41:GLU:HG2	1:A:41:GLU:O	2.07	0.54
1:B:175:LEU:CD1	1:B:177:ILE:HG23	2.36	0.54
1:C:79:VAL:HG11	1:C:81:TYR:CE2	2.42	0.54
1:C:177:ILE:HD13	1:C:177:ILE:O	2.08	0.54
1:E:172:GLU:CD	1:E:212:TRP:CZ2	2.85	0.54
1:E:172:GLU:CD	1:E:212:TRP:CH2	2.85	0.54
1:E:374:ASP:OD1	1:E:374:ASP:N	2.36	0.54
1:B:546:ARG:NH2	1:C:15:ASN:OD1	2.41	0.54
1:D:229:TYR:N	1:D:229:TYR:CD2	2.75	0.54
1:E:67:CYS:O	1:E:68:PHE:HB2	2.07	0.54
1:B:30:ASP:OD2	1:B:89:TYR:OH	2.21	0.54
1:C:175:LEU:CD1	1:C:177:ILE:HG23	2.37	0.54
1:C:190:LYS:O	1:C:190:LYS:HG2	2.06	0.54
1:D:172:GLU:HB3	1:D:212:TRP:CH2	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:206:ASN:OD1	1:D:210:MET:CE	2.56	0.54
1:A:471:ALA:HB3	1:A:472:PRO:HD3	1.90	0.54
1:C:182:ARG:CZ	1:C:267:LYS:HE2	2.37	0.54
1:E:204:ILE:HD13	1:F:468:VAL:HG23	1.90	0.54
1:F:174:ILE:HG12	1:F:176:THR:HG22	1.88	0.54
1:A:57:VAL:O	1:A:57:VAL:HG12	2.07	0.54
1:D:3:LEU:HD21	1:E:68:PHE:CE2	2.43	0.54
1:F:8:LEU:O	1:F:37:PHE:CZ	2.61	0.54
1:B:360:VAL:HG23	1:B:363:TYR:HB2	1.88	0.54
1:D:44:SER:OG	1:D:45:THR:N	2.41	0.54
1:E:44:SER:OG	1:E:45:THR:N	2.40	0.54
1:F:46:PHE:HB2	1:F:57:VAL:HG23	1.88	0.54
1:F:46:PHE:O	1:F:46:PHE:CD2	2.61	0.54
1:A:59:ILE:O	1:A:59:ILE:CG2	2.56	0.54
1:B:286:TYR:C	1:B:286:TYR:CD2	2.85	0.54
1:C:279:PHE:HB3	1:C:282:ILE:HG22	1.89	0.54
1:C:291:PHE:C	1:C:291:PHE:CD2	2.86	0.54
1:D:204:ILE:HD13	1:E:468:VAL:HG23	1.90	0.54
1:D:305:ARG:HB2	1:D:306:PRO:HD2	1.90	0.54
1:C:46:PHE:CB	1:C:57:VAL:HG23	2.37	0.54
1:C:324:ASP:OD1	1:C:324:ASP:C	2.51	0.54
1:D:46:PHE:CE1	1:D:55:LEU:CD1	2.91	0.54
1:F:542:MET:HE1	1:F:545:LEU:HD23	1.90	0.54
1:F:566:THR:C	1:F:568:VAL:N	2.64	0.54
1:E:290:MET:HE3	1:E:295:LEU:HB2	1.89	0.53
1:E:532:TRP:CZ2	1:E:546:ARG:HA	2.43	0.53
1:F:174:ILE:HD13	1:F:174:ILE:O	2.08	0.53
1:A:229:TYR:N	1:A:229:TYR:CD2	2.75	0.53
1:B:23:PHE:N	1:B:23:PHE:CD2	2.75	0.53
1:B:182:ARG:NH2	1:B:267:LYS:HE2	2.24	0.53
1:D:158:MET:O	1:D:159:ARG:CD	2.50	0.53
1:D:276:GLN:O	1:D:277:LYS:C	2.50	0.53
1:F:229:TYR:N	1:F:229:TYR:CD2	2.76	0.53
1:B:12:THR:HG21	1:B:76:TYR:HB2	1.90	0.53
1:B:534:LEU:HB2	1:B:542:MET:CE	2.37	0.53
1:F:212:TRP:CZ3	1:F:247:ILE:HG13	2.43	0.53
1:A:172:GLU:HB3	1:A:212:TRP:CH2	2.44	0.53
1:B:276:GLN:O	1:B:277:LYS:C	2.51	0.53
1:C:463:ILE:O	1:C:463:ILE:HD12	2.09	0.53
1:D:182:ARG:CZ	1:D:267:LYS:HE2	2.38	0.53
1:F:516:ASP:CG	1:F:518:THR:HG22	2.34	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:542:MET:O	1:B:543:ASN:C	2.51	0.53
1:C:164:LYS:C	1:C:282:ILE:HD11	2.32	0.53
1:D:172:GLU:CD	1:D:212:TRP:CH2	2.86	0.53
1:E:559:GLU:O	1:E:560:SER:C	2.50	0.53
1:A:470:TYR:HB3	1:A:479:PHE:CD1	2.44	0.53
1:B:286:TYR:N	1:B:331:ASN:OD1	2.41	0.53
1:C:172:GLU:CD	1:C:212:TRP:CH2	2.87	0.53
1:C:302:HIS:CD2	1:C:303:LEU:HD13	2.43	0.53
1:D:172:GLU:CD	1:D:212:TRP:CZ2	2.87	0.53
1:E:18:GLN:NE2	1:E:552:GLY:O	2.39	0.53
1:E:37:PHE:CD1	1:E:38:ASP:N	2.77	0.53
1:E:470:TYR:HB3	1:E:479:PHE:CD1	2.44	0.53
1:F:177:ILE:HD13	1:F:177:ILE:C	2.34	0.53
1:A:44:SER:OG	1:A:45:THR:N	2.40	0.53
1:A:185:PHE:CE2	1:A:259:ASN:HB2	2.43	0.53
1:B:339:THR:HG21	1:C:472:PRO:HB3	1.91	0.53
1:B:463:ILE:O	1:B:463:ILE:HD13	2.09	0.53
1:D:285:ASP:O	1:D:286:TYR:C	2.50	0.53
1:E:46:PHE:CE1	1:E:55:LEU:CD1	2.91	0.53
1:E:152:VAL:HG22	1:E:153:LEU:N	2.23	0.53
1:F:152:VAL:HG21	1:F:307:ASN:HD21	1.73	0.53
1:D:158:MET:C	1:D:159:ARG:HG2	2.34	0.53
1:D:244:SER:O	1:D:245:GLY:C	2.51	0.53
1:D:559:GLU:O	1:D:560:SER:C	2.51	0.53
1:E:175:LEU:CD1	1:E:177:ILE:HG23	2.39	0.53
1:F:496:VAL:O	1:F:497:LYS:C	2.52	0.53
1:A:37:PHE:CD1	1:A:38:ASP:N	2.75	0.53
1:A:233:GLN:O	1:A:236:ILE:HG13	2.09	0.53
1:C:46:PHE:HB3	1:C:57:VAL:HG23	1.90	0.53
1:C:60:ASP:HA	1:C:102:VAL:HG22	1.91	0.53
1:D:148:SER:HB3	1:E:156:SER:O	2.09	0.53
1:E:157:THR:O	1:E:157:THR:CG2	2.55	0.53
1:E:498:LYS:O	1:E:499:TYR:C	2.52	0.53
1:F:182:ARG:NH2	1:F:267:LYS:HE2	2.24	0.53
1:A:164:LYS:C	1:A:282:ILE:HD11	2.34	0.53
1:B:158:MET:C	1:B:159:ARG:HG2	2.33	0.53
1:D:152:VAL:HG22	1:D:153:LEU:N	2.23	0.53
1:D:152:VAL:HG21	1:D:307:ASN:HD21	1.74	0.53
1:F:177:ILE:HG21	1:F:236:ILE:HG12	1.90	0.53
1:F:471:ALA:HB3	1:F:472:PRO:HD3	1.90	0.53
1:B:559:GLU:O	1:B:560:SER:C	2.53	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:46:PHE:CD2	1:D:46:PHE:O	2.62	0.52
1:D:302:HIS:CD2	1:D:303:LEU:HD13	2.44	0.52
1:D:572:ILE:O	1:D:572:ILE:CG2	2.50	0.52
1:E:26:ASN:HB3	1:E:29:ARG:CZ	2.39	0.52
1:E:90:LEU:HA	1:E:109:PRO:HA	1.91	0.52
1:E:360:VAL:HG13	1:F:163:ILE:HD12	1.89	0.52
1:F:286:TYR:CE1	1:F:301:LYS:HE3	2.44	0.52
1:A:177:ILE:HD13	1:A:177:ILE:C	2.32	0.52
1:A:290:MET:CE	1:A:295:LEU:HB3	2.34	0.52
1:B:90:LEU:HD22	1:B:107:LEU:HD23	1.90	0.52
1:E:134:TYR:O	1:E:572:ILE:HD13	2.09	0.52
1:F:124:LEU:HD21	1:F:532:TRP:HE3	1.73	0.52
1:F:172:GLU:HB3	1:F:212:TRP:CH2	2.44	0.52
1:C:46:PHE:O	1:C:46:PHE:CD2	2.63	0.52
1:E:313:LEU:HB2	1:E:321:LEU:HB3	1.90	0.52
1:A:172:GLU:CD	1:A:212:TRP:CZ2	2.87	0.52
1:A:491:ASP:O	1:A:494:ASN:N	2.41	0.52
1:A:529:LYS:O	1:A:530:GLY:O	2.28	0.52
1:B:572:ILE:O	1:B:572:ILE:CG2	2.49	0.52
1:C:148:SER:HB3	1:D:156:SER:O	2.09	0.52
1:C:256:GLU:O	1:C:264:SER:HA	2.08	0.52
1:C:516:ASP:OD2	1:C:517:ILE:N	2.42	0.52
1:D:26:ASN:O	1:D:29:ARG:HB3	2.09	0.52
1:D:30:ASP:OD2	1:D:89:TYR:OH	2.21	0.52
1:D:177:ILE:HG22	1:D:236:ILE:HG23	1.92	0.52
1:A:217:GLU:O	1:A:220:LYS:N	2.42	0.52
1:B:563:ILE:C	1:B:564:ASN:ND2	2.68	0.52
1:C:75:ASN:O	1:C:92:VAL:N	2.40	0.52
1:C:502:MET:HG2	1:C:567:VAL:HG11	1.91	0.52
1:C:539:THR:CG2	1:D:94:ASP:HA	2.39	0.52
1:A:470:TYR:CB	1:A:479:PHE:CE1	2.93	0.52
1:B:42:PHE:CE2	1:B:44:SER:HB2	2.44	0.52
1:B:470:TYR:HB3	1:B:479:PHE:CD1	2.44	0.52
1:C:498:LYS:O	1:C:499:TYR:C	2.52	0.52
1:E:363:TYR:HD2	1:F:316:TYR:CE1	2.28	0.52
1:F:256:GLU:O	1:F:264:SER:HA	2.09	0.52
1:B:217:GLU:O	1:B:220:LYS:N	2.42	0.52
1:B:286:TYR:HE1	1:B:301:LYS:HE3	1.74	0.52
1:C:45:THR:HG23	1:C:45:THR:O	2.10	0.52
1:F:164:LYS:C	1:F:282:ILE:HD11	2.35	0.52
1:A:157:THR:HG22	1:A:488:ILE:HB	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:520:MET:SD	1:A:572:ILE:HG12	2.50	0.52
1:A:542:MET:HE1	1:A:545:LEU:HD23	1.92	0.52
1:B:285:ASP:HA	1:B:331:ASN:OD1	2.10	0.52
1:C:111:VAL:HB	1:C:545:LEU:HD13	1.92	0.52
1:D:111:VAL:HB	1:D:545:LEU:HD13	1.91	0.52
1:D:516:ASP:OD2	1:D:518:THR:HG22	2.09	0.52
1:D:546:ARG:NH2	1:E:15:ASN:OD1	2.43	0.52
1:E:177:ILE:HG22	1:E:236:ILE:HG23	1.91	0.52
1:F:542:MET:O	1:F:543:ASN:C	2.52	0.52
1:B:3:LEU:N	1:B:44:SER:O	2.43	0.52
1:C:175:LEU:HD11	1:C:177:ILE:HG23	1.92	0.52
1:F:37:PHE:CD1	1:F:38:ASP:N	2.78	0.52
1:F:37:PHE:HZ	1:F:40:HIS:O	1.92	0.52
1:F:324:ASP:C	1:F:324:ASP:OD1	2.52	0.52
1:A:217:GLU:O	1:A:218:SER:C	2.52	0.52
1:A:563:ILE:O	1:A:564:ASN:ND2	2.42	0.52
1:B:560:SER:O	1:B:564:ASN:ND2	2.41	0.52
1:E:175:LEU:HD23	1:E:239:VAL:HB	1.92	0.52
1:E:285:ASP:OD2	1:E:287:GLN:N	2.42	0.52
1:A:5:LYS:NZ	1:A:41:GLU:OE2	2.43	0.51
1:A:472:PRO:HB3	1:F:339:THR:HG21	1.92	0.51
1:C:48:TYR:OH	1:C:109:PRO:HG3	2.11	0.51
1:C:539:THR:HG23	1:D:93:THR:O	2.10	0.51
1:A:46:PHE:HB3	1:A:57:VAL:HG23	1.91	0.51
1:D:306:PRO:HD3	1:D:326:SER:HB3	1.92	0.51
1:E:359:ASN:O	1:E:360:VAL:C	2.50	0.51
1:F:90:LEU:HA	1:F:109:PRO:HA	1.93	0.51
1:B:148:SER:CB	1:C:156:SER:O	2.58	0.51
1:B:290:MET:HE3	1:B:295:LEU:HB3	1.92	0.51
1:C:41:GLU:O	1:C:41:GLU:HG2	2.11	0.51
1:C:164:LYS:CB	1:C:282:ILE:HD12	2.40	0.51
1:C:285:ASP:O	1:C:286:TYR:C	2.53	0.51
1:D:356:ARG:NH2	1:E:487:ARG:O	2.42	0.51
1:F:128:ASN:C	1:F:128:ASN:ND2	2.67	0.51
1:A:276:GLN:O	1:A:277:LYS:C	2.52	0.51
1:C:534:LEU:HB2	1:C:542:MET:CE	2.41	0.51
1:D:164:LYS:C	1:D:282:ILE:HD11	2.35	0.51
1:D:347:LYS:HE2	1:D:369:THR:CG2	2.41	0.51
1:A:182:ARG:NH2	1:A:267:LYS:HE2	2.25	0.51
1:A:286:TYR:C	1:A:286:TYR:CD2	2.88	0.51
1:A:491:ASP:O	1:A:492:GLU:C	2.51	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:356:ARG:NH2	1:D:487:ARG:O	2.38	0.51
1:E:351:LYS:O	1:E:352:ASN:HB2	2.10	0.51
1:F:6:ILE:CG2	1:F:7:LYS:N	2.73	0.51
1:A:157:THR:HG23	1:A:489:SER:H	1.75	0.51
1:B:75:ASN:HA	1:B:92:VAL:HG22	1.91	0.51
1:B:157:THR:O	1:B:157:THR:CG2	2.56	0.51
1:D:175:LEU:HD11	1:D:177:ILE:HG23	1.91	0.51
1:F:291:PHE:C	1:F:291:PHE:CD2	2.89	0.51
1:A:48:TYR:OH	1:A:109:PRO:HG3	2.11	0.51
1:A:285:ASP:O	1:A:286:TYR:C	2.53	0.51
1:A:534:LEU:HB2	1:A:542:MET:CE	2.41	0.51
1:C:46:PHE:CE1	1:C:55:LEU:CD1	2.94	0.51
1:C:351:LYS:HG2	1:C:352:ASN:OD1	2.10	0.51
1:D:290:MET:HE3	1:D:295:LEU:HB3	1.92	0.51
1:D:299:ASN:OD1	1:D:571:VAL:HG22	2.11	0.51
1:A:172:GLU:CD	1:A:212:TRP:CH2	2.88	0.51
1:B:164:LYS:CB	1:B:282:ILE:HD12	2.41	0.51
1:C:133:HIS:CD2	1:C:525:TRP:H	2.29	0.51
1:C:286:TYR:C	1:C:286:TYR:CD2	2.89	0.51
1:D:133:HIS:HB3	1:D:520:MET:CE	2.40	0.51
1:E:6:ILE:CG2	1:E:7:LYS:N	2.74	0.51
1:E:291:PHE:C	1:E:291:PHE:CD2	2.89	0.51
1:E:319:ASN:C	1:E:320:ARG:HG2	2.36	0.51
1:E:542:MET:O	1:E:543:ASN:C	2.54	0.51
1:E:566:THR:O	1:E:568:VAL:N	2.44	0.51
1:B:148:SER:HB3	1:C:156:SER:O	2.10	0.51
1:C:177:ILE:HG22	1:C:236:ILE:HG23	1.93	0.51
1:C:185:PHE:CE2	1:C:259:ASN:HB2	2.46	0.51
1:D:45:THR:HG23	1:D:45:THR:O	2.11	0.51
1:D:563:ILE:O	1:D:564:ASN:ND2	2.44	0.51
1:E:285:ASP:HA	1:E:331:ASN:OD1	2.11	0.51
1:F:111:VAL:HB	1:F:545:LEU:HD13	1.93	0.51
1:F:285:ASP:O	1:F:286:TYR:C	2.54	0.51
1:F:315:ASP:C	1:F:317:ALA:H	2.18	0.51
1:A:45:THR:O	1:A:45:THR:HG23	2.10	0.51
1:B:37:PHE:C	1:B:38:ASP:CG	2.79	0.51
1:D:553:VAL:HG12	1:D:555:LEU:HD12	1.91	0.51
1:E:79:VAL:CG1	1:E:81:TYR:CE2	2.93	0.51
1:F:572:ILE:O	1:F:572:ILE:CG2	2.54	0.51
1:B:172:GLU:CD	1:B:212:TRP:CZ2	2.88	0.50
1:C:172:GLU:HB3	1:C:212:TRP:CH2	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:233:GLN:O	1:C:236:ILE:HG13	2.11	0.50
1:E:57:VAL:O	1:E:57:VAL:CG1	2.58	0.50
1:E:358:ASN:CG	1:E:358:ASN:O	2.53	0.50
1:F:157:THR:HG22	1:F:488:ILE:HB	1.93	0.50
1:A:546:ARG:NH2	1:B:15:ASN:CG	2.69	0.50
1:B:42:PHE:CE1	1:B:59:ILE:CD1	2.93	0.50
1:D:259:ASN:O	1:D:260:GLY:C	2.55	0.50
1:D:360:VAL:HG13	1:E:163:ILE:HD12	1.93	0.50
1:E:185:PHE:CE2	1:E:259:ASN:HB2	2.46	0.50
1:E:208:TYR:CZ	1:F:463:ILE:HG12	2.45	0.50
1:E:286:TYR:HE1	1:E:301:LYS:HG3	1.75	0.50
1:F:175:LEU:HD11	1:F:177:ILE:HG23	1.93	0.50
1:A:177:ILE:CB	1:A:236:ILE:HA	2.42	0.50
1:B:46:PHE:CE1	1:B:55:LEU:CD1	2.94	0.50
1:C:44:SER:OG	1:C:45:THR:N	2.42	0.50
1:C:371:ASN:C	1:C:371:ASN:OD1	2.55	0.50
1:D:152:VAL:O	1:D:152:VAL:HG13	2.09	0.50
1:D:491:ASP:O	1:D:492:GLU:C	2.54	0.50
1:D:498:LYS:O	1:D:499:TYR:C	2.54	0.50
1:F:502:MET:O	1:F:554:ARG:NH1	2.41	0.50
1:A:12:THR:HG21	1:A:76:TYR:HB2	1.92	0.50
1:A:46:PHE:O	1:A:46:PHE:CD2	2.64	0.50
1:C:360:VAL:HG13	1:D:163:ILE:HD12	1.92	0.50
1:C:553:VAL:HG12	1:C:555:LEU:HD12	1.92	0.50
1:F:46:PHE:CE1	1:F:55:LEU:CD1	2.94	0.50
1:A:259:ASN:O	1:A:260:GLY:C	2.51	0.50
1:B:79:VAL:CG1	1:B:81:TYR:CE2	2.94	0.50
1:C:164:LYS:HB2	1:C:282:ILE:HD12	1.94	0.50
1:C:212:TRP:O	1:C:213:PHE:CD2	2.65	0.50
1:C:229:TYR:N	1:C:229:TYR:CD2	2.79	0.50
1:C:285:ASP:OD2	1:C:285:ASP:C	2.55	0.50
1:D:120:VAL:CG2	1:D:121:LEU:N	2.73	0.50
1:D:491:ASP:O	1:D:494:ASN:N	2.44	0.50
1:F:164:LYS:CB	1:F:282:ILE:HD12	2.42	0.50
1:A:46:PHE:CE1	1:A:55:LEU:CD1	2.94	0.50
1:B:172:GLU:CD	1:B:212:TRP:CH2	2.90	0.50
1:C:212:TRP:CZ3	1:C:247:ILE:HG13	2.47	0.50
1:E:59:ILE:O	1:E:59:ILE:CG2	2.59	0.50
1:A:90:LEU:HA	1:A:109:PRO:HA	1.93	0.50
1:B:175:LEU:HD11	1:B:177:ILE:HG23	1.93	0.50
1:B:306:PRO:HD3	1:B:326:SER:HB3	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:95:ILE:HG12	1:E:105:LEU:HD22	1.94	0.50
1:E:244:SER:O	1:E:245:GLY:C	2.55	0.50
1:E:541:HIS:O	1:E:545:LEU:HB2	2.11	0.50
1:F:470:TYR:HB3	1:F:479:PHE:CD1	2.47	0.50
1:F:559:GLU:O	1:F:560:SER:C	2.55	0.50
1:A:172:GLU:CD	1:A:245:GLY:H	2.20	0.50
1:B:152:VAL:HG22	1:B:153:LEU:N	2.27	0.50
1:E:106:SER:O	1:E:107:LEU:HD12	2.11	0.50
1:F:79:VAL:HG11	1:F:81:TYR:CE2	2.47	0.50
1:F:491:ASP:O	1:F:494:ASN:N	2.44	0.50
1:F:520:MET:HB3	1:F:570:ASN:OD1	2.12	0.50
1:A:226:LEU:HD12	1:A:233:GLN:HB3	1.94	0.50
1:A:559:GLU:O	1:A:560:SER:C	2.55	0.50
1:E:90:LEU:HD22	1:E:107:LEU:HD23	1.94	0.50
1:E:133:HIS:HB3	1:E:520:MET:CE	2.42	0.50
1:F:78:GLN:CG	1:F:79:VAL:N	2.73	0.50
1:A:6:ILE:CG2	1:A:7:LYS:N	2.75	0.49
1:A:324:ASP:C	1:A:324:ASP:OD1	2.54	0.49
1:A:520:MET:HE1	1:A:572:ILE:HG12	1.94	0.49
1:B:360:VAL:CG2	1:B:363:TYR:HB2	2.42	0.49
1:B:498:LYS:O	1:B:499:TYR:C	2.54	0.49
1:C:90:LEU:HD22	1:C:107:LEU:HD23	1.94	0.49
1:C:276:GLN:O	1:C:277:LYS:C	2.53	0.49
1:C:285:ASP:HA	1:C:331:ASN:OD1	2.12	0.49
1:C:358:ASN:O	1:C:358:ASN:CG	2.54	0.49
1:D:157:THR:HG22	1:D:488:ILE:HB	1.94	0.49
1:D:351:LYS:O	1:D:352:ASN:HB2	2.13	0.49
1:E:157:THR:HG22	1:E:488:ILE:HB	1.93	0.49
1:E:286:TYR:C	1:E:286:TYR:CD2	2.89	0.49
1:E:305:ARG:HB2	1:E:306:PRO:CD	2.43	0.49
1:F:172:GLU:CD	1:F:245:GLY:H	2.20	0.49
1:F:185:PHE:CE2	1:F:259:ASN:HB2	2.46	0.49
1:F:202:ASP:OD2	1:F:274:SER:OG	2.30	0.49
1:A:106:SER:C	1:A:107:LEU:HD12	2.36	0.49
1:B:48:TYR:CE1	1:B:55:LEU:HD22	2.48	0.49
1:B:172:GLU:HB3	1:B:212:TRP:CH2	2.47	0.49
1:B:282:ILE:HG23	1:B:334:PHE:CD2	2.47	0.49
1:D:29:ARG:HD2	1:D:30:ASP:OD2	2.11	0.49
1:D:92:VAL:HG23	1:D:92:VAL:O	2.12	0.49
1:E:172:GLU:OE1	1:E:212:TRP:CH2	2.64	0.49
1:F:23:PHE:CD2	1:F:23:PHE:N	2.80	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:351:LYS:HG2	1:F:352:ASN:OD1	2.12	0.49
1:A:165:SER:HA	1:A:282:ILE:HD13	1.94	0.49
1:B:26:ASN:O	1:B:29:ARG:HB3	2.12	0.49
1:B:67:CYS:SG	1:B:68:PHE:N	2.85	0.49
1:C:296:ASN:O	1:C:300:ASP:HB2	2.12	0.49
1:C:306:PRO:HD3	1:C:326:SER:HB3	1.94	0.49
1:C:339:THR:HG21	1:D:472:PRO:HB3	1.93	0.49
1:D:371:ASN:OD1	1:D:371:ASN:C	2.55	0.49
1:E:130:ILE:CG2	1:E:527:GLN:HG2	2.43	0.49
1:E:158:MET:C	1:E:159:ARG:HG2	2.37	0.49
1:E:371:ASN:C	1:E:371:ASN:OD1	2.55	0.49
1:E:532:TRP:HZ2	1:E:546:ARG:HA	1.76	0.49
1:F:152:VAL:HG13	1:F:152:VAL:O	2.11	0.49
1:F:172:GLU:OE1	1:F:212:TRP:CH2	2.64	0.49
1:A:339:THR:HG21	1:B:472:PRO:HB3	1.93	0.49
1:B:202:ASP:OD2	1:B:274:SER:OG	2.30	0.49
1:B:358:ASN:CG	1:B:358:ASN:O	2.55	0.49
1:B:546:ARG:NH2	1:C:15:ASN:CG	2.70	0.49
1:C:6:ILE:HG23	1:C:7:LYS:N	2.27	0.49
1:E:359:ASN:C	1:E:360:VAL:O	2.52	0.49
1:F:285:ASP:OD2	1:F:287:GLN:N	2.45	0.49
1:A:156:SER:O	1:F:148:SER:HB3	2.12	0.49
1:B:542:MET:HB3	1:B:546:ARG:NH1	2.27	0.49
1:A:177:ILE:HG22	1:A:236:ILE:HA	1.94	0.49
1:A:360:VAL:HG23	1:A:363:TYR:HB2	1.94	0.49
1:B:307:ASN:OD1	1:B:307:ASN:N	2.36	0.49
1:C:542:MET:O	1:C:543:ASN:C	2.56	0.49
1:C:566:THR:C	1:C:568:VAL:N	2.68	0.49
1:D:286:TYR:C	1:D:286:TYR:CD2	2.90	0.49
1:E:128:ASN:HB2	1:E:510:TYR:HA	1.94	0.49
1:E:276:GLN:O	1:E:277:LYS:C	2.56	0.49
1:A:75:ASN:HA	1:A:92:VAL:HG22	1.95	0.49
1:B:206:ASN:OD1	1:B:210:MET:HE3	2.12	0.49
1:C:106:SER:O	1:C:107:LEU:HD12	2.13	0.49
1:D:483:LEU:HD12	1:D:484:ARG:N	2.28	0.49
1:E:220:LYS:O	1:E:221:GLU:C	2.54	0.49
1:F:529:LYS:O	1:F:530:GLY:C	2.55	0.49
1:A:10:TYR:HB2	1:A:38:ASP:HB2	1.94	0.49
1:A:144:GLU:OE1	1:A:356:ARG:NH1	2.46	0.49
1:C:23:PHE:CD2	1:C:23:PHE:N	2.80	0.49
1:B:6:ILE:HG23	1:B:7:LYS:N	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:122:ASN:OD1	1:E:517:ILE:HG12	2.13	0.49
1:B:61:LEU:HD12	1:B:61:LEU:N	2.28	0.49
1:B:516:ASP:OD2	1:B:518:THR:HG22	2.13	0.49
1:C:360:VAL:HG23	1:C:363:TYR:HB2	1.95	0.49
1:E:129:VAL:CG2	1:E:130:ILE:N	2.76	0.49
1:A:124:LEU:HD21	1:A:532:TRP:HE3	1.78	0.48
1:A:239:VAL:HG22	1:A:376:ILE:HG13	1.95	0.48
1:A:282:ILE:HD11	1:A:483:LEU:HB3	1.95	0.48
1:B:177:ILE:CG2	1:B:236:ILE:HG12	2.43	0.48
1:B:299:ASN:ND2	1:B:571:VAL:HG22	2.27	0.48
1:B:360:VAL:HG13	1:C:163:ILE:HD12	1.95	0.48
1:E:26:ASN:HB3	1:E:29:ARG:NH2	2.28	0.48
1:F:45:THR:HG23	1:F:45:THR:O	2.12	0.48
1:A:572:ILE:O	1:A:573:ILE:HB	2.12	0.48
1:B:185:PHE:CE2	1:B:259:ASN:HB2	2.48	0.48
1:C:319:ASN:C	1:C:320:ARG:HG2	2.37	0.48
1:D:359:ASN:O	1:D:360:VAL:C	2.56	0.48
1:D:509:ASP:O	1:D:510:TYR:C	2.56	0.48
1:E:470:TYR:CB	1:E:479:PHE:CE1	2.95	0.48
1:F:128:ASN:HB2	1:F:510:TYR:HA	1.94	0.48
1:F:572:ILE:O	1:F:573:ILE:HB	2.12	0.48
1:A:37:PHE:CE1	1:A:40:HIS:O	2.66	0.48
1:A:148:SER:CB	1:B:156:SER:O	2.62	0.48
1:A:305:ARG:HB2	1:A:306:PRO:CD	2.42	0.48
1:A:307:ASN:OD1	1:A:307:ASN:N	2.44	0.48
1:A:351:LYS:O	1:A:352:ASN:HB2	2.13	0.48
1:A:502:MET:O	1:A:554:ARG:NH1	2.41	0.48
1:B:256:GLU:O	1:B:264:SER:HA	2.13	0.48
1:C:133:HIS:HB3	1:C:520:MET:HE3	1.95	0.48
1:C:157:THR:HG22	1:C:488:ILE:HB	1.95	0.48
1:C:177:ILE:HG22	1:C:236:ILE:HA	1.95	0.48
1:C:177:ILE:CG2	1:C:236:ILE:HG12	2.43	0.48
1:D:566:THR:C	1:D:568:VAL:N	2.70	0.48
1:E:463:ILE:O	1:E:463:ILE:HD13	2.13	0.48
1:F:120:VAL:CG2	1:F:121:LEU:N	2.76	0.48
1:A:121:LEU:O	1:A:124:LEU:HD12	2.13	0.48
1:A:470:TYR:CG	1:A:479:PHE:HE1	2.30	0.48
1:C:12:THR:HG21	1:C:76:TYR:HB2	1.95	0.48
1:E:164:LYS:CB	1:E:282:ILE:HD12	2.43	0.48
1:E:544:MET:O	1:E:548:LEU:HB2	2.13	0.48
1:F:553:VAL:HG12	1:F:555:LEU:HD12	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:129:VAL:CG2	1:B:130:ILE:N	2.77	0.48
1:B:133:HIS:HB3	1:B:520:MET:HE2	1.94	0.48
1:B:285:ASP:OD2	1:B:285:ASP:C	2.56	0.48
1:B:542:MET:HE2	1:B:545:LEU:HD23	1.95	0.48
1:C:8:LEU:CD2	1:C:77:CYS:HB2	2.44	0.48
1:C:90:LEU:HA	1:C:109:PRO:HA	1.95	0.48
1:E:23:PHE:N	1:E:23:PHE:CD2	2.80	0.48
1:E:217:GLU:O	1:E:218:SER:C	2.54	0.48
1:E:339:THR:HG21	1:F:472:PRO:HB3	1.93	0.48
1:E:537:VAL:O	1:E:538:ASP:C	2.55	0.48
1:F:463:ILE:O	1:F:463:ILE:HD12	2.14	0.48
1:A:516:ASP:OD2	1:A:518:THR:HG22	2.14	0.48
1:B:177:ILE:HD13	1:B:177:ILE:O	2.13	0.48
1:B:282:ILE:HD11	1:B:483:LEU:HB3	1.95	0.48
1:D:212:TRP:O	1:D:213:PHE:CD2	2.66	0.48
1:D:363:TYR:HD2	1:E:316:TYR:CE1	2.30	0.48
1:E:48:TYR:OH	1:E:109:PRO:HG3	2.14	0.48
1:F:26:ASN:HB3	1:F:29:ARG:CZ	2.42	0.48
1:A:42:PHE:CE2	1:A:44:SER:HB2	2.49	0.48
1:A:61:LEU:N	1:A:61:LEU:HD12	2.29	0.48
1:C:511:SER:O	1:C:511:SER:OG	2.30	0.48
1:E:380:VAL:O	1:E:462:ALA:N	2.47	0.48
1:E:516:ASP:OD2	1:E:518:THR:HG22	2.14	0.48
1:E:554:ARG:HG2	1:E:556:TRP:NE1	2.28	0.48
1:F:282:ILE:HD12	1:F:282:ILE:HA	1.71	0.48
1:F:512:THR:HG23	1:F:513:LYS:N	2.29	0.48
1:B:55:LEU:N	1:B:55:LEU:HD23	2.29	0.48
1:B:285:ASP:OD2	1:B:287:GLN:N	2.46	0.48
1:C:470:TYR:HB3	1:C:479:PHE:CD1	2.49	0.48
1:D:115:TYR:CE1	1:D:537:VAL:HG13	2.49	0.48
1:D:291:PHE:C	1:D:291:PHE:CD2	2.91	0.48
1:E:175:LEU:HD11	1:E:177:ILE:HG23	1.95	0.48
1:E:560:SER:O	1:E:564:ASN:ND2	2.44	0.48
1:F:78:GLN:HG2	1:F:79:VAL:H	1.79	0.48
1:F:92:VAL:O	1:F:92:VAL:CG2	2.59	0.48
1:F:95:ILE:HG12	1:F:105:LEU:HD22	1.96	0.48
1:A:3:LEU:HD11	1:B:68:PHE:CZ	2.49	0.48
1:A:212:TRP:CZ3	1:A:247:ILE:HG13	2.49	0.48
1:B:172:GLU:OE2	1:B:245:GLY:N	2.45	0.48
1:B:511:SER:O	1:B:511:SER:OG	2.28	0.48
1:E:12:THR:HG21	1:E:76:TYR:HB2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:498:LYS:O	1:F:499:TYR:C	2.55	0.48
1:B:212:TRP:HA	1:B:212:TRP:CE3	2.49	0.48
1:B:296:ASN:O	1:B:300:ASP:HB2	2.14	0.48
1:C:258:VAL:HG12	1:C:263:LEU:O	2.12	0.48
1:D:285:ASP:OD2	1:D:287:GLN:N	2.46	0.48
1:D:516:ASP:CG	1:D:518:THR:HG22	2.38	0.48
1:E:249:GLN:OE1	1:E:249:GLN:HA	2.13	0.48
1:F:177:ILE:HG22	1:F:236:ILE:HA	1.96	0.48
1:B:172:GLU:OE1	1:B:212:TRP:CH2	2.65	0.47
1:B:566:THR:C	1:B:568:VAL:N	2.67	0.47
1:D:172:GLU:OE1	1:D:212:TRP:CH2	2.65	0.47
1:D:220:LYS:O	1:D:221:GLU:C	2.57	0.47
1:E:45:THR:HG23	1:E:45:THR:O	2.13	0.47
1:E:212:TRP:O	1:E:213:PHE:CD2	2.67	0.47
1:F:258:VAL:HG22	1:F:259:ASN:N	2.28	0.47
1:A:496:VAL:O	1:A:497:LYS:C	2.56	0.47
1:B:463:ILE:O	1:B:463:ILE:HD12	2.15	0.47
1:C:157:THR:HG23	1:C:489:SER:H	1.79	0.47
1:C:290:MET:HE3	1:C:295:LEU:HB2	1.94	0.47
1:D:48:TYR:OH	1:D:109:PRO:HG3	2.13	0.47
1:A:291:PHE:C	1:A:291:PHE:CD2	2.92	0.47
1:A:371:ASN:OD1	1:A:371:ASN:C	2.54	0.47
1:D:29:ARG:HD3	1:D:89:TYR:CE2	2.49	0.47
1:D:258:VAL:HG22	1:D:259:ASN:N	2.30	0.47
1:D:516:ASP:OD1	1:D:518:THR:HG22	2.14	0.47
1:D:549:PHE:O	1:D:552:GLY:N	2.47	0.47
1:A:380:VAL:O	1:A:462:ALA:N	2.47	0.47
1:B:210:MET:HE2	1:B:210:MET:HB3	1.78	0.47
1:B:305:ARG:HB2	1:B:306:PRO:HD2	1.95	0.47
1:B:470:TYR:CB	1:B:479:PHE:CE1	2.98	0.47
1:C:463:ILE:O	1:C:463:ILE:HD13	2.13	0.47
1:C:571:VAL:HG13	1:C:572:ILE:N	2.30	0.47
1:D:177:ILE:HD13	1:D:177:ILE:O	2.14	0.47
1:D:470:TYR:HB3	1:D:479:PHE:CD1	2.50	0.47
1:E:61:LEU:CD2	1:E:67:CYS:SG	3.02	0.47
1:E:463:ILE:O	1:E:463:ILE:HD12	2.14	0.47
1:E:470:TYR:CG	1:E:479:PHE:HE1	2.28	0.47
1:F:177:ILE:CB	1:F:236:ILE:HA	2.44	0.47
1:F:286:TYR:C	1:F:286:TYR:CD2	2.92	0.47
1:F:353:TYR:O	1:F:354:ASN:HB3	2.15	0.47
1:B:3:LEU:CB	1:B:45:THR:HB	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3:LEU:HB3	1:B:45:THR:HB	1.96	0.47
1:B:572:ILE:O	1:B:573:ILE:HB	2.14	0.47
1:D:129:VAL:CG2	1:D:130:ILE:N	2.78	0.47
1:D:233:GLN:HG3	1:D:380:VAL:HG22	1.97	0.47
1:B:177:ILE:HG21	1:B:236:ILE:HG12	1.96	0.47
1:D:37:PHE:HZ	1:D:40:HIS:O	1.94	0.47
1:F:8:LEU:CD2	1:F:77:CYS:HB2	2.45	0.47
1:A:157:THR:HB	1:A:492:GLU:OE1	2.14	0.47
1:B:189:GLU:CD	1:B:189:GLU:N	2.73	0.47
1:B:274:SER:HB2	1:B:338:VAL:CG2	2.45	0.47
1:B:335:ASP:OD2	1:B:351:LYS:HD2	2.15	0.47
1:C:10:TYR:HB2	1:C:38:ASP:HB2	1.96	0.47
1:C:48:TYR:CE1	1:C:55:LEU:HD22	2.49	0.47
1:D:124:LEU:HD21	1:D:532:TRP:HE3	1.80	0.47
1:D:133:HIS:HB3	1:D:520:MET:HE2	1.96	0.47
1:D:155:THR:HG21	1:D:307:ASN:O	2.15	0.47
1:D:177:ILE:CB	1:D:236:ILE:HA	2.45	0.47
1:E:42:PHE:CE2	1:E:44:SER:HB2	2.49	0.47
1:E:48:TYR:CE1	1:E:55:LEU:HD22	2.50	0.47
1:E:357:GLY:HA2	1:E:358:ASN:HA	1.69	0.47
1:F:212:TRP:O	1:F:213:PHE:CD2	2.67	0.47
1:A:173:TYR:CD2	1:A:173:TYR:N	2.83	0.47
1:A:175:LEU:HD13	1:A:177:ILE:HG23	1.96	0.47
1:B:128:ASN:HB2	1:B:510:TYR:HA	1.97	0.47
1:B:470:TYR:CG	1:B:479:PHE:HE1	2.33	0.47
1:C:26:ASN:O	1:C:29:ARG:HB3	2.13	0.47
1:C:172:GLU:OE1	1:C:212:TRP:CH2	2.63	0.47
1:C:491:ASP:O	1:C:492:GLU:C	2.58	0.47
1:C:563:ILE:O	1:C:564:ASN:ND2	2.48	0.47
1:D:286:TYR:CE1	1:D:301:LYS:HE3	2.50	0.47
1:E:212:TRP:O	1:E:213:PHE:CG	2.68	0.47
1:E:572:ILE:O	1:E:572:ILE:CG2	2.51	0.47
1:F:516:ASP:OD1	1:F:518:THR:HG22	2.14	0.47
1:A:254:ASP:O	1:A:255:HIS:C	2.57	0.47
1:B:177:ILE:HG22	1:B:236:ILE:HA	1.96	0.47
1:B:177:ILE:CB	1:B:236:ILE:HA	2.45	0.47
1:B:244:SER:O	1:B:245:GLY:C	2.58	0.47
1:C:155:THR:HG21	1:C:307:ASN:O	2.15	0.47
1:E:21:LEU:HD12	1:E:556:TRP:O	2.15	0.47
1:E:537:VAL:O	1:E:539:THR:N	2.48	0.47
1:A:23:PHE:N	1:A:23:PHE:CD2	2.82	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:212:TRP:O	1:B:213:PHE:CD2	2.68	0.47
1:D:359:ASN:C	1:D:360:VAL:O	2.58	0.47
1:E:177:ILE:HD13	1:E:177:ILE:O	2.15	0.47
1:F:75:ASN:OD1	1:F:75:ASN:N	2.45	0.47
1:A:164:LYS:CB	1:A:282:ILE:HD12	2.45	0.46
1:A:487:ARG:HG2	1:A:488:ILE:N	2.30	0.46
1:B:120:VAL:CG2	1:B:121:LEU:N	2.77	0.46
1:C:282:ILE:HD11	1:C:483:LEU:HB3	1.95	0.46
1:D:185:PHE:CE2	1:D:259:ASN:HB2	2.49	0.46
1:E:37:PHE:CE1	1:E:40:HIS:O	2.68	0.46
1:F:48:TYR:CE1	1:F:55:LEU:HD22	2.50	0.46
1:A:12:THR:HG22	1:A:75:ASN:OD1	2.15	0.46
1:A:37:PHE:C	1:A:38:ASP:CG	2.83	0.46
1:C:37:PHE:HZ	1:C:40:HIS:O	1.96	0.46
1:C:359:ASN:O	1:C:360:VAL:C	2.55	0.46
1:D:571:VAL:HG13	1:D:572:ILE:N	2.31	0.46
1:D:572:ILE:O	1:D:573:ILE:HB	2.14	0.46
1:E:106:SER:C	1:E:107:LEU:HD12	2.41	0.46
1:E:311:ALA:HB2	1:E:325:LEU:HD22	1.97	0.46
1:A:120:VAL:CG2	1:A:121:LEU:N	2.77	0.46
1:C:323:ILE:HG23	1:C:353:TYR:CE1	2.49	0.46
1:D:12:THR:HG21	1:D:76:TYR:CB	2.45	0.46
1:D:210:MET:HE2	1:D:210:MET:HB3	1.80	0.46
1:D:463:ILE:O	1:D:463:ILE:HD12	2.14	0.46
1:D:529:LYS:O	1:D:530:GLY:O	2.33	0.46
1:F:155:THR:HG21	1:F:307:ASN:O	2.15	0.46
1:A:29:ARG:HD2	1:A:30:ASP:OD2	2.16	0.46
1:A:68:PHE:CE2	1:F:3:LEU:HD21	2.51	0.46
1:A:285:ASP:HA	1:A:331:ASN:OD1	2.15	0.46
1:B:516:ASP:OD2	1:B:517:ILE:N	2.47	0.46
1:D:75:ASN:HA	1:D:92:VAL:HG22	1.98	0.46
1:E:10:TYR:HB2	1:E:38:ASP:HB2	1.97	0.46
1:A:152:VAL:HG22	1:A:153:LEU:N	2.31	0.46
1:A:563:ILE:C	1:A:564:ASN:ND2	2.74	0.46
1:B:164:LYS:O	1:B:282:ILE:CD1	2.59	0.46
1:C:26:ASN:HB3	1:C:29:ARG:CZ	2.45	0.46
1:D:541:HIS:O	1:D:545:LEU:HB2	2.16	0.46
1:E:120:VAL:CG2	1:E:121:LEU:N	2.78	0.46
1:E:177:ILE:HG22	1:E:236:ILE:HA	1.96	0.46
1:E:566:THR:C	1:E:568:VAL:N	2.70	0.46
1:F:371:ASN:OD1	1:F:371:ASN:C	2.57	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:152:VAL:HG21	1:B:307:ASN:HD21	1.81	0.46
1:E:212:TRP:HA	1:E:212:TRP:CE3	2.50	0.46
1:F:10:TYR:HB2	1:F:38:ASP:HB2	1.97	0.46
1:A:95:ILE:HG12	1:A:105:LEU:HD22	1.98	0.46
1:A:177:ILE:HB	1:A:236:ILE:HA	1.97	0.46
1:A:463:ILE:O	1:A:463:ILE:HD13	2.15	0.46
1:C:79:VAL:CG1	1:C:81:TYR:CE2	2.99	0.46
1:F:38:ASP:O	1:F:39:VAL:HG23	2.16	0.46
1:B:165:SER:HA	1:B:282:ILE:HD13	1.98	0.46
1:B:212:TRP:CZ3	1:B:247:ILE:HG13	2.51	0.46
1:C:37:PHE:C	1:C:38:ASP:CG	2.83	0.46
1:C:57:VAL:O	1:C:57:VAL:CG1	2.63	0.46
1:C:177:ILE:CB	1:C:236:ILE:HA	2.45	0.46
1:D:217:GLU:O	1:D:220:LYS:N	2.49	0.46
1:D:249:GLN:HA	1:D:249:GLN:OE1	2.16	0.46
1:D:307:ASN:OD1	1:D:307:ASN:N	2.45	0.46
1:E:310:THR:HG22	1:E:486:GLY:HA3	1.98	0.46
1:F:177:ILE:HB	1:F:236:ILE:HA	1.97	0.46
1:A:158:MET:C	1:A:159:ARG:HG2	2.41	0.46
1:B:276:GLN:O	1:B:277:LYS:O	2.33	0.46
1:B:291:PHE:C	1:B:291:PHE:HD2	2.24	0.46
1:C:177:ILE:HD13	1:C:177:ILE:C	2.41	0.46
1:C:380:VAL:O	1:C:462:ALA:N	2.48	0.46
1:D:233:GLN:HG3	1:D:380:VAL:CG2	2.46	0.46
1:D:548:LEU:HD23	1:D:548:LEU:HA	1.84	0.46
1:E:152:VAL:HG21	1:E:307:ASN:HD21	1.81	0.46
1:E:571:VAL:HG13	1:E:572:ILE:N	2.31	0.46
1:F:48:TYR:OH	1:F:109:PRO:HG3	2.16	0.46
1:F:276:GLN:O	1:F:277:LYS:C	2.59	0.46
1:B:351:LYS:O	1:B:352:ASN:HB2	2.14	0.46
1:B:542:MET:HE1	1:B:545:LEU:HD23	1.97	0.46
1:D:42:PHE:CE2	1:D:44:SER:HB2	2.51	0.46
1:D:324:ASP:C	1:D:324:ASP:OD1	2.59	0.46
1:E:306:PRO:HD3	1:E:326:SER:HB3	1.98	0.46
1:A:463:ILE:O	1:A:463:ILE:HD12	2.15	0.45
1:A:563:ILE:N	1:A:563:ILE:CD1	2.78	0.45
1:B:549:PHE:O	1:B:552:GLY:N	2.49	0.45
1:C:189:GLU:N	1:C:189:GLU:CD	2.74	0.45
1:C:220:LYS:O	1:C:221:GLU:C	2.59	0.45
1:C:541:HIS:O	1:C:545:LEU:HB2	2.17	0.45
1:D:37:PHE:C	1:D:38:ASP:CG	2.85	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:157:THR:HB	1:D:492:GLU:OE1	2.17	0.45
1:D:299:ASN:ND2	1:D:299:ASN:H	2.15	0.45
1:E:224:ASP:C	1:E:226:LEU:N	2.73	0.45
1:F:6:ILE:HG23	1:F:7:LYS:N	2.31	0.45
1:F:25:SER:OG	1:F:28:GLU:HG3	2.16	0.45
1:F:380:VAL:O	1:F:462:ALA:N	2.49	0.45
1:A:148:SER:HB3	1:B:156:SER:O	2.16	0.45
1:B:165:SER:CA	1:B:282:ILE:HD13	2.46	0.45
1:C:95:ILE:HG12	1:C:105:LEU:HD22	1.99	0.45
1:C:120:VAL:CG2	1:C:121:LEU:N	2.79	0.45
1:E:8:LEU:CD2	1:E:77:CYS:HB2	2.46	0.45
1:E:92:VAL:HG23	1:E:92:VAL:O	2.16	0.45
1:E:302:HIS:CD2	1:E:303:LEU:HD13	2.51	0.45
1:F:82:ILE:HA	1:F:83:GLN:HA	1.74	0.45
1:A:38:ASP:O	1:A:39:VAL:HG23	2.16	0.45
1:A:42:PHE:CE1	1:A:59:ILE:CD1	2.99	0.45
1:B:371:ASN:OD1	1:B:371:ASN:C	2.59	0.45
1:B:538:ASP:O	1:B:541:HIS:N	2.40	0.45
1:B:545:LEU:O	1:B:546:ARG:C	2.57	0.45
1:D:177:ILE:HB	1:D:236:ILE:HA	1.98	0.45
1:D:212:TRP:CZ3	1:D:247:ILE:HG13	2.51	0.45
1:D:511:SER:O	1:D:511:SER:OG	2.28	0.45
1:E:129:VAL:HG23	1:E:130:ILE:H	1.81	0.45
1:E:177:ILE:CG2	1:E:236:ILE:HG12	2.46	0.45
1:E:210:MET:HE2	1:E:210:MET:HB3	1.81	0.45
1:E:217:GLU:O	1:E:220:LYS:N	2.49	0.45
1:E:563:ILE:C	1:E:564:ASN:ND2	2.74	0.45
1:B:189:GLU:CD	1:B:189:GLU:H	2.24	0.45
1:C:177:ILE:HG21	1:C:236:ILE:HG12	1.98	0.45
1:C:351:LYS:O	1:C:352:ASN:HB2	2.17	0.45
1:D:122:ASN:OD1	1:D:517:ILE:HG12	2.16	0.45
1:F:516:ASP:OD2	1:F:517:ILE:N	2.49	0.45
1:F:571:VAL:HG13	1:F:572:ILE:N	2.30	0.45
1:A:79:VAL:CG1	1:A:81:TYR:CE2	3.00	0.45
1:A:128:ASN:C	1:A:128:ASN:HD22	2.25	0.45
1:A:139:TYR:O	1:A:140:GLU:C	2.59	0.45
1:B:8:LEU:CD2	1:B:77:CYS:HB2	2.46	0.45
1:C:286:TYR:CE1	1:C:301:LYS:HE3	2.51	0.45
1:C:305:ARG:HB2	1:C:306:PRO:CD	2.46	0.45
1:E:38:ASP:O	1:E:39:VAL:HG23	2.16	0.45
1:F:59:ILE:O	1:F:59:ILE:CG2	2.64	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:106:SER:C	1:F:107:LEU:HD12	2.42	0.45
1:A:220:LYS:O	1:A:221:GLU:C	2.57	0.45
1:B:217:GLU:O	1:B:218:SER:C	2.60	0.45
1:C:175:LEU:HD23	1:C:239:VAL:HB	1.99	0.45
1:C:282:ILE:HD12	1:C:282:ILE:HA	1.75	0.45
1:F:26:ASN:HB3	1:F:29:ARG:NH2	2.31	0.45
1:F:463:ILE:O	1:F:463:ILE:HD13	2.16	0.45
1:A:174:ILE:CG1	1:A:176:THR:HG22	2.44	0.45
1:B:46:PHE:HB3	1:B:57:VAL:HG23	1.98	0.45
1:B:525:TRP:CZ3	1:B:554:ARG:NH1	2.84	0.45
1:C:75:ASN:HA	1:C:92:VAL:HG22	1.99	0.45
1:C:75:ASN:OD1	1:C:75:ASN:N	2.50	0.45
1:C:129:VAL:CG2	1:C:130:ILE:N	2.79	0.45
1:C:212:TRP:HA	1:C:212:TRP:CE3	2.51	0.45
1:C:560:SER:O	1:C:564:ASN:ND2	2.43	0.45
1:D:305:ARG:HB2	1:D:306:PRO:CD	2.47	0.45
1:D:496:VAL:O	1:D:497:LYS:C	2.59	0.45
1:A:48:TYR:CE1	1:A:55:LEU:HD22	2.51	0.45
1:A:175:LEU:HD11	1:A:177:ILE:HG23	1.99	0.45
1:A:306:PRO:HD3	1:A:326:SER:HB3	1.98	0.45
1:B:95:ILE:HG12	1:B:105:LEU:HD22	1.97	0.45
1:C:82:ILE:HA	1:C:83:GLN:HA	1.70	0.45
1:C:483:LEU:HD12	1:C:484:ARG:N	2.32	0.45
1:C:572:ILE:O	1:C:573:ILE:C	2.58	0.45
1:E:212:TRP:CZ3	1:E:247:ILE:HG13	2.52	0.45
1:E:351:LYS:HG2	1:E:352:ASN:OD1	2.17	0.45
1:F:3:LEU:O	1:F:82:ILE:HG13	2.17	0.45
1:F:23:PHE:HD2	1:F:117:GLN:OE1	2.00	0.45
1:A:155:THR:HG21	1:A:307:ASN:O	2.16	0.45
1:A:285:ASP:CG	1:A:288:SER:HG	2.21	0.45
1:B:129:VAL:HG23	1:B:130:ILE:H	1.82	0.45
1:B:206:ASN:OD1	1:B:210:MET:CE	2.65	0.45
1:C:71:LEU:HD12	1:C:71:LEU:O	2.16	0.45
1:C:531:ILE:HD12	1:C:531:ILE:HA	1.87	0.45
1:D:148:SER:HB2	1:E:156:SER:O	2.16	0.45
1:D:561:ASP:C	1:D:563:ILE:N	2.74	0.45
1:E:41:GLU:O	1:E:41:GLU:HG2	2.15	0.45
1:E:282:ILE:HD11	1:E:483:LEU:HB3	1.99	0.45
1:A:156:SER:O	1:F:148:SER:HB2	2.17	0.45
1:B:124:LEU:HD21	1:B:532:TRP:HE3	1.81	0.45
1:B:157:THR:HB	1:B:492:GLU:OE1	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:544:MET:O	1:B:548:LEU:HB2	2.17	0.45
1:D:182:ARG:NH2	1:D:267:LYS:HE2	2.32	0.45
1:D:212:TRP:O	1:D:213:PHE:CG	2.70	0.45
1:E:274:SER:HB2	1:E:338:VAL:CG2	2.47	0.45
1:A:189:GLU:N	1:A:189:GLU:CD	2.75	0.44
1:D:133:HIS:CD2	1:D:525:TRP:H	2.36	0.44
1:D:202:ASP:OD2	1:D:274:SER:OG	2.35	0.44
1:E:572:ILE:O	1:E:573:ILE:HB	2.17	0.44
1:F:124:LEU:CD2	1:F:532:TRP:HB2	2.45	0.44
1:F:531:ILE:HD12	1:F:531:ILE:HA	1.78	0.44
1:F:545:LEU:O	1:F:546:ARG:C	2.60	0.44
1:A:96:GLN:OE1	1:F:49:ARG:HA	2.18	0.44
1:B:122:ASN:OD1	1:B:517:ILE:HG12	2.17	0.44
1:B:525:TRP:CE3	1:B:554:ARG:NH1	2.85	0.44
1:C:190:LYS:O	1:C:190:LYS:CG	2.62	0.44
1:D:128:ASN:HB2	1:D:510:TYR:HA	1.99	0.44
1:F:115:TYR:CE1	1:F:537:VAL:HG13	2.52	0.44
1:F:164:LYS:HB2	1:F:282:ILE:HD12	1.99	0.44
1:F:360:VAL:HG23	1:F:363:TYR:HB2	2.00	0.44
1:A:152:VAL:HG21	1:A:307:ASN:HD21	1.81	0.44
1:A:177:ILE:HD13	1:A:177:ILE:H	1.82	0.44
1:A:293:LEU:HD22	1:A:309:VAL:HG11	2.00	0.44
1:A:347:LYS:HE2	1:A:369:THR:CG2	2.47	0.44
1:A:566:THR:O	1:A:568:VAL:N	2.49	0.44
1:B:65:ARG:HG2	1:B:66:SER:N	2.32	0.44
1:B:164:LYS:HB2	1:B:282:ILE:HD12	2.00	0.44
1:C:8:LEU:HD22	1:C:77:CYS:HB2	1.98	0.44
1:C:166:GLU:OE1	1:C:279:PHE:HA	2.17	0.44
1:C:529:LYS:O	1:C:530:GLY:O	2.35	0.44
1:C:572:ILE:O	1:C:573:ILE:HB	2.18	0.44
1:D:82:ILE:HA	1:D:83:GLN:HA	1.75	0.44
1:E:360:VAL:HG23	1:E:363:TYR:HB2	1.97	0.44
1:F:509:ASP:O	1:F:510:TYR:C	2.59	0.44
1:B:302:HIS:CD2	1:B:303:LEU:HD13	2.52	0.44
1:B:516:ASP:CG	1:B:518:THR:HG22	2.42	0.44
1:C:274:SER:HB2	1:C:338:VAL:CG2	2.48	0.44
1:D:157:THR:HG23	1:D:489:SER:H	1.81	0.44
1:E:61:LEU:HD12	1:E:61:LEU:N	2.33	0.44
1:E:65:ARG:HG2	1:E:66:SER:N	2.32	0.44
1:E:75:ASN:OD1	1:E:75:ASN:N	2.48	0.44
1:F:81:TYR:HE1	1:F:86:ARG:NH2	2.15	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:127:VAL:CG2	1:F:528:PHE:CD1	2.99	0.44
1:F:572:ILE:O	1:F:573:ILE:C	2.59	0.44
1:B:23:PHE:HD2	1:B:117:GLN:OE1	2.01	0.44
1:C:38:ASP:O	1:C:39:VAL:HG23	2.17	0.44
1:C:172:GLU:OE2	1:C:245:GLY:N	2.47	0.44
1:C:210:MET:HE2	1:C:210:MET:HB3	1.85	0.44
1:C:217:GLU:O	1:C:218:SER:C	2.60	0.44
1:D:177:ILE:HG22	1:D:236:ILE:HA	1.98	0.44
1:D:502:MET:O	1:D:554:ARG:NH1	2.45	0.44
1:A:212:TRP:CE3	1:A:212:TRP:HA	2.53	0.44
1:B:177:ILE:HB	1:B:236:ILE:HA	2.00	0.44
1:B:510:TYR:HB3	1:C:502:MET:HE2	2.00	0.44
1:C:189:GLU:CD	1:C:189:GLU:H	2.26	0.44
1:C:502:MET:O	1:C:554:ARG:NH1	2.44	0.44
1:D:79:VAL:CG1	1:D:81:TYR:CE2	3.00	0.44
1:D:532:TRP:CZ2	1:D:546:ARG:HA	2.53	0.44
1:F:563:ILE:C	1:F:564:ASN:ND2	2.76	0.44
1:B:41:GLU:O	1:B:41:GLU:HG2	2.16	0.44
1:C:124:LEU:HD21	1:C:532:TRP:HE3	1.82	0.44
1:C:152:VAL:HG22	1:C:153:LEU:N	2.33	0.44
1:D:38:ASP:O	1:D:39:VAL:HG23	2.17	0.44
1:E:133:HIS:CD2	1:E:525:TRP:H	2.36	0.44
1:F:175:LEU:HD13	1:F:177:ILE:HG23	2.00	0.44
1:F:313:LEU:HD23	1:F:313:LEU:HA	1.79	0.44
1:A:75:ASN:OD1	1:A:75:ASN:N	2.50	0.44
1:A:82:ILE:HA	1:A:83:GLN:HA	1.70	0.44
1:A:516:ASP:OD2	1:A:517:ILE:N	2.50	0.44
1:A:560:SER:O	1:A:564:ASN:ND2	2.44	0.44
1:B:487:ARG:HG2	1:B:488:ILE:N	2.33	0.44
1:B:494:ASN:O	1:B:495:ASN:C	2.61	0.44
1:C:164:LYS:O	1:C:282:ILE:CD1	2.60	0.44
1:C:537:VAL:O	1:C:538:ASP:C	2.60	0.44
1:F:106:SER:O	1:F:107:LEU:HD12	2.17	0.44
1:F:520:MET:HE1	1:F:572:ILE:HG12	2.00	0.44
1:A:164:LYS:HB2	1:A:282:ILE:HD12	1.99	0.44
1:A:285:ASP:OD2	1:A:287:GLN:N	2.50	0.44
1:A:299:ASN:ND2	1:A:299:ASN:N	2.65	0.44
1:B:38:ASP:O	1:B:39:VAL:HG23	2.18	0.44
1:C:491:ASP:O	1:C:494:ASN:N	2.51	0.44
1:C:520:MET:SD	1:C:572:ILE:HG12	2.58	0.44
1:D:563:ILE:C	1:D:564:ASN:ND2	2.75	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:177:ILE:HG21	1:E:236:ILE:HG12	1.99	0.44
1:F:152:VAL:HG22	1:F:153:LEU:N	2.32	0.44
1:F:279:PHE:HB3	1:F:282:ILE:HG22	2.00	0.44
1:A:502:MET:HE2	1:F:510:TYR:HB3	2.00	0.43
1:A:545:LEU:O	1:A:546:ARG:C	2.59	0.43
1:C:533:THR:HG23	1:D:15:ASN:ND2	2.33	0.43
1:D:37:PHE:CE1	1:D:40:HIS:O	2.71	0.43
1:E:516:ASP:CG	1:E:518:THR:HG22	2.43	0.43
1:F:42:PHE:CE2	1:F:44:SER:HB2	2.53	0.43
1:C:133:HIS:HB3	1:C:520:MET:HE2	2.00	0.43
1:C:165:SER:HA	1:C:282:ILE:HD13	1.99	0.43
1:C:244:SER:O	1:C:245:GLY:C	2.59	0.43
1:C:516:ASP:OD2	1:C:518:THR:HG22	2.18	0.43
1:D:6:ILE:CG2	1:D:7:LYS:N	2.80	0.43
1:D:48:TYR:CE1	1:D:55:LEU:HD22	2.53	0.43
1:D:561:ASP:O	1:D:562:MET:C	2.60	0.43
1:E:226:LEU:HD12	1:E:233:GLN:HB3	2.00	0.43
1:E:285:ASP:O	1:E:286:TYR:C	2.59	0.43
1:F:5:LYS:HB3	1:F:80:GLN:HG3	2.00	0.43
1:A:68:PHE:CZ	1:F:3:LEU:HD11	2.53	0.43
1:B:172:GLU:CD	1:B:245:GLY:H	2.25	0.43
1:B:515:SER:O	1:B:516:ASP:C	2.61	0.43
1:C:509:ASP:O	1:C:510:TYR:C	2.61	0.43
1:E:175:LEU:HA	1:E:239:VAL:HB	2.00	0.43
1:A:470:TYR:O	1:A:471:ALA:C	2.60	0.43
1:B:177:ILE:HD13	1:B:177:ILE:C	2.42	0.43
1:B:258:VAL:HG22	1:B:259:ASN:N	2.33	0.43
1:C:516:ASP:CG	1:C:518:THR:HG22	2.43	0.43
1:D:57:VAL:O	1:D:57:VAL:HG12	2.18	0.43
1:D:124:LEU:CD2	1:D:532:TRP:HB2	2.46	0.43
1:D:347:LYS:HE2	1:D:369:THR:HG22	1.99	0.43
1:E:165:SER:CA	1:E:282:ILE:HD13	2.48	0.43
1:E:542:MET:HE1	1:E:545:LEU:HD23	1.99	0.43
1:E:573:ILE:HD13	1:E:573:ILE:N	2.33	0.43
1:F:363:TYR:CD1	1:F:364:ILE:HG23	2.53	0.43
1:F:514:LEU:HD12	1:F:514:LEU:HA	1.78	0.43
1:A:189:GLU:CD	1:A:189:GLU:H	2.27	0.43
1:A:321:LEU:HA	1:A:321:LEU:HD12	1.77	0.43
1:B:282:ILE:HD12	1:B:282:ILE:HA	1.79	0.43
1:B:299:ASN:OD1	1:B:299:ASN:N	2.48	0.43
1:D:12:THR:HG22	1:D:75:ASN:OD1	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:110:ASP:OD1	1:D:113:MET:HB2	2.18	0.43
1:D:503:PHE:O	1:D:504:GLY:C	2.61	0.43
1:D:545:LEU:O	1:D:546:ARG:C	2.61	0.43
1:E:75:ASN:CA	1:E:92:VAL:HG22	2.48	0.43
1:F:21:LEU:HG	1:F:22:HIS:N	2.34	0.43
1:F:210:MET:HE2	1:F:210:MET:HB3	1.86	0.43
1:F:249:GLN:OE1	1:F:249:GLN:HA	2.19	0.43
1:A:215:ASP:OD1	1:A:217:GLU:N	2.51	0.43
1:C:212:TRP:O	1:C:213:PHE:CG	2.71	0.43
1:C:357:GLY:HA2	1:C:358:ASN:HA	1.68	0.43
1:C:471:ALA:O	1:C:472:PRO:C	2.62	0.43
1:C:516:ASP:OD2	1:C:516:ASP:C	2.62	0.43
1:D:360:VAL:HG23	1:D:363:TYR:HB2	2.00	0.43
1:D:520:MET:HB3	1:D:570:ASN:OD1	2.19	0.43
1:D:542:MET:HE1	1:D:545:LEU:HD23	2.00	0.43
1:E:12:THR:HG21	1:E:76:TYR:CB	2.47	0.43
1:E:115:TYR:CE1	1:E:537:VAL:HG13	2.53	0.43
1:E:124:LEU:HD21	1:E:532:TRP:HE3	1.83	0.43
1:E:169:THR:HG23	1:E:170:GLN:HG3	2.00	0.43
1:E:512:THR:HG23	1:E:513:LYS:N	2.34	0.43
1:F:122:ASN:OD1	1:F:517:ILE:HG12	2.18	0.43
1:B:3:LEU:HB3	1:B:45:THR:CB	2.48	0.43
1:B:520:MET:HB3	1:B:570:ASN:OD1	2.18	0.43
1:C:348:VAL:CG2	1:C:349:TYR:N	2.77	0.43
1:D:23:PHE:CD2	1:D:23:PHE:N	2.86	0.43
1:D:59:ILE:O	1:D:59:ILE:CG2	2.66	0.43
1:D:189:GLU:CD	1:D:189:GLU:N	2.77	0.43
1:D:329:GLU:CD	1:D:357:GLY:H	2.27	0.43
1:E:152:VAL:O	1:E:152:VAL:HG13	2.16	0.43
1:F:55:LEU:N	1:F:55:LEU:HD23	2.33	0.43
1:A:27:GLU:HG2	1:A:28:GLU:N	2.34	0.43
1:C:152:VAL:O	1:C:152:VAL:HG13	2.19	0.43
1:D:129:VAL:HG23	1:D:130:ILE:H	1.84	0.43
1:D:177:ILE:HD13	1:D:177:ILE:C	2.43	0.43
1:D:310:THR:HG22	1:D:486:GLY:HA3	2.01	0.43
1:E:293:LEU:HD22	1:E:309:VAL:HG11	2.00	0.43
1:E:491:ASP:O	1:E:494:ASN:N	2.51	0.43
1:F:42:PHE:CE1	1:F:59:ILE:CD1	3.02	0.43
1:F:357:GLY:HA2	1:F:358:ASN:HA	1.77	0.43
1:A:3:LEU:HD11	1:B:68:PHE:HZ	1.84	0.43
1:B:48:TYR:OH	1:B:109:PRO:HG3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:282:ILE:HG23	1:C:334:PHE:CD2	2.54	0.43
1:D:212:TRP:HA	1:D:212:TRP:CE3	2.54	0.43
1:E:23:PHE:HD2	1:E:117:GLN:OE1	2.01	0.43
1:E:177:ILE:CB	1:E:236:ILE:HA	2.49	0.43
1:F:168:PHE:CD2	1:F:480:GLY:HA2	2.54	0.43
1:A:534:LEU:HD23	1:A:534:LEU:HA	1.83	0.43
1:B:175:LEU:HD13	1:B:177:ILE:HG23	2.00	0.43
1:B:249:GLN:HA	1:B:249:GLN:OE1	2.18	0.43
1:C:12:THR:HG22	1:C:75:ASN:OD1	2.19	0.43
1:C:157:THR:HB	1:C:492:GLU:OE1	2.19	0.43
1:C:158:MET:C	1:C:159:ARG:HG2	2.42	0.43
1:C:172:GLU:CD	1:C:245:GLY:H	2.27	0.43
1:C:496:VAL:O	1:C:497:LYS:C	2.62	0.43
1:C:534:LEU:HD23	1:C:534:LEU:HA	1.90	0.43
1:E:12:THR:HA	1:E:13:PRO:HD3	1.87	0.43
1:E:374:ASP:HB3	1:E:467:HIS:O	2.19	0.43
1:F:8:LEU:HD22	1:F:77:CYS:HB2	2.01	0.43
1:F:29:ARG:HD2	1:F:30:ASP:OD2	2.18	0.43
1:F:315:ASP:C	1:F:317:ALA:N	2.76	0.43
1:F:494:ASN:O	1:F:495:ASN:C	2.62	0.43
1:A:282:ILE:HD12	1:A:282:ILE:HA	1.73	0.42
1:A:572:ILE:O	1:A:572:ILE:CG2	2.50	0.42
1:B:285:ASP:O	1:B:286:TYR:C	2.61	0.42
1:D:10:TYR:HB2	1:D:38:ASP:HB2	2.00	0.42
1:D:95:ILE:HG12	1:D:105:LEU:HD22	2.01	0.42
1:D:177:ILE:CG2	1:D:236:ILE:HG12	2.48	0.42
1:E:71:LEU:HD12	1:E:71:LEU:O	2.18	0.42
1:F:3:LEU:HB3	1:F:45:THR:HB	2.01	0.42
1:F:104:GLU:C	1:F:105:LEU:HD23	2.44	0.42
1:A:112:VAL:CG2	1:A:548:LEU:CD1	2.97	0.42
1:A:274:SER:HB2	1:A:338:VAL:CG2	2.49	0.42
1:A:563:ILE:HD13	1:A:563:ILE:H	1.80	0.42
1:C:363:TYR:CD1	1:C:364:ILE:HG23	2.54	0.42
1:C:363:TYR:HD2	1:D:316:TYR:CE1	2.37	0.42
1:D:130:ILE:CG2	1:D:527:GLN:HG2	2.49	0.42
1:D:164:LYS:CB	1:D:282:ILE:HD12	2.49	0.42
1:E:282:ILE:HD12	1:E:282:ILE:HA	1.67	0.42
1:A:16:ASN:HB3	1:F:531:ILE:CD1	2.49	0.42
1:A:65:ARG:HG2	1:A:66:SER:N	2.34	0.42
1:A:277:LYS:O	1:A:336:SER:OG	2.37	0.42
1:A:537:VAL:O	1:A:539:THR:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:112:VAL:CG2	1:B:548:LEU:CD1	2.97	0.42
1:B:491:ASP:O	1:B:494:ASN:N	2.52	0.42
1:C:470:TYR:CB	1:C:479:PHE:CE1	3.02	0.42
1:C:514:LEU:HD12	1:C:514:LEU:HA	1.90	0.42
1:C:516:ASP:OD1	1:C:518:THR:HG22	2.19	0.42
1:E:285:ASP:OD2	1:E:285:ASP:C	2.63	0.42
1:A:531:ILE:HD12	1:A:531:ILE:HA	1.84	0.42
1:B:104:GLU:C	1:B:105:LEU:HD23	2.44	0.42
1:B:111:VAL:CB	1:B:545:LEU:HD13	2.47	0.42
1:C:139:TYR:O	1:C:140:GLU:C	2.62	0.42
1:C:165:SER:CA	1:C:282:ILE:HD13	2.49	0.42
1:D:112:VAL:CG2	1:D:548:LEU:CD1	2.97	0.42
1:D:217:GLU:O	1:D:218:SER:C	2.62	0.42
1:E:157:THR:HB	1:E:492:GLU:OE1	2.19	0.42
1:F:537:VAL:O	1:F:538:ASP:C	2.62	0.42
1:A:553:VAL:HG12	1:A:555:LEU:HD12	2.00	0.42
1:B:174:ILE:CG1	1:B:176:THR:HG22	2.48	0.42
1:B:571:VAL:HG13	1:B:572:ILE:N	2.34	0.42
1:C:92:VAL:HG23	1:C:92:VAL:O	2.20	0.42
1:D:172:GLU:OE2	1:D:245:GLY:N	2.49	0.42
1:D:189:GLU:CD	1:D:189:GLU:H	2.28	0.42
1:D:542:MET:HB3	1:D:546:ARG:NH1	2.34	0.42
1:E:542:MET:HB3	1:E:546:ARG:NH1	2.34	0.42
1:F:16:ASN:CG	1:F:18:GLN:H	2.28	0.42
1:A:55:LEU:N	1:A:55:LEU:HD23	2.34	0.42
1:C:42:PHE:CE2	1:C:44:SER:HB2	2.54	0.42
1:C:48:TYR:CD2	1:C:55:LEU:HD13	2.55	0.42
1:C:226:LEU:HD12	1:C:233:GLN:HB3	2.01	0.42
1:D:41:GLU:O	1:D:41:GLU:HG2	2.20	0.42
1:D:258:VAL:HG12	1:D:263:LEU:O	2.18	0.42
1:D:279:PHE:HB3	1:D:282:ILE:HG22	2.02	0.42
1:D:315:ASP:HB3	1:D:370:ILE:HD11	2.01	0.42
1:E:494:ASN:O	1:E:495:ASN:C	2.62	0.42
1:E:516:ASP:OD1	1:E:518:THR:HG22	2.20	0.42
1:A:157:THR:CG2	1:A:157:THR:O	2.64	0.42
1:B:42:PHE:CG	1:B:43:THR:N	2.85	0.42
1:B:224:ASP:C	1:B:226:LEU:N	2.76	0.42
1:B:539:THR:CG2	1:B:540:GLY:N	2.82	0.42
1:C:177:ILE:HB	1:C:236:ILE:HA	2.01	0.42
1:C:249:GLN:OE1	1:C:249:GLN:HA	2.19	0.42
1:C:263:LEU:HD12	1:C:263:LEU:HA	1.90	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:120:VAL:HG23	1:D:121:LEU:H	1.81	0.42
1:D:124:LEU:HD22	1:D:532:TRP:CB	2.47	0.42
1:D:323:ILE:HG23	1:D:353:TYR:CE1	2.55	0.42
1:D:470:TYR:CB	1:D:479:PHE:CE1	3.02	0.42
1:E:139:TYR:O	1:E:140:GLU:C	2.61	0.42
1:F:104:GLU:O	1:F:105:LEU:HD23	2.19	0.42
1:F:165:SER:HA	1:F:282:ILE:HD13	2.01	0.42
1:A:566:THR:C	1:A:568:VAL:N	2.78	0.42
1:C:531:ILE:CD1	1:D:16:ASN:HB3	2.49	0.42
1:D:492:GLU:O	1:D:493:LEU:C	2.63	0.42
1:E:177:ILE:HD13	1:E:177:ILE:C	2.44	0.42
1:F:224:ASP:C	1:F:226:LEU:N	2.77	0.42
1:F:236:ILE:HG21	1:F:378:PHE:CE2	2.55	0.42
1:F:289:LEU:HD11	1:F:293:LEU:HD11	2.01	0.42
1:F:542:MET:O	1:F:545:LEU:CB	2.68	0.42
1:B:290:MET:HE3	1:B:295:LEU:HB2	2.01	0.42
1:C:124:LEU:HD22	1:C:532:TRP:CB	2.46	0.42
1:C:124:LEU:CD2	1:C:532:TRP:HB2	2.46	0.42
1:C:182:ARG:NH2	1:C:267:LYS:HE2	2.35	0.42
1:C:285:ASP:OD2	1:C:287:GLN:N	2.53	0.42
1:C:494:ASN:O	1:C:495:ASN:C	2.63	0.42
1:C:549:PHE:O	1:C:552:GLY:N	2.53	0.42
1:D:25:SER:OG	1:D:28:GLU:HG3	2.19	0.42
1:D:89:TYR:N	1:D:89:TYR:CD2	2.88	0.42
1:D:476:GLN:O	1:D:478:LYS:HG2	2.20	0.42
1:F:4:SER:HA	1:F:82:ILE:HG12	2.01	0.42
1:F:132:GLN:OE1	1:F:515:SER:HB3	2.20	0.42
1:F:285:ASP:HA	1:F:331:ASN:OD1	2.19	0.42
1:A:48:TYR:CD2	1:A:55:LEU:HD13	2.55	0.42
1:A:132:GLN:OE1	1:A:515:SER:HB3	2.19	0.42
1:A:164:LYS:O	1:A:282:ILE:CD1	2.60	0.42
1:A:165:SER:CA	1:A:282:ILE:HD13	2.49	0.42
1:A:356:ARG:NH2	1:B:487:ARG:O	2.52	0.42
1:B:57:VAL:O	1:B:57:VAL:HG12	2.20	0.42
1:B:533:THR:HG23	1:B:546:ARG:NH2	2.35	0.42
1:D:177:ILE:HG21	1:D:236:ILE:HG12	2.01	0.42
1:D:299:ASN:H	1:D:299:ASN:HD22	1.68	0.42
1:D:380:VAL:O	1:D:462:ALA:N	2.53	0.42
1:F:534:LEU:HD23	1:F:534:LEU:HA	1.84	0.42
1:A:12:THR:OG1	1:A:13:PRO:HD2	2.19	0.41
1:A:248:LYS:O	1:A:249:GLN:C	2.62	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:255:HIS:O	1:A:256:GLU:HG3	2.20	0.41
1:A:350:VAL:HG22	1:A:353:TYR:HB2	2.01	0.41
1:B:348:VAL:CG2	1:B:349:TYR:N	2.81	0.41
1:B:359:ASN:O	1:B:360:VAL:C	2.58	0.41
1:C:61:LEU:N	1:C:61:LEU:HD12	2.34	0.41
1:C:325:LEU:HD12	1:C:325:LEU:HA	1.90	0.41
1:D:46:PHE:CE1	1:D:55:LEU:HD12	2.55	0.41
1:F:56:ARG:HD3	1:F:104:GLU:OE1	2.20	0.41
1:F:561:ASP:OD2	1:F:566:THR:HG21	2.19	0.41
1:A:5:LYS:HB3	1:A:80:GLN:HG3	2.02	0.41
1:C:332:LEU:HA	1:C:332:LEU:HD12	1.84	0.41
1:D:61:LEU:N	1:D:61:LEU:HD12	2.35	0.41
1:D:282:ILE:HD12	1:D:282:ILE:HA	1.67	0.41
1:D:285:ASP:HA	1:D:331:ASN:OD1	2.19	0.41
1:D:544:MET:O	1:D:548:LEU:HB2	2.21	0.41
1:D:561:ASP:O	1:D:563:ILE:N	2.53	0.41
1:F:350:VAL:HG22	1:F:353:TYR:HB2	2.02	0.41
1:A:130:ILE:O	1:A:131:ARG:CG	2.69	0.41
1:A:347:LYS:HE2	1:A:369:THR:HG22	2.01	0.41
1:A:516:ASP:OD2	1:A:516:ASP:C	2.63	0.41
1:A:542:MET:O	1:A:546:ARG:N	2.53	0.41
1:C:81:TYR:HE1	1:C:86:ARG:NH2	2.18	0.41
1:D:304:LEU:HD23	1:D:304:LEU:HA	1.83	0.41
1:D:532:TRP:HZ2	1:D:546:ARG:HA	1.86	0.41
1:E:228:GLY:C	1:E:230:PRO:HD3	2.46	0.41
1:E:531:ILE:O	1:E:531:ILE:CG2	2.68	0.41
1:F:165:SER:CA	1:F:282:ILE:HD13	2.50	0.41
1:F:212:TRP:CE3	1:F:212:TRP:HA	2.55	0.41
1:A:299:ASN:ND2	1:A:299:ASN:H	2.18	0.41
1:A:514:LEU:HD21	1:A:528:PHE:CE2	2.55	0.41
1:B:128:ASN:C	1:B:128:ASN:HD22	2.25	0.41
1:B:168:PHE:CD2	1:B:480:GLY:HA2	2.55	0.41
1:B:531:ILE:HD12	1:B:531:ILE:HA	1.85	0.41
1:C:26:ASN:HB3	1:C:29:ARG:NH2	2.36	0.41
1:C:166:GLU:OE1	1:C:279:PHE:CA	2.68	0.41
1:C:502:MET:HE3	1:C:502:MET:HB3	1.91	0.41
1:C:542:MET:CE	1:C:542:MET:HA	2.48	0.41
1:C:542:MET:O	1:C:545:LEU:CB	2.69	0.41
1:E:46:PHE:CE1	1:E:55:LEU:HD12	2.54	0.41
1:E:258:VAL:HG12	1:E:263:LEU:O	2.19	0.41
1:E:487:ARG:HG2	1:E:488:ILE:N	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:531:ILE:HD12	1:E:531:ILE:HA	1.82	0.41
1:F:76:TYR:OH	1:F:113:MET:HG2	2.20	0.41
1:F:282:ILE:HG23	1:F:334:PHE:CD2	2.55	0.41
1:F:470:TYR:CB	1:F:479:PHE:CE1	3.03	0.41
1:A:541:HIS:O	1:A:545:LEU:HB2	2.19	0.41
1:B:12:THR:HG21	1:B:76:TYR:CB	2.51	0.41
1:B:48:TYR:CD2	1:B:55:LEU:HD13	2.55	0.41
1:B:133:HIS:CD2	1:B:525:TRP:H	2.39	0.41
1:B:492:GLU:O	1:B:493:LEU:C	2.63	0.41
1:C:112:VAL:CG2	1:C:548:LEU:CD1	2.99	0.41
1:C:248:LYS:O	1:C:249:GLN:C	2.64	0.41
1:D:81:TYR:HE1	1:D:86:ARG:NH2	2.19	0.41
1:D:290:MET:HE3	1:D:290:MET:HB3	1.82	0.41
1:D:293:LEU:HD22	1:D:309:VAL:HG11	2.02	0.41
1:E:360:VAL:CG2	1:E:363:TYR:HB2	2.51	0.41
1:F:121:LEU:O	1:F:124:LEU:HD12	2.19	0.41
1:F:129:VAL:CG2	1:F:130:ILE:N	2.83	0.41
1:A:95:ILE:CD1	1:A:105:LEU:HD22	2.50	0.41
1:A:104:GLU:C	1:A:105:LEU:HD23	2.45	0.41
1:A:313:LEU:HD23	1:A:313:LEU:HA	1.83	0.41
1:A:533:THR:HG23	1:A:546:ARG:NH2	2.36	0.41
1:C:224:ASP:O	1:C:225:TYR:C	2.64	0.41
1:C:359:ASN:C	1:C:360:VAL:O	2.56	0.41
1:D:106:SER:C	1:D:107:LEU:HD12	2.46	0.41
1:D:165:SER:CA	1:D:282:ILE:HD13	2.51	0.41
1:D:286:TYR:HE1	1:D:301:LYS:HE3	1.85	0.41
1:F:79:VAL:CG1	1:F:81:TYR:CE2	3.03	0.41
1:F:319:ASN:C	1:F:320:ARG:HG2	2.45	0.41
1:F:502:MET:HE3	1:F:502:MET:HB3	1.89	0.41
1:A:311:ALA:HB2	1:A:325:LEU:HD22	2.03	0.41
1:A:515:SER:O	1:A:516:ASP:C	2.63	0.41
1:A:516:ASP:CG	1:A:518:THR:HG22	2.45	0.41
1:B:516:ASP:OD2	1:B:516:ASP:C	2.64	0.41
1:B:548:LEU:HD23	1:B:548:LEU:HA	1.81	0.41
1:C:55:LEU:HD23	1:C:55:LEU:N	2.36	0.41
1:D:348:VAL:HG13	1:D:368:LEU:HB3	2.03	0.41
1:E:133:HIS:HB3	1:E:520:MET:HE3	2.03	0.41
1:E:189:GLU:N	1:E:189:GLU:CD	2.79	0.41
1:E:483:LEU:HD12	1:E:484:ARG:N	2.36	0.41
1:B:82:ILE:HA	1:B:83:GLN:HA	1.72	0.41
1:B:138:GLU:OE2	1:B:515:SER:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:359:ASN:C	1:B:360:VAL:O	2.59	0.41
1:C:12:THR:HG21	1:C:76:TYR:CB	2.50	0.41
1:C:487:ARG:HG2	1:C:488:ILE:N	2.35	0.41
1:D:16:ASN:CG	1:D:18:GLN:H	2.28	0.41
1:D:127:VAL:CG2	1:D:528:PHE:CD1	3.00	0.41
1:D:471:ALA:O	1:D:472:PRO:C	2.61	0.41
1:E:42:PHE:CE1	1:E:59:ILE:CD1	3.03	0.41
1:E:55:LEU:HD23	1:E:55:LEU:N	2.36	0.41
1:E:164:LYS:HB2	1:E:282:ILE:HD12	2.03	0.41
1:F:3:LEU:CB	1:F:45:THR:HB	2.50	0.41
1:F:244:SER:O	1:F:245:GLY:C	2.64	0.41
1:F:285:ASP:OD2	1:F:285:ASP:C	2.63	0.41
1:A:360:VAL:CG2	1:A:363:TYR:HB2	2.50	0.41
1:A:572:ILE:O	1:A:573:ILE:CB	2.67	0.41
1:C:172:GLU:CD	1:C:212:TRP:HZ2	2.28	0.41
1:C:224:ASP:C	1:C:226:LEU:N	2.78	0.41
1:C:520:MET:HB3	1:C:570:ASN:OD1	2.21	0.41
1:D:27:GLU:HG2	1:D:28:GLU:N	2.36	0.41
1:D:164:LYS:HB2	1:D:282:ILE:HD12	2.03	0.41
1:D:487:ARG:HG2	1:D:488:ILE:N	2.35	0.41
1:D:516:ASP:OD2	1:D:517:ILE:N	2.54	0.41
1:E:130:ILE:HB	1:E:527:GLN:HG2	2.03	0.41
1:E:157:THR:HG23	1:E:489:SER:H	1.82	0.41
1:E:519:SER:O	1:E:573:ILE:HG12	2.21	0.41
1:E:531:ILE:HG13	1:F:15:ASN:OD1	2.21	0.41
1:E:533:THR:HG23	1:E:546:ARG:NH2	2.35	0.41
1:F:282:ILE:HD11	1:F:483:LEU:HB3	2.02	0.41
1:F:305:ARG:HB2	1:F:306:PRO:CD	2.50	0.41
1:A:133:HIS:HB3	1:A:520:MET:HE2	2.03	0.41
1:A:210:MET:HB3	1:A:210:MET:HE2	1.87	0.41
1:A:249:GLN:OE1	1:A:249:GLN:HA	2.21	0.41
1:A:316:TYR:CE2	1:A:482:HIS:CD2	3.09	0.41
1:B:357:GLY:HA2	1:B:358:ASN:HA	1.67	0.41
1:B:516:ASP:OD1	1:B:518:THR:HG22	2.21	0.41
1:C:42:PHE:CD1	1:C:59:ILE:HD11	2.56	0.41
1:C:512:THR:HG23	1:C:513:LYS:N	2.34	0.41
1:C:563:ILE:HD13	1:C:563:ILE:H	1.85	0.41
1:D:463:ILE:O	1:D:463:ILE:HD13	2.20	0.41
1:E:8:LEU:CD1	1:E:105:LEU:HD11	2.51	0.41
1:E:124:LEU:CD2	1:E:532:TRP:HB2	2.47	0.41
1:E:177:ILE:HB	1:E:236:ILE:HA	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:561:ASP:O	1:E:562:MET:C	2.63	0.41
1:F:21:LEU:HD12	1:F:556:TRP:O	2.21	0.41
1:F:65:ARG:HG2	1:F:66:SER:N	2.35	0.41
1:F:374:ASP:HB3	1:F:467:HIS:O	2.20	0.41
1:F:529:LYS:C	1:F:530:GLY:O	2.63	0.41
1:F:532:TRP:CZ2	1:F:546:ARG:HA	2.56	0.41
1:B:573:ILE:N	1:B:573:ILE:HD13	2.36	0.40
1:C:76:TYR:OH	1:C:113:MET:HG2	2.22	0.40
1:C:89:TYR:CD2	1:C:89:TYR:N	2.89	0.40
1:C:236:ILE:HG21	1:C:378:PHE:CE2	2.55	0.40
1:C:512:THR:HG23	1:C:513:LYS:O	2.21	0.40
1:C:533:THR:HG23	1:C:546:ARG:NH2	2.36	0.40
1:D:75:ASN:OD1	1:D:75:ASN:N	2.53	0.40
1:D:139:TYR:O	1:D:140:GLU:C	2.64	0.40
1:D:215:ASP:OD1	1:D:217:GLU:N	2.52	0.40
1:D:282:ILE:HD11	1:D:483:LEU:HB3	2.03	0.40
1:E:37:PHE:C	1:E:38:ASP:CG	2.89	0.40
1:E:148:SER:CB	1:F:156:SER:O	2.69	0.40
1:E:348:VAL:CG2	1:E:349:TYR:N	2.82	0.40
1:E:509:ASP:O	1:E:510:TYR:C	2.64	0.40
1:F:189:GLU:N	1:F:189:GLU:CD	2.79	0.40
1:F:224:ASP:O	1:F:225:TYR:C	2.64	0.40
1:F:296:ASN:O	1:F:300:ASP:HB2	2.21	0.40
1:A:67:CYS:SG	1:A:68:PHE:N	2.94	0.40
1:A:570:ASN:O	1:A:571:VAL:HG23	2.21	0.40
1:A:571:VAL:HG13	1:A:572:ILE:N	2.36	0.40
1:B:329:GLU:CD	1:B:357:GLY:H	2.27	0.40
1:B:549:PHE:C	1:B:551:ALA:N	2.78	0.40
1:C:514:LEU:HD21	1:C:528:PHE:CE2	2.56	0.40
1:D:23:PHE:HD2	1:D:117:GLN:OE1	2.04	0.40
1:D:55:LEU:N	1:D:55:LEU:HD23	2.37	0.40
1:D:129:VAL:HG23	1:D:130:ILE:N	2.36	0.40
1:D:514:LEU:HD21	1:D:528:PHE:CE2	2.56	0.40
1:E:6:ILE:HG23	1:E:7:LYS:N	2.37	0.40
1:E:104:GLU:C	1:E:105:LEU:HD23	2.46	0.40
1:E:138:GLU:OE2	1:E:515:SER:HB2	2.20	0.40
1:F:16:ASN:HD21	1:F:18:GLN:HG3	1.86	0.40
1:F:37:PHE:CE1	1:F:40:HIS:O	2.74	0.40
1:F:48:TYR:CD2	1:F:55:LEU:HD13	2.56	0.40
1:F:170:GLN:O	1:F:244:SER:CB	2.70	0.40
1:F:560:SER:O	1:F:564:ASN:ND2	2.52	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:570:ASN:O	1:F:571:VAL:HG23	2.22	0.40
1:A:7:LYS:HG3	1:A:37:PHE:CE2	2.57	0.40
1:A:511:SER:HB2	1:B:567:VAL:HG21	2.02	0.40
1:A:542:MET:HB3	1:A:546:ARG:NH1	2.36	0.40
1:B:12:THR:HA	1:B:13:PRO:HD3	1.89	0.40
1:B:139:TYR:O	1:B:140:GLU:C	2.63	0.40
1:B:220:LYS:O	1:B:221:GLU:C	2.64	0.40
1:C:69:GLU:O	1:C:69:GLU:HG2	2.21	0.40
1:C:295:LEU:HD12	1:C:295:LEU:HA	1.93	0.40
1:D:8:LEU:CD2	1:D:77:CYS:HB2	2.51	0.40
1:D:12:THR:HA	1:D:13:PRO:HD3	1.89	0.40
1:D:518:THR:O	1:D:518:THR:HG23	2.21	0.40
1:E:148:SER:HB3	1:F:156:SER:O	2.22	0.40
1:E:202:ASP:OD2	1:E:274:SER:OG	2.40	0.40
1:E:502:MET:HE3	1:E:502:MET:HB3	1.94	0.40
1:F:212:TRP:O	1:F:213:PHE:CG	2.74	0.40
1:F:353:TYR:O	1:F:354:ASN:CB	2.67	0.40
1:A:224:ASP:O	1:A:225:TYR:C	2.64	0.40
1:B:5:LYS:HB3	1:B:80:GLN:HG3	2.03	0.40
1:B:130:ILE:O	1:B:131:ARG:CG	2.69	0.40
1:B:227:THR:O	1:B:230:PRO:HD3	2.22	0.40
1:C:165:SER:HB3	1:C:482:HIS:ND1	2.35	0.40
1:C:307:ASN:OD1	1:C:307:ASN:N	2.46	0.40
1:C:470:TYR:O	1:C:471:ALA:C	2.64	0.40
1:D:46:PHE:CE1	1:D:55:LEU:HD11	2.57	0.40
1:D:177:ILE:HD13	1:D:177:ILE:H	1.85	0.40
1:E:48:TYR:CD2	1:E:55:LEU:HD13	2.56	0.40
1:E:224:ASP:O	1:E:225:TYR:C	2.64	0.40
1:F:61:LEU:HD12	1:F:61:LEU:N	2.36	0.40
1:F:75:ASN:CA	1:F:92:VAL:HG22	2.51	0.40
1:F:571:VAL:CG1	1:F:572:ILE:N	2.79	0.40
1:A:71:LEU:CG	1:A:71:LEU:O	2.68	0.40
1:A:239:VAL:O	1:A:375:THR:HA	2.21	0.40
1:A:362:GLN:O	1:A:363:TYR:C	2.65	0.40
1:B:175:LEU:HD23	1:B:239:VAL:HB	2.04	0.40
1:B:538:ASP:O	1:B:540:GLY:N	2.54	0.40
1:C:538:ASP:O	1:C:541:HIS:N	2.52	0.40
1:C:541:HIS:O	1:C:545:LEU:N	2.54	0.40
1:D:42:PHE:CE1	1:D:59:ILE:CD1	3.03	0.40
1:D:111:VAL:CG2	1:D:545:LEU:HD13	2.51	0.40
1:D:274:SER:HB2	1:D:338:VAL:CG2	2.52	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:475:LYS:HD2	1:D:475:LYS:HA	1.96	0.40
1:D:494:ASN:O	1:D:495:ASN:C	2.65	0.40
1:E:174:ILE:CG1	1:E:176:THR:HG22	2.50	0.40
1:F:95:ILE:CD1	1:F:105:LEU:HD22	2.51	0.40
1:F:286:TYR:HE1	1:F:301:LYS:HE3	1.84	0.40

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:255:HIS:O	1:B:291:PHE:CZ[2_665]	1.96	0.24
1:C:295:LEU:O	1:F:65:ARG:NH2[1_556]	2.07	0.13
1:A:255:HIS:O	1:B:291:PHE:CE2[2_665]	2.09	0.11
1:A:255:HIS:C	1:B:291:PHE:CZ[2_665]	2.19	0.01

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	482/583 (83%)	386 (80%)	82 (17%)	14 (3%)	3	20
1	B	482/583 (83%)	390 (81%)	82 (17%)	10 (2%)	5	27
1	C	482/583 (83%)	387 (80%)	86 (18%)	9 (2%)	6	30
1	D	482/583 (83%)	388 (80%)	81 (17%)	13 (3%)	4	22
1	E	482/583 (83%)	390 (81%)	85 (18%)	7 (2%)	8	35
1	F	482/583 (83%)	387 (80%)	85 (18%)	10 (2%)	5	27
All	All	2892/3498 (83%)	2328 (80%)	501 (17%)	63 (2%)	5	26

All (63) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	258	VAL
1	A	530	GLY
1	A	539	THR
1	B	258	VAL
1	B	530	GLY
1	C	258	VAL
1	C	530	GLY
1	D	258	VAL
1	D	530	GLY
1	D	539	THR
1	E	258	VAL
1	E	530	GLY
1	E	539	THR
1	F	258	VAL
1	F	530	GLY
1	F	539	THR
1	A	68	PHE
1	A	233	GLN
1	A	255	HIS
1	B	68	PHE
1	B	539	THR
1	C	68	PHE
1	C	539	THR
1	D	68	PHE
1	E	68	PHE
1	F	68	PHE
1	A	36	LYS
1	D	550	GLU
1	F	567	VAL
1	A	546	ARG
1	A	567	VAL
1	B	304	LEU
1	A	39	VAL
1	A	360	VAL
1	A	538	ASP
1	B	39	VAL
1	B	277	LYS
1	B	567	VAL
1	C	567	VAL
1	D	250	GLU
1	D	567	VAL
1	F	233	GLN
1	F	304	LEU

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Mol	Chain	Res	Type
1	A	260	GLY
1	B	36	LYS
1	C	39	VAL
1	D	39	VAL
1	D	371	ASN
1	D	542	MET
1	E	39	VAL
1	F	36	LYS
1	F	39	VAL
1	B	572	ILE
1	D	245	GLY
1	E	567	VAL
1	C	190	LYS
1	D	260	GLY
1	A	572	ILE
1	C	360	VAL
1	C	572	ILE
1	D	572	ILE
1	E	572	ILE
1	F	572	ILE

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	446/529 (84%)	358 (80%)	88 (20%)	1 8
1	B	446/529 (84%)	354 (79%)	92 (21%)	1 7
1	C	446/529 (84%)	357 (80%)	89 (20%)	1 7
1	D	446/529 (84%)	361 (81%)	85 (19%)	1 8
1	E	446/529 (84%)	351 (79%)	95 (21%)	1 6
1	F	446/529 (84%)	358 (80%)	88 (20%)	1 8
All	All	2676/3174 (84%)	2139 (80%)	537 (20%)	1 7

All (537) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	ILE
1	A	16	ASN
1	A	18	GLN
1	A	23	PHE
1	A	38	ASP
1	A	46	PHE
1	A	55	LEU
1	A	57	VAL
1	A	58	THR
1	A	61	LEU
1	A	62	VAL
1	A	65	ARG
1	A	69	GLU
1	A	71	LEU
1	A	72	MET
1	A	74	VAL
1	A	82	ILE
1	A	87	VAL
1	A	92	VAL
1	A	94	ASP
1	A	95	ILE
1	A	103	CYS
1	A	108	VAL
1	A	128	ASN
1	A	129	VAL
1	A	135	THR
1	A	146	ILE
1	A	155	THR
1	A	157	THR
1	A	165	SER
1	A	174	ILE
1	A	175	LEU
1	A	176	THR
1	A	177	ILE
1	A	182	ARG
1	A	189	GLU
1	A	199	SER
1	A	200	THR
1	A	204	ILE
1	A	210	MET
1	A	215	ASP
1	A	226	LEU
1	A	227	THR

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Mol	Chain	Res	Type
1	A	229	TYR
1	A	236	ILE
1	A	239	VAL
1	A	241	ILE
1	A	249	GLN
1	A	263	LEU
1	A	267	LYS
1	A	274	SER
1	A	285	ASP
1	A	288	SER
1	A	295	LEU
1	A	299	ASN
1	A	303	LEU
1	A	320	ARG
1	A	330	THR
1	A	338	VAL
1	A	350	VAL
1	A	358	ASN
1	A	359	ASN
1	A	360	VAL
1	A	365	ASP
1	A	369	THR
1	A	370	ILE
1	A	374	ASP
1	A	376	ILE
1	A	380	VAL
1	A	463	ILE
1	A	481	VAL
1	A	484	ARG
1	A	491	ASP
1	A	513	LYS
1	A	514	LEU
1	A	518	THR
1	A	524	ASN
1	A	526	VAL
1	A	533	THR
1	A	539	THR
1	A	548	LEU
1	A	560	SER
1	A	563	ILE
1	A	567	VAL
1	A	568	VAL

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Mol	Chain	Res	Type
1	A	571	VAL
1	A	572	ILE
1	A	573	ILE
1	B	6	ILE
1	B	16	ASN
1	B	18	GLN
1	B	23	PHE
1	B	26	ASN
1	B	38	ASP
1	B	46	PHE
1	B	55	LEU
1	B	57	VAL
1	B	58	THR
1	B	61	LEU
1	B	62	VAL
1	B	65	ARG
1	B	69	GLU
1	B	71	LEU
1	B	72	MET
1	B	74	VAL
1	B	75	ASN
1	B	82	ILE
1	B	87	VAL
1	B	92	VAL
1	B	94	ASP
1	B	98	LEU
1	B	103	CYS
1	B	108	VAL
1	B	128	ASN
1	B	129	VAL
1	B	135	THR
1	B	146	ILE
1	B	155	THR
1	B	157	THR
1	B	165	SER
1	B	174	ILE
1	B	176	THR
1	B	177	ILE
1	B	182	ARG
1	B	189	GLU
1	B	199	SER
1	B	200	THR

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Mol	Chain	Res	Type
1	B	204	ILE
1	B	210	MET
1	B	215	ASP
1	B	226	LEU
1	B	227	THR
1	B	229	TYR
1	B	236	ILE
1	B	239	VAL
1	B	249	GLN
1	B	263	LEU
1	B	267	LYS
1	B	274	SER
1	B	282	ILE
1	B	285	ASP
1	B	288	SER
1	B	295	LEU
1	B	299	ASN
1	B	303	LEU
1	B	320	ARG
1	B	325	LEU
1	B	326	SER
1	B	330	THR
1	B	338	VAL
1	B	348	VAL
1	B	350	VAL
1	B	358	ASN
1	B	359	ASN
1	B	360	VAL
1	B	365	ASP
1	B	369	THR
1	B	374	ASP
1	B	376	ILE
1	B	380	VAL
1	B	463	ILE
1	B	481	VAL
1	B	484	ARG
1	B	491	ASP
1	B	502	MET
1	B	513	LYS
1	B	514	LEU
1	B	518	THR
1	B	524	ASN

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Mol	Chain	Res	Type
1	B	526	VAL
1	B	533	THR
1	B	539	THR
1	B	548	LEU
1	B	560	SER
1	B	563	ILE
1	B	567	VAL
1	B	568	VAL
1	B	571	VAL
1	B	572	ILE
1	B	573	ILE
1	C	6	ILE
1	C	16	ASN
1	C	18	GLN
1	C	23	PHE
1	C	38	ASP
1	C	46	PHE
1	C	55	LEU
1	C	57	VAL
1	C	58	THR
1	C	61	LEU
1	C	62	VAL
1	C	65	ARG
1	C	69	GLU
1	C	71	LEU
1	C	72	MET
1	C	74	VAL
1	C	87	VAL
1	C	92	VAL
1	C	94	ASP
1	C	103	CYS
1	C	108	VAL
1	C	128	ASN
1	C	129	VAL
1	C	135	THR
1	C	146	ILE
1	C	155	THR
1	C	157	THR
1	C	165	SER
1	C	174	ILE
1	C	176	THR
1	C	177	ILE

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Mol	Chain	Res	Type
1	C	182	ARG
1	C	189	GLU
1	C	199	SER
1	C	200	THR
1	C	204	ILE
1	C	210	MET
1	C	215	ASP
1	C	226	LEU
1	C	227	THR
1	C	229	TYR
1	C	236	ILE
1	C	239	VAL
1	C	249	GLN
1	C	263	LEU
1	C	267	LYS
1	C	274	SER
1	C	285	ASP
1	C	288	SER
1	C	295	LEU
1	C	299	ASN
1	C	303	LEU
1	C	320	ARG
1	C	325	LEU
1	C	330	THR
1	C	338	VAL
1	C	348	VAL
1	C	350	VAL
1	C	358	ASN
1	C	359	ASN
1	C	360	VAL
1	C	365	ASP
1	C	369	THR
1	C	370	ILE
1	C	374	ASP
1	C	376	ILE
1	C	380	VAL
1	C	463	ILE
1	C	481	VAL
1	C	484	ARG
1	C	491	ASP
1	C	502	MET
1	C	512	THR

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Mol	Chain	Res	Type
1	C	513	LYS
1	C	514	LEU
1	C	518	THR
1	C	524	ASN
1	C	526	VAL
1	C	531	ILE
1	C	533	THR
1	C	539	THR
1	C	548	LEU
1	C	560	SER
1	C	563	ILE
1	C	567	VAL
1	C	568	VAL
1	C	571	VAL
1	C	572	ILE
1	C	573	ILE
1	D	16	ASN
1	D	18	GLN
1	D	23	PHE
1	D	38	ASP
1	D	46	PHE
1	D	55	LEU
1	D	57	VAL
1	D	58	THR
1	D	61	LEU
1	D	62	VAL
1	D	65	ARG
1	D	69	GLU
1	D	71	LEU
1	D	72	MET
1	D	74	VAL
1	D	82	ILE
1	D	87	VAL
1	D	92	VAL
1	D	94	ASP
1	D	103	CYS
1	D	108	VAL
1	D	128	ASN
1	D	129	VAL
1	D	135	THR
1	D	146	ILE
1	D	155	THR

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Mol	Chain	Res	Type
1	D	157	THR
1	D	165	SER
1	D	174	ILE
1	D	176	THR
1	D	177	ILE
1	D	182	ARG
1	D	199	SER
1	D	200	THR
1	D	204	ILE
1	D	210	MET
1	D	215	ASP
1	D	219	LEU
1	D	226	LEU
1	D	227	THR
1	D	229	TYR
1	D	236	ILE
1	D	239	VAL
1	D	249	GLN
1	D	263	LEU
1	D	267	LYS
1	D	274	SER
1	D	285	ASP
1	D	288	SER
1	D	295	LEU
1	D	299	ASN
1	D	303	LEU
1	D	325	LEU
1	D	330	THR
1	D	338	VAL
1	D	348	VAL
1	D	350	VAL
1	D	358	ASN
1	D	359	ASN
1	D	360	VAL
1	D	365	ASP
1	D	369	THR
1	D	374	ASP
1	D	376	ILE
1	D	380	VAL
1	D	463	ILE
1	D	481	VAL
1	D	484	ARG

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Mol	Chain	Res	Type
1	D	502	MET
1	D	513	LYS
1	D	514	LEU
1	D	518	THR
1	D	524	ASN
1	D	526	VAL
1	D	533	THR
1	D	539	THR
1	D	548	LEU
1	D	560	SER
1	D	563	ILE
1	D	566	THR
1	D	567	VAL
1	D	568	VAL
1	D	571	VAL
1	D	572	ILE
1	D	573	ILE
1	E	16	ASN
1	E	18	GLN
1	E	23	PHE
1	E	26	ASN
1	E	38	ASP
1	E	46	PHE
1	E	55	LEU
1	E	57	VAL
1	E	58	THR
1	E	61	LEU
1	E	62	VAL
1	E	65	ARG
1	E	69	GLU
1	E	71	LEU
1	E	72	MET
1	E	74	VAL
1	E	82	ILE
1	E	87	VAL
1	E	94	ASP
1	E	103	CYS
1	E	108	VAL
1	E	128	ASN
1	E	129	VAL
1	E	135	THR
1	E	143	LEU

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Mol	Chain	Res	Type
1	E	146	ILE
1	E	155	THR
1	E	157	THR
1	E	165	SER
1	E	174	ILE
1	E	175	LEU
1	E	176	THR
1	E	177	ILE
1	E	182	ARG
1	E	189	GLU
1	E	199	SER
1	E	200	THR
1	E	204	ILE
1	E	210	MET
1	E	215	ASP
1	E	219	LEU
1	E	226	LEU
1	E	227	THR
1	E	229	TYR
1	E	236	ILE
1	E	239	VAL
1	E	244	SER
1	E	249	GLN
1	E	263	LEU
1	E	267	LYS
1	E	274	SER
1	E	278	ASP
1	E	282	ILE
1	E	285	ASP
1	E	288	SER
1	E	295	LEU
1	E	299	ASN
1	E	303	LEU
1	E	325	LEU
1	E	330	THR
1	E	338	VAL
1	E	348	VAL
1	E	350	VAL
1	E	358	ASN
1	E	359	ASN
1	E	360	VAL
1	E	365	ASP

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Mol	Chain	Res	Type
1	E	369	THR
1	E	370	ILE
1	E	374	ASP
1	E	376	ILE
1	E	380	VAL
1	E	463	ILE
1	E	475	LYS
1	E	476	GLN
1	E	481	VAL
1	E	484	ARG
1	E	512	THR
1	E	513	LYS
1	E	514	LEU
1	E	518	THR
1	E	524	ASN
1	E	526	VAL
1	E	531	ILE
1	E	533	THR
1	E	539	THR
1	E	548	LEU
1	E	560	SER
1	E	563	ILE
1	E	566	THR
1	E	567	VAL
1	E	568	VAL
1	E	571	VAL
1	E	572	ILE
1	E	573	ILE
1	F	16	ASN
1	F	18	GLN
1	F	23	PHE
1	F	38	ASP
1	F	46	PHE
1	F	55	LEU
1	F	57	VAL
1	F	58	THR
1	F	61	LEU
1	F	62	VAL
1	F	65	ARG
1	F	69	GLU
1	F	71	LEU
1	F	72	MET

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Mol	Chain	Res	Type
1	F	74	VAL
1	F	87	VAL
1	F	103	CYS
1	F	108	VAL
1	F	128	ASN
1	F	129	VAL
1	F	135	THR
1	F	143	LEU
1	F	146	ILE
1	F	155	THR
1	F	157	THR
1	F	165	SER
1	F	174	ILE
1	F	176	THR
1	F	177	ILE
1	F	182	ARG
1	F	189	GLU
1	F	199	SER
1	F	200	THR
1	F	204	ILE
1	F	210	MET
1	F	215	ASP
1	F	226	LEU
1	F	227	THR
1	F	229	TYR
1	F	230	PRO
1	F	236	ILE
1	F	239	VAL
1	F	249	GLN
1	F	263	LEU
1	F	267	LYS
1	F	274	SER
1	F	282	ILE
1	F	285	ASP
1	F	288	SER
1	F	295	LEU
1	F	299	ASN
1	F	303	LEU
1	F	325	LEU
1	F	330	THR
1	F	338	VAL
1	F	348	VAL

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Mol	Chain	Res	Type
1	F	350	VAL
1	F	358	ASN
1	F	359	ASN
1	F	360	VAL
1	F	365	ASP
1	F	369	THR
1	F	370	ILE
1	F	374	ASP
1	F	376	ILE
1	F	380	VAL
1	F	463	ILE
1	F	468	VAL
1	F	475	LYS
1	F	481	VAL
1	F	484	ARG
1	F	491	ASP
1	F	513	LYS
1	F	514	LEU
1	F	518	THR
1	F	524	ASN
1	F	526	VAL
1	F	531	ILE
1	F	533	THR
1	F	539	THR
1	F	548	LEU
1	F	560	SER
1	F	563	ILE
1	F	567	VAL
1	F	568	VAL
1	F	571	VAL
1	F	572	ILE
1	F	573	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	40	HIS
1	A	142	ASN
1	A	201	HIS
1	A	233	GLN
1	A	543	ASN
1	A	565	ASN

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Mol	Chain	Res	Type
1	B	40	HIS
1	B	145	GLN
1	B	201	HIS
1	B	206	ASN
1	B	233	GLN
1	B	543	ASN
1	B	564	ASN
1	B	565	ASN
1	C	40	HIS
1	C	206	ASN
1	C	233	GLN
1	C	299	ASN
1	C	543	ASN
1	D	40	HIS
1	D	201	HIS
1	D	233	GLN
1	D	366	ASN
1	D	543	ASN
1	D	565	ASN
1	E	40	HIS
1	E	119	ASN
1	E	233	GLN
1	E	302	HIS
1	E	366	ASN
1	E	543	ASN
1	E	557	HIS
1	E	564	ASN
1	F	40	HIS
1	F	70	GLN
1	F	96	GLN
1	F	201	HIS
1	F	233	GLN
1	F	543	ASN
1	F	565	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	488/583 (83%)	0.41	28 (5%) 29 15	48, 91, 189, 275	0
1	B	488/583 (83%)	0.40	37 (7%) 20 10	50, 92, 180, 276	0
1	C	488/583 (83%)	0.23	12 (2%) 58 35	58, 102, 192, 278	0
1	D	488/583 (83%)	0.26	17 (3%) 47 27	65, 104, 205, 279	0
1	E	488/583 (83%)	0.17	15 (3%) 51 30	58, 103, 198, 275	0
1	F	488/583 (83%)	0.21	23 (4%) 36 19	52, 94, 194, 281	0
All	All	2928/3498 (83%)	0.28	132 (4%) 38 20	48, 99, 194, 281	0

All (132) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	98	LEU	6.3
1	D	58	THR	5.9
1	F	13	PRO	4.8
1	A	40	HIS	4.6
1	A	69	GLU	4.3
1	F	565	ASN	4.0
1	B	46	PHE	4.0
1	B	60	ASP	4.0
1	B	58	THR	4.0
1	B	218	SER	3.9
1	A	193	PHE	3.9
1	B	214	ASN	3.8
1	C	39	VAL	3.8
1	D	530	GLY	3.6
1	A	71	LEU	3.6
1	A	533	THR	3.6
1	B	98	LEU	3.5
1	B	228	GLY	3.4
1	B	69	GLU	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	102	VAL	3.4
1	A	98	LEU	3.4
1	A	250	GLU	3.3
1	D	6	ILE	3.3
1	E	14	PHE	3.2
1	E	193	PHE	3.2
1	A	191	PRO	3.2
1	B	193	PHE	3.2
1	B	71	LEU	3.2
1	D	103	CYS	3.1
1	A	357	GLY	3.1
1	A	68	PHE	3.1
1	E	93	THR	3.1
1	B	205	TYR	3.1
1	B	99	ASN	3.1
1	A	530	GLY	3.0
1	B	530	GLY	3.0
1	C	11	ASN	3.0
1	A	62	VAL	3.0
1	B	72	MET	3.0
1	B	3	LEU	2.9
1	B	219	LEU	2.9
1	F	97	GLN	2.9
1	B	47	ASN	2.9
1	A	278	ASP	2.9
1	B	103	CYS	2.9
1	A	565	ASN	2.8
1	F	39	VAL	2.8
1	B	216	TYR	2.8
1	B	54	VAL	2.8
1	B	48	TYR	2.7
1	F	69	GLU	2.7
1	F	205	TYR	2.7
1	B	39	VAL	2.7
1	A	263	LEU	2.7
1	E	6	ILE	2.6
1	D	77	CYS	2.6
1	F	566	THR	2.6
1	B	56	ARG	2.6
1	B	97	GLN	2.6
1	E	530	GLY	2.6
1	C	91	PHE	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	71	LEU	2.5
1	A	335	ASP	2.5
1	C	62	VAL	2.5
1	E	46	PHE	2.4
1	D	40	HIS	2.4
1	E	205	TYR	2.4
1	D	39	VAL	2.4
1	B	531	ILE	2.4
1	B	291	PHE	2.4
1	A	275	ASN	2.4
1	B	536	ASN	2.4
1	E	58	THR	2.4
1	F	81	TYR	2.4
1	B	11	ASN	2.4
1	E	508	ASN	2.4
1	A	188	ALA	2.4
1	D	98	LEU	2.4
1	B	67	CYS	2.4
1	F	58	THR	2.3
1	E	47	ASN	2.3
1	C	98	LEU	2.3
1	C	530	GLY	2.3
1	F	93	THR	2.3
1	A	103	CYS	2.3
1	F	103	CYS	2.3
1	D	126	ASN	2.3
1	A	97	GLN	2.3
1	F	18	GLN	2.3
1	B	533	THR	2.3
1	B	565	ASN	2.3
1	F	99	ASN	2.3
1	F	59	ILE	2.3
1	D	17	MET	2.3
1	E	48	TYR	2.3
1	B	55	LEU	2.2
1	A	195	SER	2.2
1	D	62	VAL	2.2
1	F	102	VAL	2.2
1	D	67	CYS	2.2
1	E	531	ILE	2.2
1	B	90	LEU	2.2
1	F	100	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	193	PHE	2.2
1	C	40	HIS	2.2
1	E	102	VAL	2.2
1	B	62	VAL	2.2
1	F	54	VAL	2.1
1	E	573	ILE	2.1
1	C	63	SER	2.1
1	A	104	GLU	2.1
1	F	530	GLY	2.1
1	A	6	ILE	2.1
1	B	377	GLY	2.1
1	B	68	PHE	2.1
1	D	61	LEU	2.1
1	C	12	THR	2.1
1	D	68	PHE	2.1
1	A	86	ARG	2.0
1	A	72	MET	2.0
1	A	227	THR	2.0
1	C	58	THR	2.0
1	D	60	ASP	2.0
1	C	68	PHE	2.0
1	E	228	GLY	2.0
1	F	193	PHE	2.0
1	F	61	LEU	2.0
1	F	71	LEU	2.0
1	A	81	TYR	2.0
1	A	46	PHE	2.0
1	C	73	GLY	2.0
1	F	568	VAL	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 oligosaccharides 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.