



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 12:00 AM EDT

PDB ID : 1NJ8 / pdb_00001nj8
Title : Crystal Structure of Prolyl-tRNA Synthetase from Methanocaldococcus janaschii
Authors : Kamtekar, S.; Kennedy, W.D.; Wang, J.; Stathopoulos, C.; Soll, D.; Steitz, T.A.
Deposited on : 2002-12-30
Resolution : 3.20 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
Xtriage (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

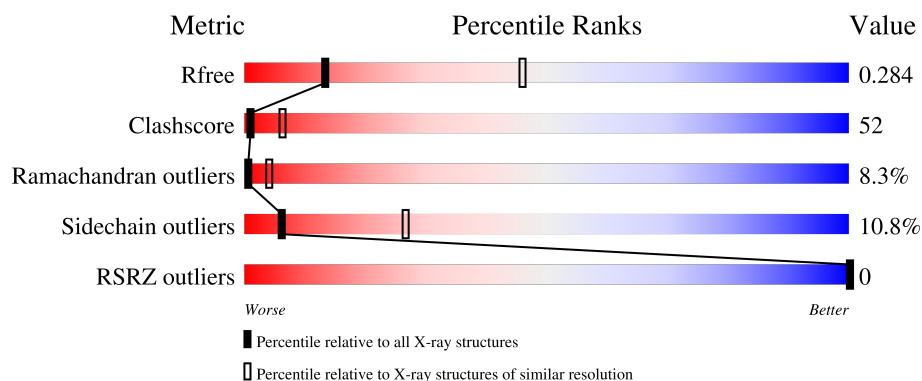
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

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	459	 27% 55% 15% ..
1	B	459	 27% 58% 14% ..
1	C	459	 25% 57% 15% ..
1	D	459	 26% 58% 14% ..

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 15182 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 Proline-tRNA Synthetase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	456	Total	C	N	O	S	0	0	0
			3772	2447	614	698	13			
1	B	456	Total	C	N	O	S	0	0	0
			3772	2447	614	698	13			
1	C	456	Total	C	N	O	S	0	0	0
			3772	2447	614	698	13			
1	D	456	Total	C	N	O	S	0	0	0
			3772	2447	614	698	13			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	expression tag	UNP Q58635
A	-2	SER	-	expression tag	UNP Q58635
A	-1	HIS	-	expression tag	UNP Q58635
A	0	MET	-	expression tag	UNP Q58635
A	1	LEU	MET	cloning artifact	UNP Q58635
B	-3	GLY	-	expression tag	UNP Q58635
B	-2	SER	-	expression tag	UNP Q58635
B	-1	HIS	-	expression tag	UNP Q58635
B	0	MET	-	expression tag	UNP Q58635
B	1	LEU	MET	cloning artifact	UNP Q58635
C	-3	GLY	-	expression tag	UNP Q58635
C	-2	SER	-	expression tag	UNP Q58635
C	-1	HIS	-	expression tag	UNP Q58635
C	0	MET	-	expression tag	UNP Q58635
C	1	LEU	MET	cloning artifact	UNP Q58635
D	-3	GLY	-	expression tag	UNP Q58635
D	-2	SER	-	expression tag	UNP Q58635
D	-1	HIS	-	expression tag	UNP Q58635
D	0	MET	-	expression tag	UNP Q58635
D	1	LEU	MET	cloning artifact	UNP Q58635

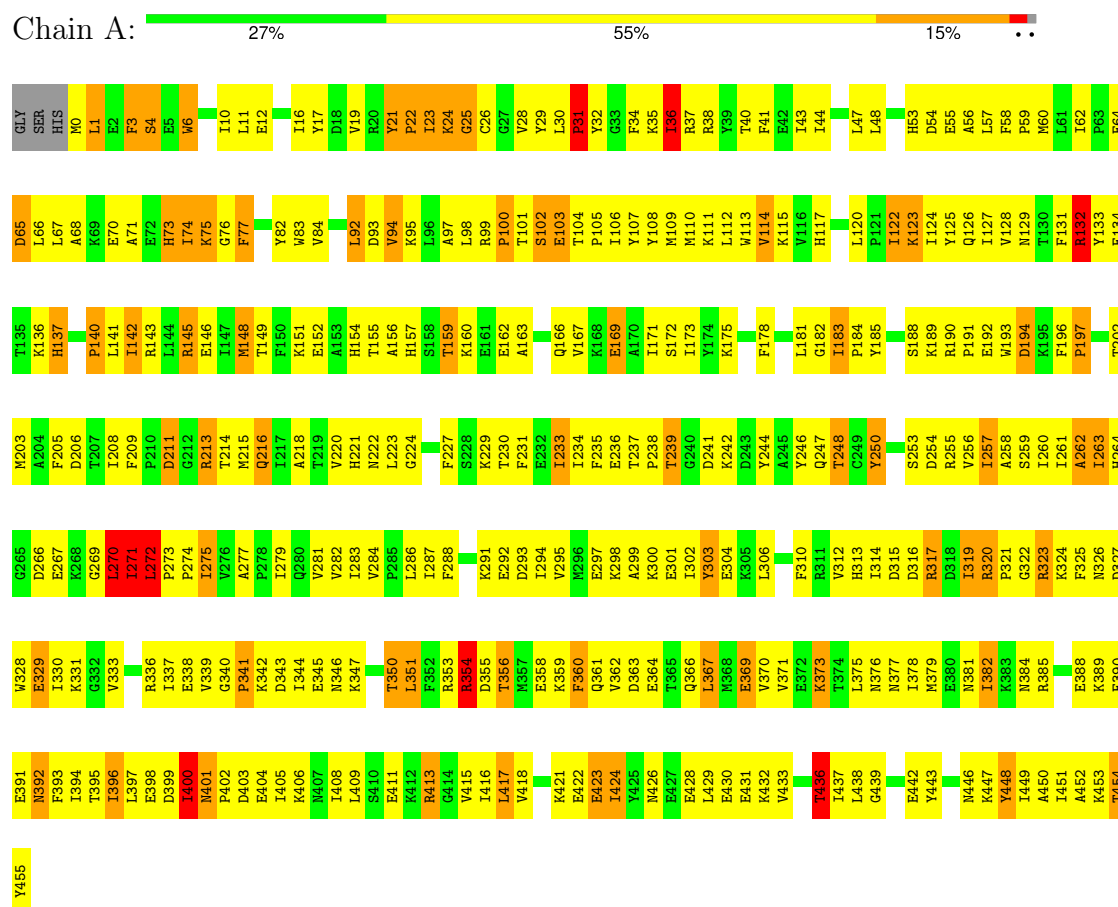
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	35	Total 35	O 35	0	0
2	B	16	Total 16	O 16	0	0
2	C	25	Total 25	O 25	0	0
2	D	18	Total 18	O 18	0	0

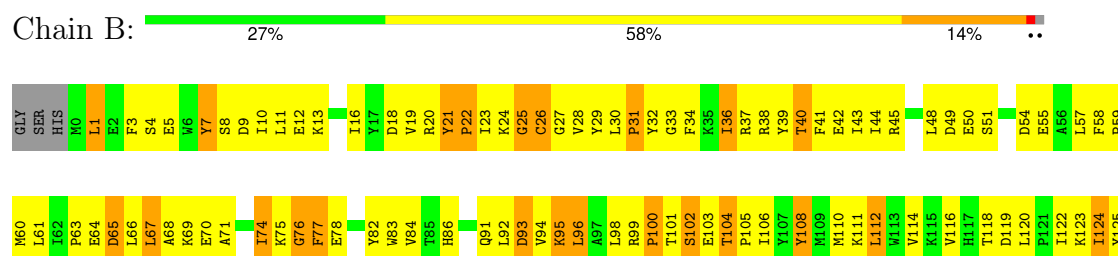
3 Residue-property plots

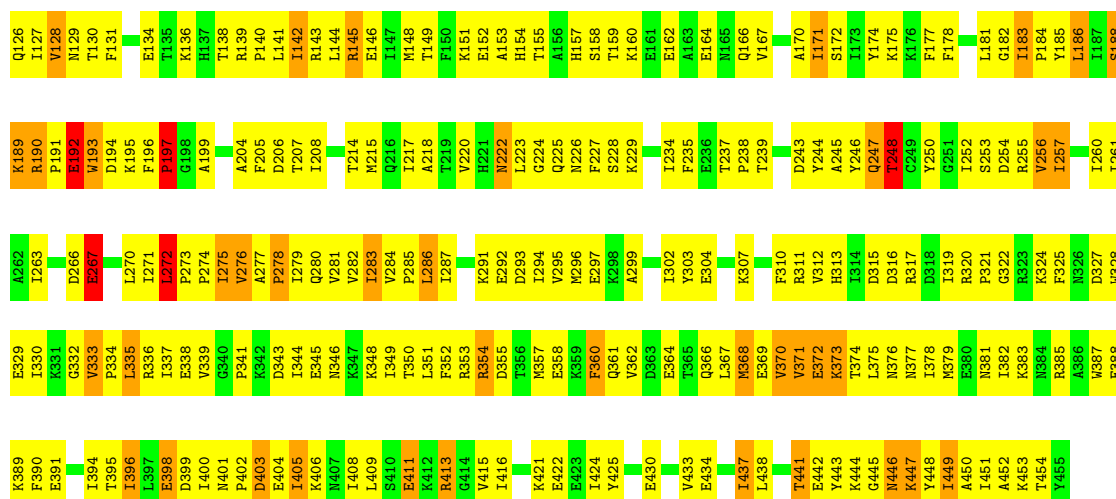
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Proline-tRNA Synthetase



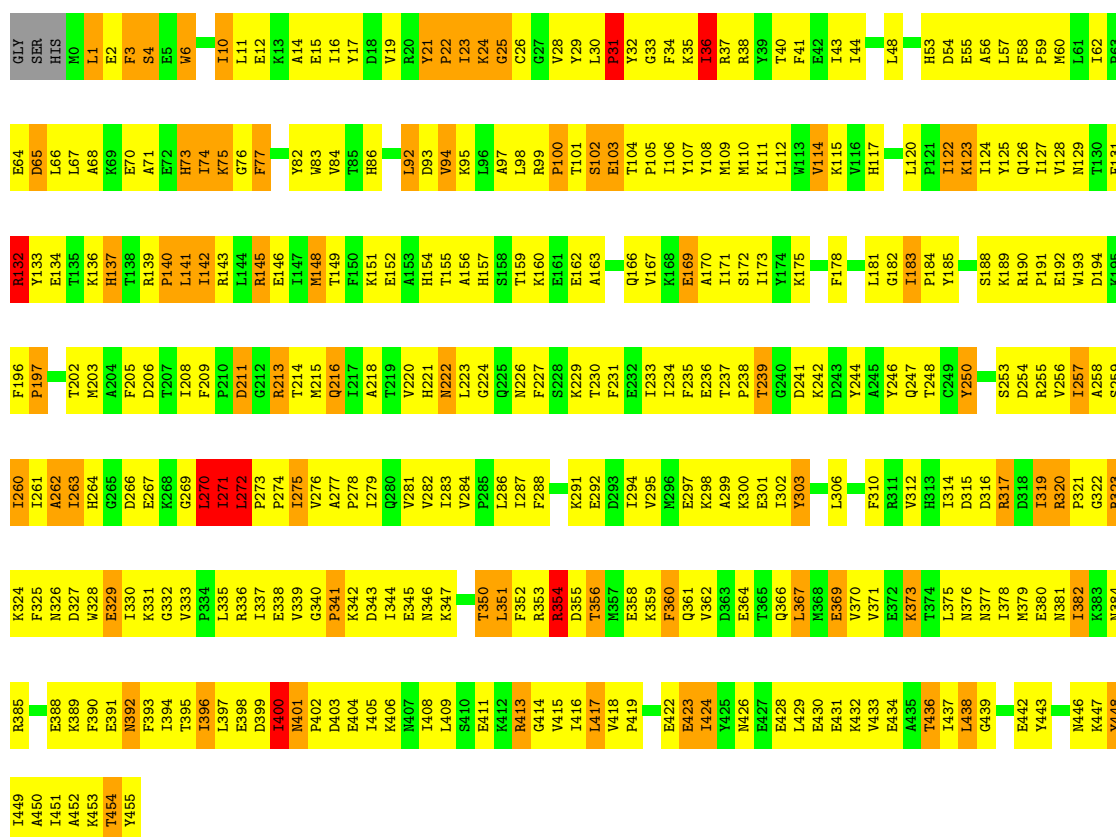
• Molecule 1: Proline-tRNA Synthetase





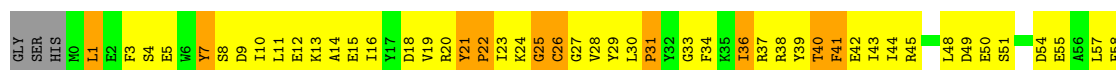
• Molecule 1: Proline-tRNA Synthetase

Chain C: 25% 57% 15% ..



• Molecule 1: Proline-tRNA Synthetase

Chain D: 26% 58% 14% ..



Y455	E388	W328	I260	K189	Y125	P59
	K389	E329	I261	R190	Q126	M60
	E391	I330	A262	P191	I127	L61
	N392	K331	I263	E192	V128	I62
	F393	G332		W193	N129	P63
	I394	V333	D266	D194	T130	E64
	T395	P334	E267	K195	F131	D65
	I396	L335		F196		L66
	L397	R336	L270	P197	E134	L67
	E398	I337	I271	G198	K136	A68
	D399	E338	I272	A199	K137	K69
	I400	V339	L273	T202	H137	E70
	N401	G340	P273	K203	T138	A71
	P402	P341	P274	M206	R139	
	D403	K342	I275	A204	P140	I74
	E404	D343	V276	F205	L141	K75
	I405	I344	A277	D206	L142	G76
	K406	E345	P278	T207	R143	F77
	M407	N346	I279	I208	L144	E78
	I408	K347	Q280		R145	
	L409	K348	V281	R213	E146	Y82
	S410	I349	V282	T214	I147	W83
	E411	T350	I283	M215	M148	W84
	K412	L351	V284	Q216	T149	T85
	R413	F352	P285	I217	F150	H86
	G414	R353	L286	A218	K151	
	I416	R354	I287	V219	E152	
		D355		V220	A153	
		T356	K291	H221	H154	Q91
		M357	E292	N222	T155	L92
		E358	D293	L223	A156	D93
		K359	I294	G224	H157	V94
	E422	F360	V295	Q225	S158	K95
	S423	Q361	M296	N226	T159	A97
	I424	V362	E297	F227	K160	L96
	Y425	D363	K298	S228	E161	R99
		E364	A299	K229	E162	P100
		T365			A163	T101
		Q366	I302	I234	E164	S102
		L367		F235	N165	E103
		M368	K307	E236	Q166	T104
		E369		T237	V167	P105
		V370	F310	P238		I106
		E372	R311	T239	I171	Y107
		K373	V312		M108	X108
		T374	H313	D243	S172	M109
	E442	L375	I314	Y244	I173	M110
	Y443	N376	D315	A245	Y174	K111
	K444	N377	D316	Y246	K175	L112
	G445	I378	R317	Q247	K176	W113
	M446	N379	D318	T248	F177	V114
	K447	E380	I319	C249	F178	K115
	Y448	N381	R320	Y250		V116
	I449	I382	P321	G251	L181	H117
	A450	K383	G322	I252	G182	T118
	I451	K384	R323	S253	I183	D119
	A452	R385	K324	D254	P184	L120
	K453	A386	F325	V255	Y185	F121
	T454	W387	D327	I257	L186	I122
					I187	K123
					S188	I124

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	108.94Å 104.84Å 91.75Å 90.00° 93.63° 90.00°	Depositor
Resolution (Å)	20.00 – 3.20 20.00 – 3.20	Depositor EDS
% Data completeness (in resolution range)	87.0 (20.00-3.20) 86.6 (20.00-3.20)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	720.88 (at 3.18Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.231 , 0.301 0.223 , 0.284	Depositor DCC
R_{free} test set	2974 reflections (9.83%)	wwPDB-VP
Wilson B-factor (Å ²)	67.4	Xtriage
Anisotropy	0.553	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 47.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	15182	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.11% 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

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.55	0/3860	1.00	24/5213 (0.5%)
1	B	0.49	0/3860	0.97	17/5213 (0.3%)
1	C	0.55	0/3860	1.00	25/5213 (0.5%)
1	D	0.47	0/3860	0.98	18/5213 (0.3%)
All	All	0.52	0/15440	0.99	84/20852 (0.4%)

There are no bond length outliers.

All (84) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	272	LEU	CA-C-N	8.68	129.32	120.38
1	D	272	LEU	C-N-CA	8.68	129.32	120.38
1	B	21	TYR	CA-C-N	8.46	130.41	119.84
1	B	21	TYR	C-N-CA	8.46	130.41	119.84
1	D	21	TYR	CA-C-N	8.29	130.20	119.84
1	D	21	TYR	C-N-CA	8.29	130.20	119.84
1	B	272	LEU	CA-C-N	7.97	128.59	120.38
1	B	272	LEU	C-N-CA	7.97	128.59	120.38
1	C	320	ARG	NE-CZ-NH2	7.48	125.94	119.20
1	A	21	TYR	CA-C-N	7.45	129.15	119.84
1	A	21	TYR	C-N-CA	7.45	129.15	119.84
1	C	21	TYR	CA-C-N	7.35	129.03	119.84
1	C	21	TYR	C-N-CA	7.35	129.03	119.84
1	B	195	LYS	N-CA-C	7.06	120.82	110.17
1	C	320	ARG	NE-CZ-NH1	-6.90	114.60	121.50
1	D	195	LYS	N-CA-C	6.89	120.57	110.17
1	A	145	ARG	N-CA-C	-6.78	103.59	110.97
1	C	145	ARG	N-CA-C	-6.72	103.65	110.97
1	D	108	TYR	N-CA-C	-6.40	104.34	111.71
1	D	183	ILE	N-CA-C	6.34	115.17	108.95
1	A	260	ILE	N-CA-C	-6.33	104.34	110.42
1	A	310	PHE	N-CA-C	6.28	119.77	109.85
1	C	310	PHE	N-CA-C	6.11	119.16	109.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	183	ILE	N-CA-C	6.09	114.67	107.73
1	C	350	THR	N-CA-C	6.05	119.10	109.24
1	C	258	ALA	N-CA-C	-5.96	104.71	111.14
1	A	350	THR	N-CA-C	5.89	118.84	109.24
1	C	6	TRP	N-CA-C	-5.88	104.78	111.07
1	B	145	ARG	N-CA-C	-5.82	105.27	112.90
1	A	169	GLU	N-CA-C	-5.80	104.87	111.14
1	A	233	ILE	CB-CA-C	-5.79	106.74	113.22
1	B	108	TYR	N-CA-C	-5.78	104.36	111.75
1	A	6	TRP	N-CA-C	-5.77	104.90	111.07
1	C	356	THR	N-CA-C	-5.73	105.94	113.17
1	B	183	ILE	N-CA-C	5.72	114.56	108.95
1	D	453	LYS	N-CA-C	-5.72	101.16	110.20
1	D	145	ARG	N-CA-C	-5.71	105.42	112.90
1	C	233	ILE	CB-CA-C	-5.69	106.85	113.22
1	A	272	LEU	CA-C-N	5.63	126.18	120.38
1	A	272	LEU	C-N-CA	5.63	126.18	120.38
1	C	329	GLU	N-CA-C	-5.61	105.08	111.14
1	C	260	ILE	N-CA-C	-5.52	104.99	110.62
1	D	42	GLU	N-CA-C	-5.50	105.44	111.82
1	A	73	HIS	N-CA-C	-5.47	102.70	111.02
1	A	25	GLY	N-CA-C	-5.46	107.49	114.85
1	B	413	ARG	CB-CA-C	-5.44	109.31	115.79
1	D	41	PHE	N-CA-C	5.43	119.90	113.28
1	D	263	ILE	N-CA-C	5.42	115.87	110.23
1	D	413	ARG	CB-CA-C	-5.42	109.34	115.79
1	B	192	GLU	N-CA-C	5.41	117.63	111.02
1	C	183	ILE	N-CA-C	5.41	113.89	107.73
1	C	454	THR	N-CA-C	5.38	118.48	110.14
1	C	272	LEU	CA-C-N	5.38	125.92	120.38
1	C	272	LEU	C-N-CA	5.38	125.92	120.38
1	C	73	HIS	N-CA-C	-5.37	102.86	111.02
1	A	400	ILE	N-CA-C	5.36	120.50	109.34
1	A	258	ALA	N-CA-C	-5.34	105.37	111.14
1	A	454	THR	N-CA-C	5.33	118.40	110.14
1	D	202	THR	N-CA-C	5.32	118.38	107.69
1	C	148	MET	N-CA-C	5.31	117.15	111.36
1	C	400	ILE	N-CA-C	5.30	120.36	109.34
1	A	356	THR	N-CA-C	-5.26	106.55	113.17
1	D	40	THR	N-CA-C	-5.22	104.85	111.11
1	B	263	ILE	N-CA-C	5.22	115.66	110.23
1	A	320	ARG	NE-CZ-NH2	-5.21	114.52	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	92	LEU	N-CA-C	5.20	120.48	113.72
1	D	333	VAL	CA-C-N	5.18	126.32	119.84
1	D	333	VAL	C-N-CA	5.18	126.32	119.84
1	A	148	MET	N-CA-C	5.17	117.00	111.36
1	B	42	GLU	N-CA-C	-5.17	105.83	111.82
1	C	25	GLY	N-CA-C	-5.17	107.87	114.85
1	B	333	VAL	CA-C-N	5.16	126.28	119.84
1	B	333	VAL	C-N-CA	5.16	126.28	119.84
1	C	438	LEU	N-CA-C	-5.14	106.84	113.01
1	A	194	ASP	N-CA-C	-5.10	104.53	111.56
1	D	213	ARG	N-CA-C	-5.07	102.98	110.48
1	B	96	LEU	N-CA-C	-5.06	102.27	110.32
1	A	92	LEU	N-CA-C	5.06	120.30	113.72
1	C	169	GLU	N-CA-C	-5.05	105.68	111.14
1	A	329	GLU	N-CA-C	-5.05	105.68	111.14
1	B	40	THR	N-CA-C	-5.05	105.05	111.11
1	B	453	LYS	N-CA-C	-5.03	101.51	109.96
1	C	38	ARG	N-CA-C	-5.02	105.69	111.07
1	A	159	THR	N-CA-C	5.01	116.85	108.99

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3772	0	3804	422	2
1	B	3772	0	3804	380	0
1	C	3772	0	3804	435	1
1	D	3772	0	3804	396	1
2	A	35	0	0	2	0
2	B	16	0	0	1	0
2	C	25	0	0	6	0
2	D	18	0	0	3	0
All	All	15182	0	15216	1587	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 52.

All (1587) 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:B:275:ILE:HD12	1:B:275:ILE:H	1.06	1.14
1:D:275:ILE:HD12	1:D:275:ILE:H	1.08	1.11
1:B:48:LEU:HD11	1:B:151:LYS:HD2	1.32	1.10
1:D:48:LEU:HD11	1:D:151:LYS:HD2	1.34	1.07
1:A:337:ILE:HG12	1:A:351:LEU:HD12	1.36	1.02
1:A:396:ILE:HD12	1:A:396:ILE:H	1.22	1.02
1:B:16:ILE:HD13	1:B:261:ILE:HD11	1.41	1.01
1:C:337:ILE:HG12	1:C:351:LEU:HD12	1.39	1.00
1:A:71:ALA:HA	1:A:75:LYS:HE2	1.42	1.00
1:C:71:ALA:HA	1:C:75:LYS:HE2	1.43	0.99
1:D:16:ILE:HD13	1:D:261:ILE:HD11	1.44	0.99
1:B:58:PHE:H	1:B:126:GLN:HE22	1.03	0.98
1:D:18:ASP:HB2	1:D:30:LEU:HD11	1.43	0.97
1:C:396:ILE:HD12	1:C:396:ILE:H	1.24	0.97
1:D:99:ARG:NH2	1:D:128:VAL:HB	1.79	0.97
1:D:58:PHE:H	1:D:126:GLN:HE22	1.07	0.96
1:B:10:ILE:HD11	1:B:270:LEU:HB2	1.48	0.96
1:D:10:ILE:HD11	1:D:270:LEU:HB2	1.48	0.95
1:B:18:ASP:HB2	1:B:30:LEU:HD11	1.48	0.95
1:D:286:LEU:HD12	1:D:286:LEU:H	1.29	0.95
1:B:99:ARG:NH2	1:B:128:VAL:HB	1.83	0.93
1:C:430:GLU:HG3	1:C:437:ILE:HG12	1.51	0.92
1:B:286:LEU:HD12	1:B:286:LEU:H	1.32	0.92
1:A:430:GLU:HG3	1:A:437:ILE:HG12	1.51	0.91
1:D:83:TRP:CE3	1:D:95:LYS:HE2	2.03	0.91
1:D:141:LEU:H	1:D:144:LEU:HD21	1.35	0.91
1:D:271:ILE:HG12	1:D:354:ARG:NH1	1.85	0.91
1:D:190:ARG:HH11	1:D:204:ALA:HB3	1.35	0.90
1:C:82:TYR:HD2	1:D:84:VAL:HG11	1.35	0.90
1:B:141:LEU:H	1:B:144:LEU:HD21	1.36	0.90
1:B:275:ILE:H	1:B:275:ILE:CD1	1.82	0.90
1:D:403:ASP:HA	1:D:406:LYS:HD3	1.51	0.90
1:B:190:ARG:HH11	1:B:204:ALA:HB3	1.36	0.90
1:B:83:TRP:CE3	1:B:95:LYS:HE2	2.06	0.89
1:D:275:ILE:H	1:D:275:ILE:CD1	1.84	0.88
1:B:362:VAL:HG11	1:B:370:VAL:HG21	1.56	0.88
1:B:271:ILE:HG12	1:B:354:ARG:NH1	1.87	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:403:ASP:HA	1:B:406:LYS:HD3	1.53	0.88
1:A:82:TYR:HD2	1:B:84:VAL:HG11	1.37	0.87
1:D:127:ILE:HG12	1:D:151:LYS:HG3	1.57	0.87
1:A:10:ILE:HD11	1:A:270:LEU:N	1.90	0.87
1:B:127:ILE:HG12	1:B:151:LYS:HG3	1.57	0.87
1:D:362:VAL:HG11	1:D:370:VAL:HG21	1.57	0.87
1:A:360:PHE:H	1:A:360:PHE:HD2	1.22	0.86
1:A:101:THR:HG23	1:A:102:SER:H	1.41	0.86
1:C:101:THR:HG23	1:C:102:SER:H	1.41	0.85
1:C:306:LEU:HD21	1:C:371:VAL:HG21	1.55	0.85
1:D:336:ARG:HB3	1:D:352:PHE:HB3	1.57	0.85
1:C:360:PHE:H	1:C:360:PHE:HD2	1.22	0.85
1:C:256:VAL:HG23	1:C:257:ILE:H	1.42	0.85
1:C:275:ILE:HD12	1:C:275:ILE:H	1.41	0.85
1:B:275:ILE:HD12	1:B:275:ILE:N	1.91	0.84
1:B:389:LYS:NZ	1:B:389:LYS:HB3	1.93	0.84
1:B:58:PHE:H	1:B:126:GLN:NE2	1.74	0.84
1:C:10:ILE:HD11	1:C:270:LEU:N	1.94	0.83
1:A:70:GLU:HG2	1:A:77:PHE:CE2	2.13	0.83
1:D:275:ILE:HD12	1:D:275:ILE:N	1.93	0.83
1:B:336:ARG:HB3	1:B:352:PHE:HB3	1.59	0.82
1:D:389:LYS:NZ	1:D:389:LYS:HB3	1.95	0.82
1:A:275:ILE:H	1:A:275:ILE:HD12	1.43	0.82
1:D:167:VAL:HG13	1:D:220:VAL:HG11	1.61	0.81
1:A:282:VAL:HG23	1:A:333:VAL:HG11	1.61	0.81
1:A:306:LEU:HD21	1:A:371:VAL:HG21	1.60	0.81
1:A:256:VAL:HG23	1:A:257:ILE:H	1.46	0.81
1:C:55:GLU:HB2	1:C:125:TYR:CZ	2.16	0.81
1:C:70:GLU:HG2	1:C:77:PHE:CE2	2.15	0.80
1:B:413:ARG:HB2	1:B:413:ARG:NH1	1.96	0.80
1:D:413:ARG:NH1	1:D:413:ARG:HB2	1.96	0.80
1:B:286:LEU:HD11	1:B:338:GLU:HB3	1.64	0.79
1:B:167:VAL:HG13	1:B:220:VAL:HG11	1.62	0.79
1:A:106:ILE:HD12	1:A:154:HIS:CD2	2.18	0.79
1:D:58:PHE:H	1:D:126:GLN:NE2	1.80	0.79
1:D:33:GLY:O	1:D:36:ILE:HG22	1.83	0.79
1:B:33:GLY:O	1:B:36:ILE:HG22	1.83	0.79
1:D:405:ILE:O	1:D:408:ILE:HG22	1.83	0.79
1:A:55:GLU:HB2	1:A:125:TYR:CZ	2.18	0.79
1:A:99:ARG:NH2	1:A:128:VAL:HB	1.98	0.79
1:A:275:ILE:HD12	1:A:275:ILE:N	1.97	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:36:ILE:HA	1:D:278:PRO:HG3	1.64	0.78
1:A:10:ILE:HD11	1:A:270:LEU:H	1.48	0.78
1:C:371:VAL:O	1:C:375:LEU:HB2	1.83	0.78
1:C:353:ARG:HB3	1:C:355:ASP:OD2	1.83	0.78
1:A:371:VAL:O	1:A:375:LEU:HB2	1.84	0.77
1:A:223:LEU:HD13	1:A:227:PHE:CD2	2.18	0.77
1:C:64:GLU:HG2	1:C:95:LYS:HB2	1.65	0.77
1:C:99:ARG:NH2	1:C:128:VAL:HB	2.00	0.77
1:C:106:ILE:HD12	1:C:154:HIS:CD2	2.19	0.77
1:B:405:ILE:O	1:B:408:ILE:HG22	1.85	0.77
1:D:215:MET:HE3	1:D:215:MET:HA	1.68	0.76
1:D:286:LEU:HD11	1:D:338:GLU:HB3	1.68	0.76
1:A:32:TYR:O	1:A:36:ILE:HG22	1.84	0.76
1:C:275:ILE:HD12	1:C:275:ILE:N	1.99	0.76
1:A:401:ASN:C	1:A:401:ASN:HD22	1.94	0.76
1:B:155:THR:OG1	1:B:248:THR:HG23	1.84	0.76
1:D:208:ILE:HG12	1:D:214:THR:HG22	1.66	0.76
1:A:102:SER:HB3	1:A:152:GLU:OE2	1.85	0.75
1:D:283:ILE:HD12	1:D:283:ILE:N	2.01	0.75
1:B:215:MET:HE3	1:B:215:MET:HA	1.69	0.75
1:B:283:ILE:HD12	1:B:283:ILE:N	2.01	0.75
1:C:181:LEU:HB3	1:C:183:ILE:CD1	2.16	0.75
1:D:16:ILE:HD13	1:D:261:ILE:CD1	2.16	0.75
1:D:155:THR:OG1	1:D:248:THR:HG23	1.85	0.75
1:A:22:PRO:HD3	1:B:108:TYR:CE2	2.21	0.75
1:B:16:ILE:HD13	1:B:261:ILE:CD1	2.15	0.75
1:C:401:ASN:C	1:C:401:ASN:HD22	1.95	0.75
1:A:159:THR:HG23	1:A:162:GLU:H	1.51	0.75
1:A:64:GLU:HG2	1:A:95:LYS:HB2	1.67	0.75
1:A:397:LEU:HD21	1:A:404:GLU:OE2	1.87	0.75
1:C:75:LYS:O	1:C:77:PHE:N	2.20	0.75
1:A:175:LYS:HG2	1:A:185:TYR:OH	1.86	0.75
1:D:349:ILE:HG22	1:D:362:VAL:O	1.87	0.75
1:B:208:ILE:HG12	1:B:214:THR:HG22	1.67	0.74
1:B:40:THR:HG21	1:B:257:ILE:HG22	1.68	0.74
1:C:32:TYR:O	1:C:36:ILE:HG22	1.86	0.74
1:C:159:THR:HG23	1:C:162:GLU:H	1.52	0.74
1:C:10:ILE:HD11	1:C:270:LEU:H	1.53	0.74
1:B:344:ILE:HD12	1:B:345:GLU:N	2.01	0.74
1:C:222:ASN:HD22	1:C:223:LEU:N	1.85	0.74
1:A:92:LEU:C	1:A:94:VAL:H	1.92	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:349:ILE:HG22	1:B:362:VAL:O	1.87	0.74
1:C:35:LYS:C	1:C:37:ARG:H	1.94	0.74
1:C:92:LEU:C	1:C:94:VAL:H	1.91	0.74
1:C:282:VAL:HG23	1:C:333:VAL:HG11	1.68	0.74
1:D:344:ILE:HD12	1:D:345:GLU:N	2.01	0.74
1:A:75:LYS:O	1:A:77:PHE:N	2.21	0.74
1:B:1:LEU:HD12	1:B:1:LEU:H	1.52	0.74
1:B:36:ILE:HA	1:B:278:PRO:HG3	1.69	0.74
1:D:127:ILE:HG12	1:D:151:LYS:CG	2.17	0.73
1:D:335:LEU:HD11	1:D:374:THR:HG21	1.69	0.73
1:B:127:ILE:HG12	1:B:151:LYS:CG	2.17	0.73
1:C:181:LEU:HB3	1:C:183:ILE:HD13	1.69	0.73
1:A:181:LEU:HB3	1:A:183:ILE:CD1	2.19	0.73
1:A:273:PRO:HG3	1:A:382:ILE:HD11	1.71	0.73
1:C:175:LYS:HG2	1:C:185:TYR:OH	1.88	0.73
1:D:10:ILE:CD1	1:D:270:LEU:HB2	2.19	0.73
1:D:24:LYS:HG3	1:D:138:THR:HG23	1.70	0.73
1:A:222:ASN:HD22	1:A:223:LEU:N	1.86	0.72
1:B:10:ILE:CD1	1:B:270:LEU:HB2	2.19	0.72
1:A:329:GLU:HG3	1:A:354:ARG:CD	2.19	0.72
1:A:101:THR:O	1:A:102:SER:HB2	1.88	0.72
1:A:353:ARG:HB3	1:A:355:ASP:OD2	1.88	0.72
1:D:1:LEU:HD12	1:D:1:LEU:H	1.53	0.72
1:D:40:THR:HG21	1:D:257:ILE:HG22	1.70	0.72
1:C:22:PRO:HD3	1:D:108:TYR:CE2	2.24	0.72
1:C:101:THR:O	1:C:102:SER:HB2	1.89	0.72
1:B:281:VAL:HB	1:B:312:VAL:HG12	1.69	0.71
1:C:275:ILE:H	1:C:275:ILE:CD1	2.02	0.71
1:D:127:ILE:HA	1:D:151:LYS:HA	1.71	0.71
1:D:270:LEU:O	1:D:332:GLY:HA2	1.90	0.71
1:A:100:PRO:HG2	1:A:101:THR:H	1.56	0.71
1:B:24:LYS:HG3	1:B:138:THR:HG23	1.71	0.71
1:B:181:LEU:HB3	1:B:183:ILE:HD12	1.72	0.71
1:C:223:LEU:HD13	1:C:227:PHE:CD2	2.25	0.71
1:C:295:VAL:HG13	1:C:339:VAL:HG12	1.73	0.71
1:C:329:GLU:HG3	1:C:354:ARG:CD	2.20	0.71
1:D:182:GLY:HA2	1:D:383:LYS:HG3	1.73	0.71
1:A:409:LEU:HD21	1:A:416:ILE:HG12	1.73	0.71
1:B:127:ILE:HA	1:B:151:LYS:HA	1.72	0.71
1:C:100:PRO:HG2	1:C:101:THR:H	1.56	0.71
1:B:43:ILE:HD11	1:B:275:ILE:HG21	1.73	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:256:VAL:HG23	1:C:257:ILE:N	2.05	0.71
1:C:397:LEU:HD21	1:C:404:GLU:OE2	1.91	0.71
1:A:275:ILE:H	1:A:275:ILE:CD1	2.03	0.70
1:A:101:THR:HG23	1:A:102:SER:N	2.06	0.70
1:B:102:SER:HB3	1:B:152:GLU:OE1	1.91	0.70
1:A:378:ILE:O	1:A:382:ILE:HG23	1.92	0.70
1:C:60:MET:HE1	1:D:60:MET:HE1	1.72	0.70
1:C:48:LEU:O	1:C:53:HIS:HB2	1.91	0.70
1:C:353:ARG:C	1:C:355:ASP:H	2.00	0.70
1:D:178:PHE:HE2	1:D:256:VAL:HG12	1.55	0.70
1:A:295:VAL:HG13	1:A:339:VAL:HG12	1.74	0.70
1:C:273:PRO:HG3	1:C:382:ILE:HD11	1.74	0.70
1:D:281:VAL:HB	1:D:312:VAL:HG12	1.73	0.70
1:C:102:SER:HB3	1:C:152:GLU:OE2	1.91	0.70
1:D:181:LEU:HB3	1:D:183:ILE:HD12	1.74	0.70
1:A:36:ILE:O	1:A:36:ILE:HD13	1.92	0.69
1:B:182:GLY:HA2	1:B:383:LYS:HG3	1.74	0.69
1:C:378:ILE:O	1:C:382:ILE:HG23	1.92	0.69
1:A:35:LYS:C	1:A:37:ARG:H	1.99	0.69
1:A:342:LYS:O	1:A:342:LYS:HD3	1.92	0.69
1:B:253:SER:O	1:B:256:VAL:HG22	1.91	0.69
1:B:272:LEU:HD11	1:B:278:PRO:HD2	1.73	0.69
1:B:48:LEU:CD1	1:B:151:LYS:HD2	2.18	0.69
1:B:270:LEU:O	1:B:332:GLY:HA2	1.92	0.69
1:D:24:LYS:HG3	1:D:138:THR:CG2	2.23	0.69
1:B:276:VAL:O	1:B:278:PRO:HD3	1.93	0.69
1:C:36:ILE:HD13	1:C:36:ILE:O	1.93	0.69
1:A:396:ILE:H	1:A:396:ILE:CD1	1.97	0.69
1:D:102:SER:HB3	1:D:152:GLU:OE1	1.93	0.69
1:A:181:LEU:HB3	1:A:183:ILE:HD13	1.74	0.68
1:C:405:ILE:HA	1:C:408:ILE:HG22	1.75	0.68
1:A:48:LEU:O	1:A:53:HIS:HB2	1.92	0.68
1:A:110:MET:O	1:A:114:VAL:HG23	1.93	0.68
1:B:190:ARG:NH2	1:B:438:LEU:HD22	2.08	0.68
1:C:101:THR:HG23	1:C:102:SER:N	2.08	0.68
1:C:254:ASP:O	1:C:257:ILE:HG23	1.93	0.68
1:C:396:ILE:H	1:C:396:ILE:CD1	2.02	0.68
1:D:190:ARG:NH2	1:D:438:LEU:HD22	2.07	0.68
1:D:43:ILE:HD11	1:D:275:ILE:HG21	1.75	0.68
1:D:207:THR:CG2	1:D:215:MET:HB3	2.23	0.68
1:A:156:ALA:HB2	1:A:247:GLN:HE22	1.58	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:405:ILE:HA	1:A:408:ILE:HG22	1.75	0.68
1:A:329:GLU:HG3	1:A:354:ARG:HD2	1.75	0.68
1:C:342:LYS:O	1:C:342:LYS:HD3	1.94	0.68
1:A:256:VAL:HG23	1:A:257:ILE:N	2.07	0.68
1:C:178:PHE:CZ	1:C:218:ALA:HB2	2.29	0.68
1:D:140:PRO:O	1:D:142:ILE:HD12	1.93	0.68
1:B:181:LEU:HB3	1:B:183:ILE:CD1	2.24	0.68
1:B:343:ASP:HB3	1:B:348:LYS:O	1.94	0.68
1:C:110:MET:O	1:C:114:VAL:HG23	1.94	0.68
1:A:178:PHE:CZ	1:A:218:ALA:HB2	2.29	0.67
1:D:343:ASP:HB3	1:D:348:LYS:O	1.94	0.67
1:B:335:LEU:HD11	1:B:374:THR:HG21	1.74	0.67
1:C:409:LEU:HD21	1:C:416:ILE:HG12	1.77	0.67
1:C:10:ILE:C	1:C:12:GLU:H	2.02	0.67
1:D:205:PHE:HB2	1:D:218:ALA:HB3	1.76	0.67
1:C:443:TYR:H	1:C:448:TYR:HE1	1.43	0.67
1:D:151:LYS:O	1:D:151:LYS:HE2	1.95	0.67
1:A:67:LEU:HD11	1:A:77:PHE:HE2	1.60	0.67
1:A:353:ARG:C	1:A:355:ASP:H	2.03	0.67
1:B:24:LYS:HG3	1:B:138:THR:CG2	2.25	0.67
1:D:48:LEU:CD1	1:D:151:LYS:HD2	2.19	0.67
1:D:253:SER:O	1:D:256:VAL:HG22	1.93	0.67
1:D:272:LEU:HD11	1:D:278:PRO:HD2	1.74	0.67
1:B:101:THR:HG23	1:B:103:GLU:HG2	1.75	0.67
1:B:413:ARG:HB2	1:B:413:ARG:HH11	1.59	0.66
1:C:156:ALA:HB2	1:C:247:GLN:HE22	1.60	0.66
1:A:288:PHE:O	1:A:292:GLU:HG3	1.96	0.66
1:A:326:ASN:O	1:A:330:ILE:HG13	1.95	0.66
1:D:413:ARG:HB2	1:D:413:ARG:HH11	1.59	0.66
1:A:10:ILE:C	1:A:12:GLU:H	2.02	0.66
1:A:48:LEU:HD11	1:A:151:LYS:HD2	1.77	0.66
1:A:74:ILE:HG22	1:A:74:ILE:O	1.96	0.66
1:A:92:LEU:O	1:A:94:VAL:HG23	1.94	0.66
1:C:270:LEU:O	1:C:271:ILE:HG13	1.96	0.66
1:B:205:PHE:HB2	1:B:218:ALA:HB3	1.77	0.66
1:C:48:LEU:HD11	1:C:151:LYS:HD2	1.77	0.66
1:B:167:VAL:HG13	1:B:220:VAL:CG1	2.26	0.66
1:C:10:ILE:CD1	1:C:270:LEU:HD13	2.25	0.66
1:D:167:VAL:HG13	1:D:220:VAL:CG1	2.26	0.66
1:C:92:LEU:O	1:C:94:VAL:HG23	1.95	0.66
1:C:413:ARG:NH1	1:C:413:ARG:HB2	2.10	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:178:PHE:HE2	1:B:256:VAL:HG12	1.61	0.66
1:C:288:PHE:O	1:C:292:GLU:HG3	1.96	0.66
1:D:181:LEU:HB3	1:D:183:ILE:CD1	2.25	0.66
1:A:413:ARG:NH1	1:A:413:ARG:HB2	2.11	0.66
1:C:397:LEU:HD23	1:C:399:ASP:O	1.96	0.66
1:C:35:LYS:O	1:C:37:ARG:N	2.26	0.66
1:A:338:GLU:HB2	1:A:350:THR:HG23	1.78	0.65
1:A:353:ARG:O	1:A:355:ASP:N	2.30	0.65
1:B:207:THR:CG2	1:B:215:MET:HB3	2.26	0.65
1:C:329:GLU:HG3	1:C:354:ARG:HD2	1.77	0.65
1:B:140:PRO:O	1:B:142:ILE:HD12	1.96	0.65
1:C:353:ARG:O	1:C:355:ASP:N	2.30	0.65
1:D:353:ARG:HD3	1:D:358:GLU:OE2	1.96	0.65
1:B:353:ARG:HD3	1:B:358:GLU:OE2	1.96	0.65
1:C:73:HIS:O	1:C:74:ILE:HG13	1.96	0.65
1:B:389:LYS:HB3	1:B:389:LYS:HZ3	1.62	0.65
1:D:445:GLY:O	1:D:447:LYS:N	2.30	0.65
1:B:151:LYS:HE2	1:B:151:LYS:O	1.97	0.65
1:A:443:TYR:H	1:A:448:TYR:HE1	1.45	0.65
1:D:36:ILE:CA	1:D:278:PRO:HG3	2.26	0.65
1:A:73:HIS:O	1:A:74:ILE:HG13	1.97	0.65
1:D:101:THR:HG23	1:D:103:GLU:HG2	1.77	0.65
1:D:283:ILE:HA	1:D:337:ILE:HB	1.78	0.65
1:B:283:ILE:HD12	1:B:283:ILE:H	1.62	0.64
1:C:16:ILE:HD11	1:C:270:LEU:HD21	1.79	0.64
1:C:74:ILE:HG22	1:C:74:ILE:O	1.98	0.64
1:B:445:GLY:O	1:B:447:LYS:N	2.31	0.64
1:C:82:TYR:CD2	1:D:84:VAL:HG11	2.26	0.64
1:B:415:VAL:HA	1:B:452:ALA:HB2	1.79	0.64
1:C:67:LEU:HD11	1:C:77:PHE:HE2	1.63	0.64
1:B:149:THR:HB	1:B:254:ASP:OD2	1.97	0.64
1:C:395:THR:HB	1:C:416:ILE:CD1	2.28	0.64
1:D:291:LYS:HB3	1:D:294:ILE:HG21	1.78	0.64
1:A:102:SER:HB3	1:A:152:GLU:CD	2.22	0.64
1:A:397:LEU:HD23	1:A:399:ASP:O	1.98	0.64
1:B:291:LYS:HB3	1:B:294:ILE:HG21	1.78	0.64
1:B:396:ILE:HD12	1:B:396:ILE:N	2.13	0.64
1:C:60:MET:HE1	1:D:60:MET:CE	2.27	0.64
1:C:338:GLU:HB2	1:C:350:THR:HG23	1.80	0.64
1:A:401:ASN:C	1:A:401:ASN:ND2	2.53	0.63
1:D:16:ILE:HD11	1:D:270:LEU:HD22	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:220:VAL:HA	1:D:250:TYR:HB3	1.80	0.63
1:A:60:MET:HE1	1:B:60:MET:HE1	1.80	0.63
1:A:70:GLU:HG2	1:A:77:PHE:CZ	2.32	0.63
1:D:69:LYS:C	1:D:71:ALA:H	2.05	0.63
1:D:178:PHE:CE2	1:D:256:VAL:HG12	2.33	0.63
1:D:214:THR:OG1	1:D:454:THR:HG22	1.98	0.63
1:D:286:LEU:H	1:D:286:LEU:CD1	2.09	0.63
1:B:69:LYS:C	1:B:71:ALA:H	2.04	0.63
1:B:266:ASP:CG	1:B:271:ILE:HD11	2.23	0.63
1:C:102:SER:HB3	1:C:152:GLU:CD	2.23	0.63
1:C:369:GLU:HG3	1:C:370:VAL:N	2.12	0.63
1:D:92:LEU:C	1:D:94:VAL:H	2.07	0.63
1:D:276:VAL:O	1:D:278:PRO:HD3	1.97	0.63
1:D:415:VAL:HA	1:D:452:ALA:HB2	1.80	0.63
1:A:337:ILE:HG12	1:A:351:LEU:CD1	2.20	0.63
1:B:64:GLU:HG2	1:B:83:TRP:CH2	2.33	0.63
1:B:142:ILE:HG22	1:B:143:ARG:N	2.13	0.63
1:D:396:ILE:N	1:D:396:ILE:HD12	2.14	0.63
1:A:58:PHE:H	1:A:126:GLN:HE22	1.46	0.63
1:B:214:THR:OG1	1:B:454:THR:HG22	1.99	0.63
1:B:220:VAL:HA	1:B:250:TYR:HB3	1.81	0.63
1:C:354:ARG:O	1:C:354:ARG:NE	2.32	0.63
1:D:266:ASP:CG	1:D:271:ILE:HD11	2.24	0.63
1:D:350:THR:HA	1:D:361:GLN:HG2	1.81	0.63
1:A:55:GLU:HA	1:A:125:TYR:O	1.99	0.62
1:C:401:ASN:C	1:C:401:ASN:ND2	2.54	0.62
1:A:430:GLU:C	1:A:432:LYS:H	2.04	0.62
1:C:36:ILE:HG13	1:C:272:LEU:HD22	1.81	0.62
1:C:127:ILE:HG22	1:C:127:ILE:O	1.99	0.62
1:C:178:PHE:HZ	1:C:218:ALA:HB2	1.63	0.62
1:C:326:ASN:O	1:C:330:ILE:HG13	1.99	0.62
1:A:328:TRP:CZ3	1:A:331:LYS:HD2	2.35	0.62
1:C:58:PHE:HD1	1:C:126:GLN:NE2	1.97	0.62
1:D:283:ILE:HD12	1:D:283:ILE:H	1.64	0.62
1:A:82:TYR:CD2	1:B:84:VAL:HG11	2.28	0.62
1:A:178:PHE:HZ	1:A:218:ALA:HB2	1.62	0.62
1:B:178:PHE:CE2	1:B:217:ILE:HD12	2.35	0.62
1:C:323:ARG:O	1:C:327:ASP:N	2.25	0.62
1:D:190:ARG:HH21	1:D:438:LEU:HD22	1.64	0.62
1:C:10:ILE:HD13	1:C:270:LEU:HD13	1.82	0.62
1:C:234:ILE:HD12	1:C:234:ILE:C	2.25	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:64:GLU:HG2	1:D:83:TRP:CH2	2.34	0.62
1:D:389:LYS:HB3	1:D:389:LYS:HZ3	1.65	0.62
1:B:127:ILE:HG12	1:B:151:LYS:CB	2.29	0.62
1:C:58:PHE:H	1:C:126:GLN:HE22	1.48	0.62
1:C:360:PHE:HD2	1:C:360:PHE:N	1.96	0.62
1:D:127:ILE:HG12	1:D:151:LYS:CB	2.29	0.62
1:D:149:THR:HB	1:D:254:ASP:OD2	1.99	0.62
1:A:65:ASP:O	1:A:68:ALA:HB3	1.99	0.62
1:A:215:MET:HA	2:A:460:HOH:O	1.98	0.62
1:B:379:MET:O	1:B:382:ILE:HG12	2.00	0.62
1:C:1:LEU:HD13	1:C:6:TRP:HB2	1.81	0.62
1:C:70:GLU:HG2	1:C:77:PHE:CZ	2.34	0.62
1:C:208:ILE:HD11	1:C:415:VAL:HG12	1.81	0.62
1:C:222:ASN:HD22	1:C:222:ASN:C	2.05	0.62
1:D:379:MET:O	1:D:382:ILE:HG12	2.00	0.62
1:A:1:LEU:HD13	1:A:6:TRP:HB2	1.81	0.62
1:A:224:GLY:O	1:A:246:TYR:HA	2.00	0.62
1:A:254:ASP:O	1:A:257:ILE:HG23	2.00	0.62
1:A:395:THR:HB	1:A:416:ILE:CD1	2.30	0.62
1:B:291:LYS:HD2	1:B:291:LYS:N	2.14	0.62
1:D:142:ILE:HG22	1:D:143:ARG:N	2.13	0.62
1:A:369:GLU:HG3	1:A:370:VAL:N	2.14	0.61
1:B:322:GLY:HA2	1:B:325:PHE:HD2	1.63	0.61
1:D:191:PRO:HB2	1:D:193:TRP:CZ3	2.35	0.61
1:A:234:ILE:HD12	1:A:234:ILE:C	2.25	0.61
1:A:360:PHE:HD2	1:A:360:PHE:N	1.97	0.61
1:B:58:PHE:N	1:B:126:GLN:HE22	1.88	0.61
1:B:274:PRO:HD2	1:B:379:MET:HB2	1.81	0.61
1:A:142:ILE:HG22	1:A:143:ARG:N	2.13	0.61
1:A:328:TRP:HZ3	1:A:331:LYS:HD2	1.64	0.61
1:C:48:LEU:HD22	1:C:53:HIS:CD2	2.36	0.61
1:A:36:ILE:HG13	1:A:272:LEU:HD22	1.83	0.61
1:B:270:LEU:HB3	1:B:330:ILE:O	2.00	0.61
1:A:48:LEU:HD22	1:A:53:HIS:CD2	2.36	0.61
1:A:354:ARG:NE	1:A:354:ARG:O	2.33	0.61
1:B:16:ILE:HD11	1:B:270:LEU:HD22	1.82	0.61
1:B:36:ILE:CA	1:B:278:PRO:HG3	2.29	0.61
1:B:283:ILE:HA	1:B:337:ILE:HB	1.82	0.61
1:A:127:ILE:O	1:A:127:ILE:HG22	2.01	0.61
1:A:223:LEU:HD13	1:A:227:PHE:HD2	1.62	0.61
1:A:323:ARG:O	1:A:327:ASP:N	2.26	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:190:ARG:NH2	1:C:216:GLN:HE21	1.99	0.61
1:B:272:LEU:CD1	1:B:277:ALA:HA	2.29	0.61
1:B:286:LEU:H	1:B:286:LEU:CD1	2.11	0.61
1:A:211:ASP:OD2	1:A:213:ARG:HB2	2.01	0.61
1:B:92:LEU:C	1:B:94:VAL:H	2.09	0.61
1:B:373:LYS:HB2	1:B:373:LYS:NZ	2.16	0.61
1:C:430:GLU:C	1:C:432:LYS:H	2.06	0.61
1:B:123:LYS:HA	1:B:155:THR:HG22	1.82	0.61
1:B:178:PHE:CE2	1:B:256:VAL:HG12	2.35	0.61
1:D:373:LYS:HB2	1:D:373:LYS:NZ	2.16	0.61
1:A:21:TYR:HB3	1:A:26:CYS:O	2.00	0.61
1:A:270:LEU:O	1:A:271:ILE:HG13	2.01	0.61
1:B:43:ILE:HD11	1:B:275:ILE:CG2	2.31	0.61
1:C:211:ASP:OD2	1:C:213:ARG:HB2	2.01	0.61
1:D:256:VAL:HG23	1:D:257:ILE:H	1.66	0.61
1:C:55:GLU:HA	1:C:125:TYR:O	2.01	0.60
1:C:337:ILE:HG12	1:C:351:LEU:CD1	2.23	0.60
1:D:291:LYS:HD2	1:D:291:LYS:N	2.15	0.60
1:B:41:PHE:CE2	1:B:149:THR:HG22	2.36	0.60
1:C:157:HIS:CD2	1:C:163:ALA:HA	2.36	0.60
1:D:274:PRO:HD2	1:D:379:MET:HB2	1.83	0.60
1:D:295:VAL:C	1:D:297:GLU:H	2.08	0.60
1:B:190:ARG:HH21	1:B:438:LEU:HD22	1.65	0.60
1:D:43:ILE:HD11	1:D:275:ILE:CG2	2.31	0.60
1:D:322:GLY:HA2	1:D:325:PHE:HD2	1.64	0.60
1:B:191:PRO:HB2	1:B:193:TRP:CZ3	2.36	0.60
1:C:55:GLU:HB2	1:C:125:TYR:CE1	2.35	0.60
1:A:55:GLU:HB2	1:A:125:TYR:CE1	2.35	0.60
1:B:75:LYS:O	1:B:77:PHE:HB3	2.02	0.60
1:B:295:VAL:C	1:B:297:GLU:H	2.08	0.60
1:D:237:THR:CG2	1:D:243:ASP:HB2	2.32	0.60
1:D:270:LEU:HB3	1:D:330:ILE:O	2.02	0.60
1:A:59:PRO:HG2	1:B:21:TYR:CD1	2.36	0.60
1:A:236:GLU:HG3	1:A:242:LYS:HE2	1.84	0.60
1:B:30:LEU:O	1:B:33:GLY:N	2.34	0.60
1:C:21:TYR:HB3	1:C:26:CYS:O	2.01	0.60
1:C:373:LYS:HB2	1:C:373:LYS:NZ	2.16	0.60
1:A:266:ASP:CG	1:A:354:ARG:HH22	2.09	0.60
1:B:355:ASP:OD1	1:B:378:ILE:HA	2.00	0.60
1:C:124:ILE:HA	2:C:476:HOH:O	2.01	0.60
1:D:178:PHE:CE2	1:D:217:ILE:HD12	2.37	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:320:ARG:NH1	1:A:322:GLY:HA3	2.17	0.60
1:B:237:THR:CG2	1:B:243:ASP:HB2	2.32	0.60
1:B:350:THR:HA	1:B:361:GLN:HG2	1.84	0.60
1:C:142:ILE:HG22	1:C:143:ARG:N	2.15	0.60
1:A:120:LEU:HD13	1:A:157:HIS:C	2.27	0.59
1:A:157:HIS:CD2	1:A:163:ALA:HA	2.37	0.59
1:A:275:ILE:N	1:A:275:ILE:CD1	2.65	0.59
1:A:388:GLU:OE1	1:C:108:TYR:HE1	1.85	0.59
1:D:29:TYR:HE2	1:D:257:ILE:CD1	2.15	0.59
1:D:104:THR:N	1:D:105:PRO:HD2	2.17	0.59
1:B:285:PRO:O	1:B:287:ILE:HG23	2.02	0.59
1:D:229:LYS:HA	1:D:244:TYR:CD2	2.37	0.59
1:B:196:PHE:CD1	1:B:197:PRO:HD2	2.37	0.59
1:B:214:THR:HG1	1:B:454:THR:HG22	1.67	0.59
1:A:190:ARG:NH2	1:A:216:GLN:HE21	2.00	0.59
1:C:325:PHE:HB3	1:C:336:ARG:NH2	2.17	0.59
1:C:328:TRP:HZ3	1:C:331:LYS:HD2	1.67	0.59
1:D:196:PHE:CD1	1:D:197:PRO:HD2	2.37	0.59
1:D:385:ARG:O	1:D:388:GLU:HB3	2.02	0.59
1:A:10:ILE:HD13	1:A:270:LEU:HD13	1.85	0.59
1:A:396:ILE:HD12	1:A:396:ILE:N	2.06	0.59
1:C:299:ALA:HB1	1:C:314:ILE:HD13	1.84	0.59
1:C:328:TRP:CZ3	1:C:331:LYS:HD2	2.38	0.59
1:B:229:LYS:HA	1:B:244:TYR:CD2	2.38	0.59
1:C:236:GLU:HG3	1:C:242:LYS:HE2	1.85	0.59
1:D:355:ASP:OD1	1:D:378:ILE:HA	2.02	0.59
1:A:66:LEU:H	1:A:66:LEU:HD12	1.67	0.59
1:B:127:ILE:CG1	1:B:151:LYS:HG3	2.32	0.59
1:D:60:MET:HA	1:D:99:ARG:HD3	1.85	0.59
1:D:75:LYS:O	1:D:77:PHE:HB3	2.03	0.59
1:D:41:PHE:CE2	1:D:149:THR:HG22	2.38	0.59
1:A:284:VAL:O	1:A:286:LEU:HD12	2.02	0.59
1:A:10:ILE:CD1	1:A:270:LEU:HD13	2.33	0.59
1:B:256:VAL:HG23	1:B:257:ILE:H	1.68	0.59
1:C:65:ASP:O	1:C:68:ALA:HB3	2.02	0.59
1:C:350:THR:HB	1:C:361:GLN:HG2	1.85	0.59
1:D:58:PHE:N	1:D:126:GLN:HE22	1.90	0.59
1:A:114:VAL:HG22	1:A:122:ILE:HD11	1.85	0.58
1:A:222:ASN:HD22	1:A:222:ASN:C	2.08	0.58
1:B:116:VAL:HG23	1:B:118:THR:HB	1.84	0.58
1:C:59:PRO:HG2	1:D:21:TYR:CD1	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:120:LEU:HD13	1:C:157:HIS:C	2.27	0.58
1:D:67:LEU:O	1:D:70:GLU:HB3	2.02	0.58
1:D:123:LYS:HA	1:D:155:THR:HG22	1.84	0.58
1:D:127:ILE:CG1	1:D:151:LYS:HG3	2.32	0.58
1:C:395:THR:HB	1:C:416:ILE:HD12	1.86	0.58
1:D:282:VAL:HG23	1:D:333:VAL:HG11	1.85	0.58
1:B:237:THR:HG23	1:B:243:ASP:HB2	1.86	0.58
1:C:114:VAL:HG22	1:C:122:ILE:HD11	1.86	0.58
1:A:58:PHE:H	1:A:126:GLN:NE2	2.00	0.58
1:A:350:THR:HB	1:A:361:GLN:HG2	1.86	0.58
1:B:385:ARG:O	1:B:388:GLU:HB3	2.03	0.58
1:B:399:ASP:OD2	1:B:401:ASN:HB2	2.03	0.58
1:C:92:LEU:C	1:C:94:VAL:N	2.60	0.58
1:D:190:ARG:NH1	1:D:204:ALA:HB3	2.14	0.58
1:D:389:LYS:HB3	1:D:389:LYS:HZ2	1.68	0.58
1:B:67:LEU:O	1:B:70:GLU:HB3	2.02	0.58
1:B:29:TYR:HE2	1:B:257:ILE:CD1	2.17	0.58
1:B:402:PRO:HG2	1:B:403:ASP:H	1.67	0.58
1:A:92:LEU:C	1:A:94:VAL:N	2.61	0.58
1:A:184:PRO:HB3	1:A:390:PHE:CG	2.39	0.58
1:A:373:LYS:HB2	1:A:373:LYS:NZ	2.18	0.58
1:B:181:LEU:HD22	1:B:260:ILE:HD11	1.86	0.58
1:C:351:LEU:HB2	1:C:360:PHE:CE2	2.38	0.58
1:D:10:ILE:O	1:D:11:LEU:C	2.47	0.58
1:D:214:THR:HG1	1:D:454:THR:HG22	1.69	0.58
1:D:402:PRO:C	1:D:404:GLU:N	2.61	0.58
1:C:266:ASP:CG	1:C:354:ARG:HH22	2.11	0.58
1:D:399:ASP:OD2	1:D:401:ASN:HB2	2.04	0.58
1:A:54:ASP:O	1:A:124:ILE:HG13	2.04	0.58
1:A:344:ILE:HD12	1:A:345:GLU:N	2.19	0.58
1:B:66:LEU:C	1:B:68:ALA:H	2.12	0.58
1:B:175:LYS:HG3	1:B:185:TYR:OH	2.04	0.58
1:B:234:ILE:C	1:B:234:ILE:HD12	2.29	0.58
1:C:54:ASP:O	1:C:124:ILE:HG13	2.04	0.58
1:C:284:VAL:O	1:C:286:LEU:HD12	2.03	0.58
1:C:159:THR:HG23	1:C:162:GLU:HB2	1.85	0.57
1:D:116:VAL:HG23	1:D:118:THR:HB	1.85	0.57
1:A:437:ILE:HG22	1:A:439:GLY:H	1.69	0.57
1:B:10:ILE:O	1:B:11:LEU:C	2.47	0.57
1:C:184:PRO:HB3	1:C:390:PHE:CG	2.39	0.57
1:C:205:PHE:HB2	1:C:218:ALA:HB3	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:224:GLY:O	1:C:246:TYR:HA	2.04	0.57
1:A:229:LYS:HA	1:A:244:TYR:CD2	2.40	0.57
1:A:298:LYS:O	1:A:302:ILE:HG13	2.04	0.57
1:C:41:PHE:O	1:C:44:ILE:HG22	2.04	0.57
1:C:396:ILE:HD12	1:C:396:ILE:N	2.07	0.57
1:D:402:PRO:HG2	1:D:403:ASP:H	1.68	0.57
1:A:34:PHE:O	1:A:37:ARG:HB3	2.04	0.57
1:C:142:ILE:HD13	1:C:215:MET:HE1	1.87	0.57
1:D:75:LYS:O	1:D:76:GLY:C	2.46	0.57
1:D:237:THR:HG23	1:D:243:ASP:HB2	1.87	0.57
1:D:395:THR:HB	1:D:416:ILE:CD1	2.33	0.57
1:A:331:LYS:NZ	2:A:485:HOH:O	2.27	0.57
1:B:190:ARG:NH1	1:B:204:ALA:HB3	2.14	0.57
1:C:391:GLU:HA	1:C:394:ILE:HD12	1.84	0.57
1:D:234:ILE:C	1:D:234:ILE:HD12	2.29	0.57
1:A:60:MET:HE1	1:B:60:MET:CE	2.34	0.57
1:A:123:LYS:HA	1:A:155:THR:HA	1.87	0.57
1:A:351:LEU:HB2	1:A:360:PHE:CE2	2.38	0.57
1:C:58:PHE:H	1:C:126:GLN:NE2	2.02	0.57
1:D:18:ASP:CB	1:D:30:LEU:HD11	2.29	0.57
1:D:92:LEU:O	1:D:94:VAL:N	2.38	0.57
1:B:104:THR:N	1:B:105:PRO:HD2	2.20	0.57
1:A:35:LYS:O	1:A:37:ARG:N	2.35	0.57
1:B:402:PRO:C	1:B:404:GLU:N	2.62	0.57
1:B:60:MET:HA	1:B:99:ARG:HD3	1.87	0.57
1:B:122:ILE:O	1:B:122:ILE:HG13	2.05	0.57
1:C:319:ILE:HG13	1:C:320:ARG:N	2.20	0.57
1:D:449:ILE:HG22	1:D:449:ILE:O	2.04	0.57
1:A:405:ILE:HG23	1:A:416:ILE:HG21	1.86	0.57
1:D:272:LEU:CD1	1:D:277:ALA:HA	2.34	0.57
1:A:319:ILE:HG13	1:A:320:ARG:N	2.20	0.56
1:A:395:THR:HB	1:A:416:ILE:HD12	1.88	0.56
1:B:353:ARG:HB3	1:B:355:ASP:OD2	2.03	0.56
1:B:395:THR:HG21	1:B:408:ILE:HD11	1.87	0.56
1:D:175:LYS:HG3	1:D:185:TYR:OH	2.05	0.56
1:D:395:THR:HG21	1:D:408:ILE:HD11	1.87	0.56
1:A:41:PHE:HD2	1:A:127:ILE:HD13	1.70	0.56
1:A:430:GLU:HG3	1:A:437:ILE:CG1	2.31	0.56
1:C:123:LYS:HA	1:C:155:THR:HA	1.87	0.56
1:C:262:ALA:O	1:C:263:ILE:C	2.48	0.56
1:C:344:ILE:C	1:C:344:ILE:HD12	2.30	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:344:ILE:HD12	1:C:345:GLU:N	2.20	0.56
1:A:29:TYR:HE1	1:A:148:MET:HB2	1.70	0.56
1:A:286:LEU:HD12	1:A:286:LEU:N	2.20	0.56
1:A:325:PHE:HB3	1:A:336:ARG:NH2	2.19	0.56
1:A:344:ILE:HD12	1:A:344:ILE:C	2.30	0.56
1:B:64:GLU:HG2	1:B:83:TRP:HH2	1.70	0.56
1:B:282:VAL:HG23	1:B:333:VAL:HG11	1.87	0.56
1:C:196:PHE:CG	1:C:197:PRO:HD2	2.40	0.56
1:D:66:LEU:C	1:D:68:ALA:H	2.13	0.56
1:D:141:LEU:N	1:D:144:LEU:HD21	2.14	0.56
1:D:270:LEU:O	1:D:332:GLY:CA	2.52	0.56
1:D:402:PRO:C	1:D:404:GLU:H	2.13	0.56
1:A:196:PHE:CG	1:A:197:PRO:HD2	2.40	0.56
1:A:205:PHE:HB2	1:A:218:ALA:HB3	1.86	0.56
1:A:381:ASN:HD21	1:A:385:ARG:CZ	2.18	0.56
1:A:391:GLU:HA	1:A:394:ILE:HD12	1.87	0.56
1:B:75:LYS:O	1:B:76:GLY:C	2.47	0.56
1:C:298:LYS:O	1:C:302:ILE:HG13	2.06	0.56
1:D:122:ILE:O	1:D:122:ILE:HG13	2.05	0.56
1:D:207:THR:HG22	1:D:215:MET:HB3	1.87	0.56
1:D:353:ARG:HB3	1:D:355:ASP:OD2	2.04	0.56
1:A:156:ALA:HB2	1:A:247:GLN:NE2	2.20	0.56
1:C:29:TYR:HE1	1:C:148:MET:HB2	1.71	0.56
1:C:169:GLU:O	1:C:173:ILE:HG12	2.06	0.56
1:C:430:GLU:HG3	1:C:437:ILE:CG1	2.32	0.56
1:D:229:LYS:HA	1:D:244:TYR:CE2	2.41	0.56
1:A:142:ILE:HD13	1:A:215:MET:HE1	1.88	0.56
1:A:223:LEU:HD13	1:A:227:PHE:CE2	2.41	0.56
1:A:302:ILE:HG23	1:A:367:LEU:HD21	1.88	0.56
1:A:394:ILE:HG12	1:A:415:VAL:CG1	2.34	0.56
1:B:99:ARG:HD2	1:B:102:SER:HB2	1.86	0.56
1:B:196:PHE:CG	1:B:197:PRO:HD2	2.40	0.56
1:C:229:LYS:HA	1:C:244:TYR:CD2	2.41	0.56
1:D:5:GLU:O	1:D:9:ASP:HB2	2.05	0.56
1:D:64:GLU:HG2	1:D:83:TRP:HH2	1.71	0.56
1:B:66:LEU:C	1:B:68:ALA:N	2.64	0.56
1:B:74:ILE:O	1:B:74:ILE:HG22	2.06	0.56
1:C:262:ALA:O	1:C:264:HIS:N	2.38	0.56
1:D:127:ILE:HG12	1:D:151:LYS:HB2	1.88	0.56
1:B:413:ARG:HH11	1:B:413:ARG:CB	2.18	0.56
1:C:101:THR:HG21	1:C:103:GLU:OE1	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:286:LEU:HD12	1:C:286:LEU:N	2.21	0.56
1:A:190:ARG:HG3	1:A:194:ASP:OD2	2.05	0.55
1:C:35:LYS:C	1:C:37:ARG:N	2.63	0.55
1:C:92:LEU:O	1:C:93:ASP:HB2	2.05	0.55
1:C:142:ILE:CG2	1:C:215:MET:HE1	2.35	0.55
1:C:190:ARG:HG3	1:C:194:ASP:OD2	2.05	0.55
1:A:58:PHE:HD1	1:A:126:GLN:NE2	2.03	0.55
1:A:159:THR:HG23	1:A:162:GLU:HB2	1.88	0.55
1:A:294:ILE:HG23	1:A:295:VAL:N	2.21	0.55
1:B:322:GLY:HA2	1:B:325:PHE:CD2	2.42	0.55
1:B:402:PRO:C	1:B:404:GLU:H	2.14	0.55
1:C:417:LEU:HA	1:C:449:ILE:O	2.07	0.55
1:B:19:VAL:HG11	1:B:140:PRO:HG3	1.88	0.55
1:B:127:ILE:HG12	1:B:151:LYS:HB2	1.88	0.55
1:C:127:ILE:HG12	1:C:151:LYS:CB	2.36	0.55
1:D:181:LEU:HD22	1:D:260:ILE:HD11	1.89	0.55
1:D:285:PRO:O	1:D:287:ILE:HG23	2.06	0.55
1:A:29:TYR:HE1	1:A:148:MET:CB	2.19	0.55
1:C:437:ILE:HG22	1:C:439:GLY:H	1.72	0.55
1:B:229:LYS:HA	1:B:244:TYR:CE2	2.42	0.55
1:D:66:LEU:C	1:D:68:ALA:N	2.64	0.55
1:D:196:PHE:CG	1:D:197:PRO:HD2	2.41	0.55
1:D:413:ARG:HH11	1:D:413:ARG:CB	2.19	0.55
1:A:41:PHE:CD2	1:A:127:ILE:HD13	2.42	0.55
1:A:220:VAL:HG22	1:A:250:TYR:HB3	1.88	0.55
1:B:159:THR:HG23	1:B:162:GLU:H	1.72	0.55
1:C:394:ILE:HG12	1:C:415:VAL:CG1	2.36	0.55
1:D:19:VAL:HG11	1:D:140:PRO:HG3	1.89	0.55
1:D:74:ILE:HG22	1:D:74:ILE:O	2.07	0.55
1:D:390:PHE:CE2	1:D:394:ILE:HD11	2.42	0.55
1:A:155:THR:OG1	1:A:248:THR:HG22	2.05	0.55
1:C:196:PHE:CD2	1:C:197:PRO:HD2	2.41	0.55
1:B:141:LEU:N	1:B:144:LEU:HD21	2.16	0.55
1:B:346:ASN:O	1:B:348:LYS:HG3	2.06	0.55
1:C:62:ILE:HD13	1:C:105:PRO:HD3	1.89	0.55
1:D:188:SER:HB3	1:D:438:LEU:O	2.07	0.55
1:A:62:ILE:HD13	1:A:105:PRO:HD3	1.89	0.55
1:A:417:LEU:HD12	1:A:450:ALA:HA	1.89	0.55
1:B:449:ILE:O	1:B:449:ILE:HG22	2.07	0.55
1:C:223:LEU:HD13	1:C:227:PHE:HD2	1.69	0.55
1:D:10:ILE:HD11	1:D:270:LEU:CB	2.32	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:134:GLU:H	1:D:145:ARG:HD2	1.71	0.55
1:D:159:THR:HG23	1:D:162:GLU:H	1.72	0.55
1:A:169:GLU:O	1:A:172:SER:HB3	2.07	0.54
1:A:417:LEU:HA	1:A:449:ILE:O	2.07	0.54
1:C:169:GLU:O	1:C:172:SER:HB3	2.07	0.54
1:C:302:ILE:HG23	1:C:367:LEU:HD21	1.89	0.54
1:D:322:GLY:HA2	1:D:325:PHE:CD2	2.42	0.54
1:C:247:GLN:HE21	1:C:247:GLN:HA	1.72	0.54
1:D:99:ARG:HD2	1:D:102:SER:HB2	1.88	0.54
1:D:222:ASN:C	1:D:222:ASN:HD22	2.15	0.54
1:A:299:ALA:HB1	1:A:314:ILE:HD13	1.90	0.54
1:C:60:MET:SD	1:D:60:MET:SD	3.04	0.54
1:B:86:HIS:ND1	1:B:91:GLN:HA	2.22	0.54
1:B:125:TYR:CB	1:B:153:ALA:HA	2.37	0.54
1:D:272:LEU:HD11	1:D:278:PRO:CD	2.36	0.54
1:A:17:TYR:CE2	1:A:19:VAL:HG12	2.42	0.54
1:A:209:PHE:CE1	1:A:215:MET:SD	3.01	0.54
1:C:17:TYR:CE2	1:C:19:VAL:HG12	2.42	0.54
1:C:156:ALA:HB2	1:C:247:GLN:NE2	2.22	0.54
1:C:294:ILE:HG23	1:C:295:VAL:N	2.23	0.54
1:C:397:LEU:HB2	1:C:418:VAL:HG12	1.89	0.54
1:D:189:LYS:O	1:D:190:ARG:C	2.51	0.54
1:A:25:GLY:HA3	1:A:145:ARG:HB2	1.89	0.54
1:A:167:VAL:HG13	1:A:220:VAL:HG11	1.89	0.54
1:A:190:ARG:HH21	1:A:216:GLN:HE21	1.55	0.54
1:B:389:LYS:HB3	1:B:389:LYS:HZ2	1.69	0.54
1:B:395:THR:HB	1:B:416:ILE:CD1	2.36	0.54
1:C:127:ILE:HG12	1:C:151:LYS:HB2	1.89	0.54
1:C:353:ARG:C	1:C:355:ASP:N	2.63	0.54
1:D:274:PRO:CD	1:D:379:MET:HB2	2.36	0.54
1:B:92:LEU:O	1:B:94:VAL:N	2.41	0.54
1:C:272:LEU:HD12	1:C:272:LEU:O	2.08	0.54
1:A:196:PHE:CD2	1:A:197:PRO:HD2	2.42	0.54
1:A:277:ALA:C	1:A:279:ILE:N	2.65	0.54
1:C:124:ILE:N	1:C:154:HIS:O	2.41	0.54
1:C:159:THR:CG2	1:C:162:GLU:HB2	2.37	0.54
1:C:167:VAL:HG13	1:C:220:VAL:HG11	1.89	0.54
1:D:125:TYR:CB	1:D:153:ALA:HA	2.37	0.54
1:D:286:LEU:HD12	1:D:286:LEU:N	2.12	0.54
1:D:295:VAL:C	1:D:297:GLU:N	2.65	0.54
1:A:430:GLU:CG	1:A:437:ILE:HG12	2.29	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:295:VAL:C	1:B:297:GLU:N	2.66	0.54
1:B:325:PHE:CD1	1:B:336:ARG:HD3	2.43	0.54
1:C:190:ARG:HH21	1:C:216:GLN:HE21	1.55	0.54
1:D:30:LEU:O	1:D:33:GLY:N	2.41	0.54
1:D:332:GLY:O	1:D:333:VAL:C	2.49	0.54
1:A:400:ILE:HD13	1:A:424:ILE:HD11	1.89	0.53
1:C:237:THR:C	1:C:239:THR:H	2.17	0.53
1:A:430:GLU:C	1:A:432:LYS:N	2.64	0.53
1:C:430:GLU:CG	1:C:437:ILE:HG12	2.31	0.53
1:D:86:HIS:ND1	1:D:91:GLN:HA	2.23	0.53
1:D:335:LEU:HD11	1:D:374:THR:CG2	2.38	0.53
1:A:92:LEU:O	1:A:93:ASP:HB2	2.07	0.53
1:A:262:ALA:O	1:A:263:ILE:C	2.51	0.53
1:C:381:ASN:HD21	1:C:385:ARG:CZ	2.22	0.53
1:A:30:LEU:O	1:A:31:PRO:C	2.51	0.53
1:A:262:ALA:O	1:A:264:HIS:N	2.41	0.53
1:C:25:GLY:HA3	1:C:145:ARG:HB2	1.90	0.53
1:C:277:ALA:C	1:C:279:ILE:N	2.66	0.53
1:A:53:HIS:NE2	1:A:250:TYR:OH	2.38	0.53
1:B:18:ASP:CB	1:B:30:LEU:HD11	2.32	0.53
1:C:209:PHE:CE1	1:C:215:MET:SD	3.02	0.53
1:C:320:ARG:NH1	1:C:322:GLY:HA3	2.23	0.53
1:A:101:THR:HG21	1:A:103:GLU:OE1	2.09	0.53
1:A:247:GLN:HE21	1:A:247:GLN:HA	1.74	0.53
1:B:222:ASN:C	1:B:222:ASN:HD22	2.17	0.53
1:B:332:GLY:O	1:B:333:VAL:C	2.51	0.53
1:C:99:ARG:O	1:C:99:ARG:HG3	2.09	0.53
1:C:417:LEU:HD12	1:C:450:ALA:HA	1.90	0.53
1:D:196:PHE:HB3	1:D:199:ALA:HB3	1.89	0.53
1:D:346:ASN:O	1:D:348:LYS:HG3	2.08	0.53
1:A:155:THR:OG1	1:A:248:THR:CG2	2.56	0.53
1:A:267:GLU:OE2	1:A:267:GLU:N	2.42	0.53
1:B:270:LEU:O	1:B:332:GLY:CA	2.56	0.53
1:C:41:PHE:CD2	1:C:127:ILE:HD13	2.44	0.53
1:C:112:LEU:HB3	1:D:20:ARG:NH2	2.23	0.53
1:D:402:PRO:O	1:D:404:GLU:N	2.42	0.53
1:A:401:ASN:HD22	1:A:402:PRO:N	2.06	0.53
1:B:189:LYS:O	1:B:190:ARG:C	2.52	0.53
1:C:110:MET:HE2	1:C:122:ILE:HG13	1.90	0.53
1:C:215:MET:HA	2:C:468:HOH:O	2.08	0.53
1:C:350:THR:C	1:C:351:LEU:HD13	2.34	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:397:LEU:HB2	1:A:418:VAL:HG12	1.91	0.53
1:B:160:LYS:HA	1:B:246:TYR:CD2	2.44	0.53
1:C:34:PHE:O	1:C:37:ARG:HB3	2.09	0.53
1:B:45:ARG:O	1:B:48:LEU:HB2	2.08	0.52
1:C:267:GLU:OE2	1:C:267:GLU:N	2.42	0.52
1:A:41:PHE:O	1:A:44:ILE:HG22	2.09	0.52
1:B:142:ILE:HA	1:B:255:ARG:HD3	1.91	0.52
1:B:175:LYS:HG3	1:B:185:TYR:CZ	2.44	0.52
1:B:272:LEU:HD12	1:B:277:ALA:HA	1.90	0.52
1:B:446:ASN:HB2	1:B:448:TYR:CE1	2.45	0.52
1:C:66:LEU:HD12	1:C:66:LEU:H	1.74	0.52
1:C:102:SER:C	1:C:105:PRO:HD2	2.34	0.52
1:C:202:THR:HG23	1:C:221:HIS:ND1	2.24	0.52
1:A:16:ILE:HD11	1:A:270:LEU:HD21	1.91	0.52
1:A:114:VAL:HG22	1:A:122:ILE:CD1	2.39	0.52
1:B:274:PRO:CD	1:B:379:MET:HB2	2.38	0.52
1:C:405:ILE:HG23	1:C:416:ILE:HG21	1.90	0.52
1:A:237:THR:C	1:A:239:THR:H	2.18	0.52
1:B:5:GLU:O	1:B:9:ASP:HB2	2.09	0.52
1:B:134:GLU:H	1:B:145:ARG:HD2	1.74	0.52
1:A:1:LEU:HD12	1:A:1:LEU:H	1.75	0.52
1:A:272:LEU:CD1	1:A:277:ALA:HA	2.40	0.52
1:B:188:SER:HB3	1:B:438:LEU:O	2.10	0.52
1:B:196:PHE:HB3	1:B:199:ALA:HB3	1.90	0.52
1:C:10:ILE:HD11	1:C:270:LEU:HD13	1.92	0.52
1:C:29:TYR:HE1	1:C:148:MET:CB	2.22	0.52
1:C:184:PRO:HB3	1:C:390:PHE:CD2	2.44	0.52
1:A:270:LEU:O	1:A:354:ARG:NH1	2.42	0.52
1:B:390:PHE:CE2	1:B:394:ILE:HD11	2.45	0.52
1:C:256:VAL:CG2	1:C:257:ILE:H	2.19	0.52
1:D:171:ILE:HG23	1:D:205:PHE:HZ	1.75	0.52
1:A:253:SER:O	1:A:256:VAL:HG22	2.09	0.52
1:A:350:THR:C	1:A:351:LEU:HD13	2.34	0.52
1:C:298:LYS:HG3	1:C:344:ILE:HG21	1.90	0.52
1:D:55:GLU:HA	1:D:125:TYR:O	2.10	0.52
1:A:35:LYS:C	1:A:37:ARG:N	2.67	0.52
1:A:316:ASP:O	1:A:317:ARG:O	2.27	0.52
1:B:396:ILE:HD12	1:B:396:ILE:H	1.74	0.52
1:B:430:GLU:CG	1:B:437:ILE:HG12	2.40	0.52
1:B:430:GLU:HG3	1:B:437:ILE:HG12	1.92	0.52
1:C:114:VAL:HG22	1:C:122:ILE:CD1	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:381:ASN:HD21	1:C:385:ARG:NH2	2.08	0.52
1:D:283:ILE:N	1:D:283:ILE:CD1	2.71	0.52
1:B:171:ILE:HG23	1:B:205:PHE:HZ	1.75	0.52
1:B:283:ILE:N	1:B:283:ILE:CD1	2.71	0.52
1:C:401:ASN:HD22	1:C:402:PRO:N	2.07	0.52
1:C:430:GLU:C	1:C:432:LYS:N	2.66	0.52
1:D:68:ALA:C	1:D:70:GLU:N	2.68	0.52
1:D:325:PHE:CD1	1:D:336:ARG:HD3	2.45	0.52
1:D:401:ASN:O	1:D:404:GLU:HB3	2.10	0.52
1:A:271:ILE:O	1:A:272:LEU:O	2.28	0.51
1:B:272:LEU:HD11	1:B:278:PRO:CD	2.39	0.51
1:C:1:LEU:HD12	1:C:1:LEU:H	1.75	0.51
1:D:381:ASN:O	1:D:385:ARG:HG2	2.10	0.51
1:A:400:ILE:HG22	1:A:418:VAL:HG21	1.93	0.51
1:D:105:PRO:HG2	1:D:106:ILE:H	1.75	0.51
1:D:396:ILE:HD12	1:D:396:ILE:H	1.75	0.51
1:B:223:LEU:HD13	1:B:227:PHE:CD2	2.46	0.51
1:B:387:TRP:O	1:B:388:GLU:C	2.54	0.51
1:C:64:GLU:CG	1:C:95:LYS:HB2	2.39	0.51
1:C:385:ARG:HG3	1:C:385:ARG:NH1	2.25	0.51
1:D:341:PRO:O	1:D:344:ILE:HG13	2.10	0.51
1:A:142:ILE:CG2	1:A:215:MET:HE1	2.40	0.51
1:A:159:THR:CG2	1:A:162:GLU:HB2	2.40	0.51
1:A:208:ILE:HD11	1:A:415:VAL:HG12	1.92	0.51
1:B:106:ILE:O	1:B:110:MET:HG3	2.10	0.51
1:C:223:LEU:HD13	1:C:227:PHE:CE2	2.45	0.51
1:D:175:LYS:HG3	1:D:185:TYR:CZ	2.45	0.51
1:D:387:TRP:O	1:D:388:GLU:C	2.54	0.51
1:A:298:LYS:HG3	1:A:344:ILE:HG21	1.92	0.51
1:A:409:LEU:CD2	1:A:416:ILE:HG12	2.40	0.51
1:B:30:LEU:O	1:B:31:PRO:C	2.53	0.51
1:B:44:ILE:HG12	1:B:151:LYS:HD3	1.92	0.51
1:B:207:THR:HG22	1:B:215:MET:HB3	1.92	0.51
1:B:302:ILE:HG23	1:B:367:LEU:HD21	1.92	0.51
1:B:381:ASN:O	1:B:385:ARG:HG2	2.11	0.51
1:B:416:ILE:O	1:B:450:ALA:HA	2.10	0.51
1:C:30:LEU:O	1:C:31:PRO:C	2.53	0.51
1:A:127:ILE:HG12	1:A:151:LYS:CB	2.41	0.51
1:B:178:PHE:CZ	1:B:217:ILE:HD12	2.45	0.51
1:C:272:LEU:CD1	1:C:277:ALA:HA	2.40	0.51
1:D:92:LEU:C	1:D:94:VAL:N	2.69	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:160:LYS:HA	1:D:246:TYR:CD2	2.45	0.51
1:D:171:ILE:O	1:D:172:SER:C	2.54	0.51
1:A:23:ILE:O	1:A:24:LYS:O	2.28	0.51
1:B:57:LEU:HA	1:B:126:GLN:HE21	1.76	0.51
1:B:66:LEU:O	1:B:68:ALA:N	2.42	0.51
1:C:41:PHE:HD2	1:C:127:ILE:HD13	1.75	0.51
1:D:430:GLU:CG	1:D:437:ILE:HG12	2.41	0.51
1:D:430:GLU:HG3	1:D:437:ILE:HG12	1.93	0.51
1:A:99:ARG:O	1:A:99:ARG:HG3	2.11	0.51
1:A:112:LEU:HB3	1:B:20:ARG:NH2	2.26	0.51
1:A:184:PRO:HB3	1:A:390:PHE:CD2	2.45	0.51
1:B:64:GLU:O	1:B:65:ASP:C	2.54	0.51
1:D:44:ILE:HG12	1:D:151:LYS:HD3	1.92	0.51
1:D:114:VAL:HG12	1:D:235:PHE:HB3	1.92	0.51
1:B:55:GLU:HA	1:B:125:TYR:O	2.11	0.51
1:B:402:PRO:O	1:B:404:GLU:N	2.44	0.51
1:D:353:ARG:O	1:D:357:MET:N	2.43	0.51
1:D:360:PHE:H	1:D:360:PHE:HD2	1.59	0.51
1:B:360:PHE:H	1:B:360:PHE:HD2	1.59	0.51
1:C:253:SER:O	1:C:256:VAL:HG22	2.10	0.51
1:A:56:ALA:HB3	1:A:124:ILE:HD11	1.93	0.50
1:B:49:ASP:C	1:B:51:SER:H	2.20	0.50
1:B:68:ALA:C	1:B:70:GLU:N	2.69	0.50
1:B:295:VAL:O	1:B:297:GLU:N	2.44	0.50
1:C:271:ILE:O	1:C:272:LEU:C	2.53	0.50
1:D:295:VAL:O	1:D:297:GLU:N	2.44	0.50
1:A:211:ASP:CG	1:A:213:ARG:HB2	2.36	0.50
1:B:443:TYR:O	1:B:444:LYS:HB2	2.11	0.50
1:A:10:ILE:HD12	1:A:269:GLY:HA2	1.92	0.50
1:A:271:ILE:O	1:A:272:LEU:C	2.53	0.50
1:A:328:TRP:HA	1:A:328:TRP:CE3	2.46	0.50
1:B:196:PHE:O	1:B:197:PRO:C	2.53	0.50
1:C:112:LEU:HB3	1:D:20:ARG:HH21	1.75	0.50
1:D:45:ARG:O	1:D:48:LEU:HB2	2.10	0.50
1:D:64:GLU:O	1:D:65:ASP:C	2.55	0.50
1:A:98:LEU:HD11	1:B:61:LEU:HD21	1.93	0.50
1:A:124:ILE:N	1:A:154:HIS:O	2.44	0.50
1:A:175:LYS:HG2	1:A:185:TYR:CZ	2.46	0.50
1:C:211:ASP:CG	1:C:213:ARG:HB2	2.36	0.50
1:C:385:ARG:HG3	1:C:385:ARG:HH11	1.77	0.50
1:D:106:ILE:O	1:D:110:MET:HG3	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:160:LYS:HB2	1:A:246:TYR:CE2	2.46	0.50
1:A:235:PHE:CD1	1:A:235:PHE:C	2.89	0.50
1:B:10:ILE:HA	1:B:13:LYS:HB3	1.93	0.50
1:B:69:LYS:C	1:B:71:ALA:N	2.69	0.50
1:D:378:ILE:O	1:D:382:ILE:HG23	2.11	0.50
1:A:353:ARG:C	1:A:355:ASP:N	2.66	0.50
1:C:220:VAL:HG22	1:C:250:TYR:HB3	1.93	0.50
1:C:400:ILE:HD13	1:C:424:ILE:HD11	1.93	0.50
1:A:48:LEU:CD1	1:A:151:LYS:HD2	2.41	0.50
1:A:66:LEU:HB3	1:A:104:THR:CG2	2.42	0.50
1:A:205:PHE:CD1	1:A:218:ALA:HB3	2.47	0.50
1:A:266:ASP:OD2	1:A:354:ARG:NH2	2.45	0.50
1:B:401:ASN:O	1:B:404:GLU:HB3	2.12	0.50
1:D:277:ALA:O	1:D:278:PRO:C	2.55	0.50
1:A:110:MET:HE2	1:A:122:ILE:HG13	1.93	0.50
1:A:381:ASN:HD21	1:A:385:ARG:NH2	2.10	0.50
1:A:385:ARG:NH1	1:A:385:ARG:HG3	2.27	0.50
1:A:388:GLU:O	1:A:392:ASN:HB2	2.12	0.50
1:B:171:ILE:O	1:B:172:SER:C	2.55	0.50
1:B:237:THR:HB	1:B:238:PRO:HD2	1.94	0.50
1:D:178:PHE:CZ	1:D:217:ILE:HD12	2.46	0.50
1:A:405:ILE:O	1:A:408:ILE:HG22	2.12	0.49
1:D:157:HIS:NE2	1:D:166:GLN:HG2	2.27	0.49
1:D:237:THR:HB	1:D:238:PRO:HD2	1.94	0.49
1:D:292:GLU:N	1:D:292:GLU:CD	2.70	0.49
1:A:131:PHE:CE2	1:A:146:GLU:HG3	2.47	0.49
1:A:428:GLU:O	1:A:431:GLU:N	2.45	0.49
1:B:229:LYS:HG2	1:B:244:TYR:CD2	2.46	0.49
1:C:3:PHE:O	1:C:6:TRP:N	2.45	0.49
1:C:272:LEU:HD11	1:C:277:ALA:HA	1.93	0.49
1:D:30:LEU:O	1:D:31:PRO:C	2.54	0.49
1:A:188:SER:O	1:A:203:MET:HA	2.12	0.49
1:A:202:THR:HG23	1:A:221:HIS:ND1	2.28	0.49
1:B:292:GLU:N	1:B:292:GLU:CD	2.71	0.49
1:C:56:ALA:HB3	1:C:124:ILE:HD11	1.94	0.49
1:C:102:SER:O	1:C:106:ILE:HG13	2.13	0.49
1:D:10:ILE:HA	1:D:13:LYS:HB3	1.94	0.49
1:D:134:GLU:H	1:D:145:ARG:CD	2.25	0.49
1:D:284:VAL:O	1:D:286:LEU:HD12	2.11	0.49
1:A:428:GLU:O	1:A:429:LEU:C	2.56	0.49
1:B:223:LEU:HB2	1:B:247:GLN:HB2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:353:ARG:O	1:B:357:MET:N	2.44	0.49
1:C:160:LYS:HB2	1:C:246:TYR:CE2	2.47	0.49
1:D:71:ALA:HB2	1:D:77:PHE:CE2	2.47	0.49
1:D:443:TYR:O	1:D:444:LYS:HB2	2.12	0.49
1:D:446:ASN:HB2	1:D:448:TYR:CE1	2.48	0.49
1:A:191:PRO:HD3	1:A:439:GLY:HA2	1.92	0.49
1:A:223:LEU:HB2	1:A:247:GLN:HB2	1.94	0.49
1:B:272:LEU:HD11	1:B:277:ALA:HA	1.94	0.49
1:B:405:ILE:O	1:B:406:LYS:C	2.55	0.49
1:C:74:ILE:O	1:C:75:LYS:O	2.31	0.49
1:C:235:PHE:CD1	1:C:235:PHE:C	2.90	0.49
1:D:69:LYS:C	1:D:71:ALA:N	2.70	0.49
1:D:223:LEU:O	1:D:224:GLY:C	2.55	0.49
1:D:405:ILE:O	1:D:406:LYS:C	2.54	0.49
1:D:437:ILE:HG23	1:D:451:ILE:HG12	1.93	0.49
1:A:343:ASP:OD1	1:A:350:THR:HG22	2.13	0.49
1:B:16:ILE:HD11	1:B:270:LEU:CD2	2.43	0.49
1:B:275:ILE:HD11	1:B:379:MET:HG2	1.94	0.49
1:C:178:PHE:O	1:C:182:GLY:N	2.46	0.49
1:C:205:PHE:CD1	1:C:218:ALA:HB3	2.47	0.49
1:A:149:THR:HB	1:A:254:ASP:OD2	2.13	0.49
1:A:429:LEU:O	1:A:432:LYS:HB3	2.12	0.49
1:B:92:LEU:C	1:B:94:VAL:N	2.71	0.49
1:B:171:ILE:HG23	1:B:205:PHE:CZ	2.48	0.49
1:C:294:ILE:O	1:C:297:GLU:HB3	2.12	0.49
1:D:66:LEU:O	1:D:68:ALA:N	2.45	0.49
1:D:141:LEU:HA	1:D:144:LEU:HD11	1.94	0.49
1:D:416:ILE:O	1:D:450:ALA:HA	2.12	0.49
1:B:11:LEU:O	1:B:16:ILE:HB	2.12	0.49
1:B:71:ALA:HB2	1:B:77:PHE:CE2	2.47	0.49
1:C:300:LYS:O	1:C:301:GLU:C	2.54	0.49
1:D:16:ILE:HD11	1:D:270:LEU:CD2	2.43	0.49
1:D:272:LEU:HD12	1:D:277:ALA:HA	1.93	0.49
1:D:275:ILE:HD11	1:D:379:MET:HG2	1.94	0.49
1:D:335:LEU:CD1	1:D:378:ILE:HD11	2.43	0.49
1:B:223:LEU:O	1:B:224:GLY:C	2.56	0.49
1:C:400:ILE:HG22	1:C:418:VAL:HG21	1.95	0.49
1:A:272:LEU:HD11	1:A:277:ALA:HA	1.94	0.49
1:A:283:ILE:HG22	1:A:314:ILE:HG23	1.95	0.49
1:A:385:ARG:HG3	1:A:385:ARG:HH11	1.78	0.49
1:B:23:ILE:O	1:B:24:LYS:C	2.54	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:58:PHE:N	1:B:126:GLN:NE2	2.55	0.49
1:B:103:GLU:O	1:B:104:THR:C	2.55	0.49
1:B:367:LEU:C	1:B:369:GLU:N	2.71	0.49
1:C:16:ILE:CD1	1:C:270:LEU:HD21	2.41	0.49
1:C:60:MET:HE1	1:C:129:ASN:OD1	2.13	0.49
1:C:66:LEU:HB3	1:C:104:THR:CG2	2.43	0.49
1:C:302:ILE:HG22	1:C:306:LEU:HD12	1.94	0.49
1:C:328:TRP:CE3	1:C:328:TRP:HA	2.47	0.49
1:C:409:LEU:CD2	1:C:416:ILE:HG12	2.42	0.49
1:A:74:ILE:O	1:A:75:LYS:O	2.31	0.48
1:A:114:VAL:CG2	1:A:122:ILE:HD11	2.42	0.48
1:B:114:VAL:HG22	1:B:120:LEU:HD21	1.94	0.48
1:D:11:LEU:O	1:D:16:ILE:HB	2.13	0.48
1:D:196:PHE:O	1:D:197:PRO:C	2.55	0.48
1:A:191:PRO:C	1:A:193:TRP:H	2.21	0.48
1:B:114:VAL:HG12	1:B:235:PHE:HB3	1.95	0.48
1:B:228:SER:OG	1:B:245:ALA:O	2.30	0.48
1:C:98:LEU:HD11	1:D:61:LEU:HD21	1.95	0.48
1:C:175:LYS:HG2	1:C:185:TYR:CZ	2.47	0.48
1:C:271:ILE:O	1:C:272:LEU:O	2.31	0.48
1:C:316:ASP:O	1:C:317:ARG:O	2.30	0.48
1:D:103:GLU:O	1:D:104:THR:C	2.55	0.48
1:B:19:VAL:HG11	1:B:140:PRO:CG	2.43	0.48
1:C:114:VAL:CG2	1:C:122:ILE:HD11	2.42	0.48
1:C:384:ASN:O	1:C:385:ARG:C	2.55	0.48
1:C:428:GLU:O	1:C:431:GLU:N	2.47	0.48
1:D:280:GLN:OE1	1:D:311:ARG:HG3	2.14	0.48
1:A:169:GLU:O	1:A:173:ILE:HG12	2.13	0.48
1:A:320:ARG:C	1:A:322:GLY:N	2.69	0.48
1:B:141:LEU:HA	1:B:144:LEU:HD11	1.95	0.48
1:B:378:ILE:O	1:B:382:ILE:HG23	2.13	0.48
1:C:274:PRO:HD2	1:C:275:ILE:HD12	1.95	0.48
1:A:102:SER:C	1:A:105:PRO:HD2	2.39	0.48
1:A:306:LEU:HB2	1:A:312:VAL:HG11	1.94	0.48
1:B:108:TYR:O	1:B:111:LYS:HB3	2.13	0.48
1:B:119:ASP:O	1:B:120:LEU:HD23	2.13	0.48
1:B:341:PRO:O	1:B:344:ILE:HG13	2.13	0.48
1:C:188:SER:O	1:C:203:MET:HA	2.13	0.48
1:D:57:LEU:HA	1:D:126:GLN:HE21	1.78	0.48
1:A:256:VAL:CG2	1:A:257:ILE:H	2.23	0.48
1:B:437:ILE:HG23	1:B:451:ILE:HG12	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:343:ASP:OD1	1:C:350:THR:HG22	2.14	0.48
1:D:284:VAL:HG11	1:D:325:PHE:CE1	2.49	0.48
1:A:36:ILE:O	1:A:36:ILE:CD1	2.60	0.48
1:A:208:ILE:HG13	1:A:390:PHE:HE1	1.79	0.48
1:C:191:PRO:C	1:C:193:TRP:H	2.22	0.48
1:C:321:PRO:O	1:C:324:LYS:HB2	2.14	0.48
1:D:70:GLU:O	1:D:70:GLU:HG3	2.12	0.48
1:D:229:LYS:HG2	1:D:244:TYR:CD2	2.48	0.48
1:B:131:PHE:CE2	1:B:146:GLU:HG3	2.48	0.48
1:C:48:LEU:CD1	1:C:151:LYS:HD2	2.43	0.48
1:A:294:ILE:O	1:A:297:GLU:HB3	2.14	0.48
1:A:300:LYS:O	1:A:301:GLU:C	2.55	0.48
1:A:401:ASN:OD1	1:A:404:GLU:HB2	2.14	0.48
1:B:286:LEU:HD11	1:B:338:GLU:CB	2.41	0.48
1:C:281:VAL:O	1:C:312:VAL:HA	2.14	0.48
1:D:49:ASP:C	1:D:51:SER:H	2.22	0.48
1:D:99:ARG:HH21	1:D:129:ASN:H	1.60	0.48
1:A:60:MET:SD	1:B:60:MET:SD	3.11	0.48
1:A:66:LEU:HD12	1:A:66:LEU:N	2.29	0.48
1:B:39:TYR:CD2	1:B:311:ARG:NH1	2.81	0.48
1:C:266:ASP:OD2	1:C:354:ARG:NH2	2.47	0.48
1:D:367:LEU:C	1:D:369:GLU:N	2.72	0.48
1:A:215:MET:HE3	1:A:455:TYR:CB	2.44	0.47
1:A:291:LYS:HB3	1:A:294:ILE:CG2	2.43	0.47
1:A:415:VAL:HA	1:A:452:ALA:HB2	1.96	0.47
1:C:53:HIS:CE1	1:C:250:TYR:HH	2.24	0.47
1:D:223:LEU:HB2	1:D:247:GLN:HB2	1.95	0.47
1:A:112:LEU:HB3	1:B:20:ARG:HH21	1.79	0.47
1:C:191:PRO:HD3	1:C:439:GLY:HA2	1.94	0.47
1:C:401:ASN:O	1:C:404:GLU:HB3	2.14	0.47
1:D:63:PRO:HA	1:D:96:LEU:HD23	1.96	0.47
1:A:171:ILE:O	1:A:175:LYS:HB2	2.14	0.47
1:B:280:GLN:OE1	1:B:311:ARG:HG3	2.15	0.47
1:C:60:MET:HE1	1:D:60:MET:SD	2.53	0.47
1:C:376:ASN:O	1:C:377:ASN:C	2.57	0.47
1:D:171:ILE:HG23	1:D:205:PHE:CZ	2.50	0.47
1:B:104:THR:HB	1:B:105:PRO:CD	2.44	0.47
1:C:36:ILE:O	1:C:36:ILE:CD1	2.61	0.47
1:C:155:THR:OG1	1:C:248:THR:HG22	2.13	0.47
1:D:302:ILE:HG23	1:D:367:LEU:HD21	1.96	0.47
1:A:60:MET:HE1	1:A:129:ASN:OD1	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:141:LEU:HD13	1:A:257:ILE:HG12	1.95	0.47
1:A:376:ASN:O	1:A:377:ASN:C	2.57	0.47
1:B:157:HIS:NE2	1:B:166:GLN:HG2	2.30	0.47
1:C:370:VAL:O	1:C:371:VAL:C	2.57	0.47
1:C:388:GLU:O	1:C:392:ASN:HB2	2.14	0.47
1:D:319:ILE:HG13	1:D:320:ARG:N	2.29	0.47
1:A:3:PHE:O	1:A:6:TRP:N	2.47	0.47
1:B:25:GLY:HA2	2:B:461:HOH:O	2.14	0.47
1:B:364:GLU:C	1:B:366:GLN:N	2.71	0.47
1:B:433:VAL:O	1:B:434:GLU:C	2.58	0.47
1:C:291:LYS:HB3	1:C:294:ILE:CG2	2.44	0.47
1:C:320:ARG:C	1:C:322:GLY:N	2.70	0.47
1:D:112:LEU:N	1:D:112:LEU:HD22	2.30	0.47
1:D:282:VAL:HG11	1:D:328:TRP:CD1	2.50	0.47
1:A:43:ILE:HD11	1:A:275:ILE:HG22	1.97	0.47
1:A:60:MET:HA	1:A:99:ARG:NH1	2.30	0.47
1:A:257:ILE:O	1:A:261:ILE:HG13	2.15	0.47
1:A:272:LEU:O	1:A:272:LEU:HD12	2.15	0.47
1:A:341:PRO:C	1:A:343:ASP:H	2.22	0.47
1:A:346:ASN:O	1:A:347:LYS:HB2	2.13	0.47
1:A:355:ASP:OD2	1:A:356:THR:N	2.46	0.47
1:B:134:GLU:H	1:B:145:ARG:CD	2.27	0.47
1:B:158:SER:HA	1:B:235:PHE:CZ	2.50	0.47
1:B:222:ASN:HD22	1:B:224:GLY:H	1.62	0.47
1:B:284:VAL:O	1:B:286:LEU:HD12	2.13	0.47
1:B:319:ILE:HG13	1:B:320:ARG:N	2.30	0.47
1:B:367:LEU:O	1:B:369:GLU:N	2.48	0.47
1:C:208:ILE:HD11	1:C:415:VAL:CG1	2.45	0.47
1:C:364:GLU:O	1:C:364:GLU:HG2	2.14	0.47
1:C:366:GLN:HE21	1:C:366:GLN:HA	1.80	0.47
1:D:19:VAL:HG11	1:D:140:PRO:CG	2.44	0.47
1:D:142:ILE:HA	1:D:255:ARG:HD3	1.97	0.47
1:D:364:GLU:C	1:D:366:GLN:N	2.73	0.47
1:D:373:LYS:HB2	1:D:373:LYS:HZ2	1.80	0.47
1:D:406:LYS:O	1:D:409:LEU:HB2	2.15	0.47
1:A:125:TYR:CD1	1:A:125:TYR:C	2.92	0.47
1:C:111:LYS:HG2	1:C:112:LEU:HD12	1.97	0.47
1:A:171:ILE:HD11	1:A:203:MET:HG3	1.96	0.47
1:A:341:PRO:C	1:A:343:ASP:N	2.71	0.47
1:B:247:GLN:C	1:B:248:THR:HG22	2.40	0.47
1:C:117:HIS:CD2	1:C:238:PRO:HA	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:131:PHE:CE2	1:C:146:GLU:HG3	2.50	0.47
1:C:405:ILE:O	1:C:408:ILE:HG22	2.15	0.47
1:D:313:HIS:HD2	1:D:328:TRP:CZ2	2.33	0.47
1:A:111:LYS:HG2	1:A:112:LEU:HD12	1.97	0.47
1:A:356:THR:OG1	1:A:358:GLU:HG2	2.15	0.47
1:B:159:THR:HG23	1:B:162:GLU:HB2	1.95	0.47
1:B:277:ALA:O	1:B:278:PRO:C	2.59	0.47
1:B:325:PHE:CE1	1:B:338:GLU:HG2	2.50	0.47
1:C:66:LEU:HB3	1:C:104:THR:HG22	1.97	0.47
1:D:247:GLN:C	1:D:248:THR:HG22	2.40	0.47
1:D:271:ILE:HG12	1:D:354:ARG:HH12	1.74	0.47
1:A:64:GLU:CG	1:A:95:LYS:HB2	2.42	0.46
1:A:205:PHE:CD1	1:A:205:PHE:N	2.83	0.46
1:C:341:PRO:C	1:C:343:ASP:H	2.22	0.46
1:C:413:ARG:HB2	1:C:413:ARG:CZ	2.46	0.46
1:C:428:GLU:O	1:C:429:LEU:C	2.58	0.46
1:D:33:GLY:O	1:D:36:ILE:CG2	2.60	0.46
1:D:114:VAL:CG1	1:D:235:PHE:HB3	2.45	0.46
1:A:401:ASN:O	1:A:404:GLU:HB3	2.16	0.46
1:B:344:ILE:HD12	1:B:344:ILE:C	2.39	0.46
1:C:54:ASP:HB2	2:C:476:HOH:O	2.15	0.46
1:C:142:ILE:HG21	1:C:215:MET:HE1	1.96	0.46
1:C:171:ILE:HD11	1:C:203:MET:HG3	1.97	0.46
1:C:205:PHE:CD1	1:C:205:PHE:N	2.83	0.46
1:C:306:LEU:HB2	1:C:312:VAL:HG11	1.97	0.46
1:D:39:TYR:O	1:D:40:THR:C	2.58	0.46
1:A:37:ARG:NE	1:A:149:THR:OG1	2.48	0.46
1:A:120:LEU:HD13	1:A:157:HIS:O	2.15	0.46
1:A:306:LEU:HD22	1:A:371:VAL:HG11	1.96	0.46
1:A:340:GLY:O	1:A:344:ILE:HG23	2.16	0.46
1:A:364:GLU:O	1:A:364:GLU:HG2	2.14	0.46
1:B:373:LYS:HB2	1:B:373:LYS:HZ2	1.81	0.46
1:C:43:ILE:HD11	1:C:275:ILE:HG22	1.97	0.46
1:C:223:LEU:HB2	1:C:247:GLN:HB2	1.97	0.46
1:A:58:PHE:N	1:A:126:GLN:HE22	2.13	0.46
1:A:117:HIS:CD2	1:A:238:PRO:HA	2.50	0.46
1:B:101:THR:O	1:B:103:GLU:N	2.48	0.46
1:C:125:TYR:CD1	1:C:125:TYR:C	2.93	0.46
1:C:215:MET:HE3	1:C:455:TYR:CB	2.46	0.46
1:C:360:PHE:N	1:C:360:PHE:CD2	2.68	0.46
1:D:140:PRO:HA	2:D:457:HOH:O	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:158:SER:HA	1:D:235:PHE:CZ	2.51	0.46
1:A:248:THR:O	1:A:248:THR:HG23	2.15	0.46
1:B:284:VAL:HG11	1:B:325:PHE:CE1	2.51	0.46
1:B:336:ARG:NH1	1:B:338:GLU:OE2	2.46	0.46
1:C:104:THR:HB	1:C:105:PRO:HD3	1.97	0.46
1:C:222:ASN:C	1:C:222:ASN:ND2	2.72	0.46
1:D:65:ASP:O	1:D:68:ALA:HB3	2.15	0.46
1:A:132:ARG:O	1:A:134:GLU:N	2.48	0.46
1:A:413:ARG:HB2	1:A:413:ARG:CZ	2.46	0.46
1:B:291:LYS:CB	1:B:294:ILE:HG21	2.45	0.46
1:C:102:SER:HB3	1:C:152:GLU:OE1	2.16	0.46
1:C:126:GLN:HG3	1:C:128:VAL:HG22	1.97	0.46
1:D:68:ALA:C	1:D:70:GLU:H	2.24	0.46
1:D:100:PRO:HG2	1:D:101:THR:H	1.80	0.46
1:B:63:PRO:HA	1:B:96:LEU:HD23	1.98	0.46
1:B:191:PRO:HB3	1:B:425:TYR:OH	2.16	0.46
1:C:281:VAL:HB	1:C:312:VAL:HG12	1.98	0.46
1:C:340:GLY:O	1:C:344:ILE:HG23	2.16	0.46
1:C:346:ASN:O	1:C:347:LYS:HB2	2.14	0.46
1:D:119:ASP:O	1:D:120:LEU:HD23	2.16	0.46
1:D:291:LYS:CB	1:D:294:ILE:HG21	2.45	0.46
1:A:281:VAL:O	1:A:312:VAL:HA	2.16	0.46
1:B:39:TYR:O	1:B:40:THR:C	2.59	0.46
1:B:189:LYS:O	1:B:189:LYS:HG2	2.16	0.46
1:B:324:LYS:O	1:B:325:PHE:C	2.59	0.46
1:C:84:VAL:HG11	1:D:82:TYR:CD2	2.51	0.46
1:D:66:LEU:HB3	1:D:104:THR:CG2	2.44	0.46
1:D:223:LEU:HD13	1:D:227:PHE:CD2	2.51	0.46
1:A:384:ASN:O	1:A:385:ARG:C	2.58	0.46
1:B:33:GLY:O	1:B:36:ILE:CG2	2.62	0.46
1:B:70:GLU:O	1:B:70:GLU:HG3	2.15	0.46
1:B:159:THR:CG2	1:B:162:GLU:HB2	2.45	0.46
1:C:58:PHE:C	1:D:148:MET:HE1	2.41	0.46
1:C:132:ARG:O	1:C:134:GLU:N	2.49	0.46
1:C:341:PRO:C	1:C:343:ASP:N	2.72	0.46
1:C:401:ASN:OD1	1:C:404:GLU:HB2	2.16	0.46
1:C:415:VAL:HA	1:C:452:ALA:HB2	1.98	0.46
1:D:99:ARG:HH21	1:D:128:VAL:HB	1.76	0.46
1:D:225:GLN:O	1:D:226:ASN:C	2.58	0.46
1:B:29:TYR:HE2	1:B:257:ILE:HD11	1.81	0.45
1:C:37:ARG:NE	1:C:149:THR:OG1	2.48	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:108:TYR:CE2	1:D:22:PRO:HD3	2.51	0.45
1:C:112:LEU:HD12	1:C:112:LEU:N	2.32	0.45
1:C:149:THR:HB	1:C:254:ASP:OD2	2.16	0.45
1:C:373:LYS:HB2	1:C:373:LYS:HZ2	1.79	0.45
1:D:272:LEU:HA	1:D:273:PRO:HD3	1.82	0.45
1:A:31:PRO:HG3	1:B:54:ASP:HB3	1.99	0.45
1:A:127:ILE:HG12	1:A:151:LYS:HB2	1.97	0.45
1:A:360:PHE:N	1:A:360:PHE:CD2	2.68	0.45
1:A:405:ILE:CA	1:A:408:ILE:HG22	2.43	0.45
1:B:114:VAL:CG1	1:B:235:PHE:HB3	2.46	0.45
1:C:320:ARG:CZ	1:C:322:GLY:HA3	2.45	0.45
1:C:351:LEU:HD13	1:C:351:LEU:N	2.31	0.45
1:D:153:ALA:HB3	1:D:250:TYR:CE1	2.51	0.45
1:A:102:SER:O	1:A:106:ILE:HG13	2.16	0.45
1:A:126:GLN:HG3	1:A:128:VAL:HG22	1.98	0.45
1:A:406:LYS:HB3	1:A:433:VAL:O	2.16	0.45
1:B:21:TYR:CD2	1:B:22:PRO:HD2	2.50	0.45
1:B:297:GLU:C	1:B:299:ALA:N	2.74	0.45
1:C:64:GLU:OE2	1:C:64:GLU:HA	2.15	0.45
1:D:29:TYR:HE2	1:D:257:ILE:HD11	1.82	0.45
1:D:409:LEU:C	1:D:411:GLU:H	2.23	0.45
1:A:112:LEU:HD12	1:A:112:LEU:N	2.32	0.45
1:A:366:GLN:O	1:A:370:VAL:HG23	2.16	0.45
1:B:409:LEU:C	1:B:411:GLU:H	2.23	0.45
1:C:58:PHE:N	1:C:126:GLN:HE22	2.14	0.45
1:C:155:THR:OG1	1:C:248:THR:CG2	2.64	0.45
1:D:324:LYS:O	1:D:325:PHE:C	2.60	0.45
1:D:367:LEU:O	1:D:369:GLU:N	2.50	0.45
1:A:191:PRO:HD3	1:A:439:GLY:CA	2.47	0.45
1:A:283:ILE:O	1:A:314:ILE:HG23	2.16	0.45
1:B:37:ARG:HA	1:B:40:THR:HB	1.99	0.45
1:B:237:THR:C	1:B:239:THR:H	2.24	0.45
1:C:56:ALA:HB1	1:D:29:TYR:O	2.17	0.45
1:C:107:TYR:N	1:C:107:TYR:CD2	2.83	0.45
1:C:141:LEU:HD13	1:C:257:ILE:HG12	1.97	0.45
1:C:191:PRO:HD3	1:C:439:GLY:CA	2.47	0.45
1:C:196:PHE:CG	1:C:197:PRO:CD	2.99	0.45
1:C:306:LEU:HD22	1:C:371:VAL:HG11	1.97	0.45
1:D:7:TYR:O	1:D:8:SER:C	2.58	0.45
1:D:159:THR:HG23	1:D:162:GLU:HB2	1.97	0.45
1:D:266:ASP:OD1	1:D:271:ILE:HD11	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:272:LEU:HD11	1:D:277:ALA:HA	1.98	0.45
1:A:60:MET:HG3	1:A:99:ARG:HG2	1.97	0.45
1:A:108:TYR:CE2	1:B:22:PRO:HD3	2.51	0.45
1:A:286:LEU:HD12	1:A:286:LEU:H	1.82	0.45
1:A:351:LEU:HD13	1:A:351:LEU:N	2.31	0.45
1:B:41:PHE:CE1	1:B:256:VAL:HG21	2.52	0.45
1:B:112:LEU:N	1:B:112:LEU:HD22	2.32	0.45
1:C:405:ILE:CA	1:C:408:ILE:HG22	2.43	0.45
1:D:11:LEU:HD12	1:D:11:LEU:HA	1.74	0.45
1:D:23:ILE:O	1:D:24:LYS:C	2.58	0.45
1:D:286:LEU:HD11	1:D:338:GLU:CB	2.43	0.45
1:D:336:ARG:NH1	1:D:338:GLU:OE2	2.48	0.45
1:D:387:TRP:O	1:D:391:GLU:HG3	2.17	0.45
1:A:266:ASP:O	1:A:269:GLY:N	2.36	0.45
1:A:338:GLU:HB2	1:A:350:THR:CG2	2.45	0.45
1:A:405:ILE:HD13	1:A:451:ILE:CD1	2.46	0.45
1:B:10:ILE:C	1:B:12:GLU:N	2.73	0.45
1:B:23:ILE:O	1:B:26:CYS:HB2	2.15	0.45
1:B:60:MET:HG3	1:B:99:ARG:HG2	1.99	0.45
1:B:370:VAL:O	1:B:371:VAL:C	2.60	0.45
1:C:10:ILE:HD12	1:C:269:GLY:HA2	1.97	0.45
1:C:60:MET:HA	1:C:99:ARG:NH1	2.32	0.45
1:D:131:PHE:CE2	1:D:146:GLU:HG3	2.51	0.45
1:D:222:ASN:HD22	1:D:224:GLY:H	1.65	0.45
1:A:35:LYS:HZ3	1:A:38:ARG:NH2	2.14	0.45
1:A:107:TYR:O	1:A:108:TYR:C	2.60	0.45
1:A:428:GLU:O	1:A:432:LYS:N	2.50	0.45
1:C:62:ILE:CD1	1:C:105:PRO:HD3	2.46	0.45
1:C:104:THR:N	1:C:105:PRO:HD2	2.32	0.45
1:C:107:TYR:C	1:C:109:MET:N	2.73	0.45
1:C:237:THR:C	1:C:239:THR:N	2.75	0.45
1:C:256:VAL:O	1:C:260:ILE:N	2.45	0.45
1:C:430:GLU:O	1:C:434:GLU:N	2.50	0.45
1:D:37:ARG:O	1:D:37:ARG:HG2	2.16	0.45
1:D:252:ILE:O	1:D:252:ILE:HG13	2.17	0.45
1:A:60:MET:SD	1:A:131:PHE:HE1	2.40	0.45
1:B:65:ASP:O	1:B:68:ALA:HB3	2.17	0.45
1:B:141:LEU:HD13	1:B:257:ILE:HD11	1.98	0.45
1:B:283:ILE:H	1:B:283:ILE:CD1	2.28	0.45
1:B:335:LEU:CD1	1:B:378:ILE:HD11	2.47	0.45
1:C:157:HIS:HB3	1:C:162:GLU:HB3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:256:VAL:HG23	1:C:257:ILE:HG22	1.99	0.45
1:D:350:THR:CA	1:D:361:GLN:HG2	2.46	0.45
1:D:351:LEU:N	1:D:351:LEU:HD22	2.32	0.45
1:B:7:TYR:O	1:B:8:SER:C	2.59	0.45
1:B:99:ARG:O	1:B:99:ARG:HG3	2.16	0.45
1:C:306:LEU:CD2	1:C:371:VAL:HG21	2.39	0.45
1:B:153:ALA:HB3	1:B:250:TYR:CE1	2.52	0.44
1:C:31:PRO:HG3	1:D:54:ASP:HB3	1.99	0.44
1:C:424:ILE:C	1:C:424:ILE:HD12	2.42	0.44
1:D:191:PRO:HB3	1:D:425:TYR:OH	2.17	0.44
1:D:451:ILE:O	1:D:452:ALA:HB2	2.16	0.44
1:A:134:GLU:OE1	1:A:134:GLU:HA	2.16	0.44
1:A:157:HIS:NE2	1:A:166:GLN:HG2	2.33	0.44
1:A:295:VAL:O	1:A:298:LYS:N	2.50	0.44
1:A:302:ILE:HG22	1:A:306:LEU:HD12	1.98	0.44
1:B:387:TRP:O	1:B:391:GLU:HG3	2.17	0.44
1:C:55:GLU:N	2:C:477:HOH:O	2.50	0.44
1:C:107:TYR:O	1:C:108:TYR:C	2.60	0.44
1:C:283:ILE:HG22	1:C:314:ILE:HG23	1.99	0.44
1:D:159:THR:CG2	1:D:162:GLU:HB2	2.47	0.44
1:D:159:THR:HG21	2:D:464:HOH:O	2.16	0.44
1:A:64:GLU:OE2	1:A:64:GLU:HA	2.17	0.44
1:A:402:PRO:O	1:A:406:LYS:HG2	2.17	0.44
1:A:403:ASP:HA	1:A:406:LYS:HD3	1.98	0.44
1:B:11:LEU:HD12	1:B:11:LEU:HA	1.74	0.44
1:B:225:GLN:O	1:B:226:ASN:C	2.60	0.44
1:C:56:ALA:CA	1:D:34:PHE:HD1	2.29	0.44
1:C:120:LEU:HD13	1:C:157:HIS:O	2.17	0.44
1:C:338:GLU:HB2	1:C:350:THR:CG2	2.45	0.44
1:D:344:ILE:HD12	1:D:344:ILE:C	2.41	0.44
1:B:68:ALA:C	1:B:70:GLU:H	2.25	0.44
1:C:55:GLU:OE1	1:D:38:ARG:NH2	2.47	0.44
1:C:100:PRO:CG	1:C:101:THR:H	2.27	0.44
1:C:320:ARG:O	1:C:321:PRO:C	2.59	0.44
1:D:282:VAL:HG11	1:D:328:TRP:NE1	2.33	0.44
1:D:297:GLU:C	1:D:299:ALA:N	2.75	0.44
1:D:325:PHE:CE1	1:D:338:GLU:HG2	2.52	0.44
1:A:62:ILE:CD1	1:A:105:PRO:HD3	2.47	0.44
1:A:66:LEU:HB3	1:A:104:THR:HG22	2.00	0.44
1:A:67:LEU:HD11	1:A:77:PHE:CE2	2.48	0.44
1:A:73:HIS:C	1:A:74:ILE:HG13	2.42	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:100:PRO:HG2	1:B:101:THR:H	1.82	0.44
1:B:130:THR:C	1:B:131:PHE:CD1	2.95	0.44
1:B:252:ILE:HG13	1:B:252:ILE:O	2.17	0.44
1:B:313:HIS:HD2	1:B:328:TRP:CZ2	2.35	0.44
1:B:343:ASP:O	1:B:348:LYS:N	2.47	0.44
1:B:406:LYS:O	1:B:409:LEU:HB2	2.17	0.44
1:C:23:ILE:O	1:C:24:LYS:O	2.35	0.44
1:D:266:ASP:O	1:D:267:GLU:C	2.61	0.44
1:A:56:ALA:HB1	1:B:29:TYR:O	2.18	0.44
1:A:320:ARG:O	1:A:321:PRO:C	2.60	0.44
1:C:83:TRP:CE3	1:C:97:ALA:HB2	2.53	0.44
1:C:319:ILE:CG1	1:C:320:ARG:N	2.80	0.44
1:A:60:MET:HE1	1:B:60:MET:SD	2.57	0.44
1:A:83:TRP:CE3	1:A:97:ALA:HB2	2.53	0.44
1:A:196:PHE:CG	1:A:197:PRO:CD	3.00	0.44
1:B:177:PHE:CZ	1:B:181:LEU:HD11	2.53	0.44
1:B:270:LEU:HG	1:B:272:LEU:HD23	1.98	0.44
1:B:364:GLU:C	1:B:366:GLN:H	2.25	0.44
1:B:375:LEU:C	1:B:377:ASN:N	2.75	0.44
1:C:86:HIS:CD2	2:C:460:HOH:O	2.71	0.44
1:C:142:ILE:HG23	1:C:215:MET:HE1	1.99	0.44
1:D:104:THR:HB	1:D:105:PRO:CD	2.48	0.44
1:D:114:VAL:HG22	1:D:120:LEU:HD21	1.98	0.44
1:D:123:LYS:HG2	1:D:155:THR:HG22	2.00	0.44
1:D:183:ILE:HA	1:D:184:PRO:HD3	1.75	0.44
1:D:343:ASP:O	1:D:348:LYS:N	2.48	0.44
1:A:100:PRO:CG	1:A:101:THR:H	2.28	0.44
1:A:107:TYR:C	1:A:109:MET:N	2.74	0.44
1:A:178:PHE:O	1:A:182:GLY:N	2.51	0.44
1:A:214:THR:HG23	1:A:453:LYS:O	2.17	0.44
1:A:274:PRO:HD2	1:A:275:ILE:HD12	1.99	0.44
1:A:424:ILE:C	1:A:424:ILE:HD12	2.43	0.44
1:B:3:PHE:O	1:B:4:SER:C	2.61	0.44
1:C:36:ILE:O	1:C:36:ILE:CG1	2.66	0.44
1:C:185:TYR:CD1	1:C:185:TYR:C	2.95	0.44
1:D:21:TYR:CD2	1:D:22:PRO:HD2	2.52	0.44
1:D:130:THR:C	1:D:131:PHE:CD1	2.95	0.44
1:D:141:LEU:HD13	1:D:257:ILE:HD11	1.99	0.44
1:D:174:TYR:O	1:D:177:PHE:HB3	2.18	0.44
1:D:273:PRO:HB3	1:D:379:MET:SD	2.57	0.44
1:A:185:TYR:CD1	1:A:185:TYR:C	2.95	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:319:ILE:CG1	1:A:320:ARG:N	2.81	0.44
1:C:270:LEU:O	1:C:354:ARG:NH1	2.51	0.44
1:C:355:ASP:OD2	1:C:356:THR:N	2.49	0.44
1:D:92:LEU:O	1:D:93:ASP:CG	2.60	0.44
1:D:101:THR:O	1:D:103:GLU:N	2.50	0.44
1:D:108:TYR:O	1:D:111:LYS:HB3	2.18	0.44
1:A:21:TYR:CG	1:B:59:PRO:HG2	2.53	0.43
1:A:115:LYS:O	1:A:235:PHE:HA	2.18	0.43
1:A:321:PRO:O	1:A:324:LYS:HB2	2.18	0.43
1:A:366:GLN:HE21	1:A:366:GLN:HA	1.83	0.43
1:A:448:TYR:N	1:A:448:TYR:CD1	2.86	0.43
1:B:92:LEU:O	1:B:93:ASP:CG	2.60	0.43
1:C:60:MET:HE2	1:C:129:ASN:O	2.18	0.43
1:C:73:HIS:C	1:C:74:ILE:HG13	2.42	0.43
1:C:279:ILE:O	1:C:333:VAL:HG13	2.18	0.43
1:C:405:ILE:HD13	1:C:451:ILE:CD1	2.47	0.43
1:D:37:ARG:HA	1:D:40:THR:HB	2.00	0.43
1:D:189:LYS:O	1:D:189:LYS:HG2	2.18	0.43
1:D:237:THR:C	1:D:239:THR:H	2.26	0.43
1:A:102:SER:HB3	1:A:152:GLU:OE1	2.18	0.43
1:A:189:LYS:O	1:A:190:ARG:C	2.60	0.43
1:B:266:ASP:OD1	1:B:271:ILE:HD11	2.18	0.43
1:C:286:LEU:HD12	1:C:286:LEU:H	1.83	0.43
1:C:428:GLU:O	1:C:432:LYS:N	2.52	0.43
1:D:291:LYS:N	1:D:292:GLU:OE2	2.51	0.43
1:A:303:TYR:CD1	1:A:303:TYR:C	2.96	0.43
1:B:398:GLU:OE1	1:B:399:ASP:N	2.51	0.43
1:C:60:MET:CE	1:D:60:MET:HE1	2.45	0.43
1:C:214:THR:HG23	1:C:453:LYS:O	2.17	0.43
1:C:448:TYR:CD1	1:C:448:TYR:N	2.86	0.43
1:D:60:MET:HG3	1:D:99:ARG:HG2	2.00	0.43
1:D:91:GLN:HG2	1:D:93:ASP:H	1.83	0.43
1:D:207:THR:HG23	1:D:215:MET:HB3	1.99	0.43
1:A:55:GLU:OE1	1:B:38:ARG:NH2	2.49	0.43
1:A:58:PHE:C	1:B:148:MET:HE1	2.43	0.43
1:A:142:ILE:HG21	1:A:215:MET:HE1	1.99	0.43
1:A:157:HIS:HB3	1:A:162:GLU:HB3	2.00	0.43
1:A:237:THR:C	1:A:239:THR:N	2.76	0.43
1:A:373:LYS:HB2	1:A:373:LYS:HZ2	1.81	0.43
1:A:437:ILE:HG22	1:A:439:GLY:N	2.32	0.43
1:B:183:ILE:HA	1:B:184:PRO:HD3	1.75	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:291:LYS:N	1:B:292:GLU:OE2	2.51	0.43
1:B:335:LEU:HD11	1:B:374:THR:CG2	2.45	0.43
1:C:127:ILE:HA	1:C:151:LYS:HA	2.00	0.43
1:D:82:TYR:HB2	1:D:98:LEU:HB2	1.99	0.43
1:D:186:LEU:HD21	1:D:441:THR:OG1	2.17	0.43
1:D:370:VAL:O	1:D:371:VAL:C	2.62	0.43
1:A:16:ILE:HG21	1:A:261:ILE:HD11	2.01	0.43
1:A:36:ILE:O	1:A:36:ILE:CG1	2.66	0.43
1:C:105:PRO:O	1:C:109:MET:HG2	2.18	0.43
1:C:157:HIS:NE2	1:C:166:GLN:HG2	2.34	0.43
1:C:429:LEU:O	1:C:432:LYS:HB3	2.18	0.43
1:D:261:ILE:HG22	1:D:262:ALA:N	2.33	0.43
1:D:351:LEU:HB2	1:D:360:PHE:CE2	2.53	0.43
1:A:60:MET:HE2	1:A:129:ASN:O	2.19	0.43
1:A:222:ASN:C	1:A:222:ASN:ND2	2.75	0.43
1:A:283:ILE:O	1:A:314:ILE:HA	2.19	0.43
1:B:82:TYR:HB2	1:B:98:LEU:HB2	2.00	0.43
1:C:66:LEU:O	1:C:67:LEU:C	2.59	0.43
1:C:208:ILE:HG21	1:C:414:GLY:HA2	2.00	0.43
1:C:226:ASN:N	1:C:226:ASN:HD22	2.16	0.43
1:C:295:VAL:O	1:C:298:LYS:N	2.51	0.43
1:D:58:PHE:N	1:D:126:GLN:NE2	2.59	0.43
1:D:292:GLU:CD	1:D:292:GLU:H	2.27	0.43
1:A:24:LYS:NZ	1:A:137:HIS:CD2	2.86	0.43
1:A:59:PRO:HG2	1:B:21:TYR:CE1	2.54	0.43
1:A:71:ALA:HA	1:A:75:LYS:CE	2.31	0.43
1:A:370:VAL:O	1:A:371:VAL:C	2.62	0.43
1:B:266:ASP:O	1:B:267:GLU:C	2.62	0.43
1:B:272:LEU:HA	1:B:273:PRO:HD3	1.85	0.43
1:B:315:ASP:OD2	1:B:324:LYS:HD3	2.19	0.43
1:B:421:LYS:O	1:B:422:GLU:C	2.61	0.43
1:C:362:VAL:HG21	1:C:370:VAL:HG21	2.01	0.43
1:D:3:PHE:O	1:D:4:SER:C	2.61	0.43
1:D:360:PHE:N	1:D:360:PHE:CD2	2.84	0.43
1:D:364:GLU:C	1:D:366:GLN:H	2.27	0.43
1:B:104:THR:HB	1:B:105:PRO:HD3	2.01	0.43
1:B:207:THR:HG23	1:B:215:MET:HB3	1.99	0.43
1:B:277:ALA:C	1:B:279:ILE:N	2.75	0.43
1:B:286:LEU:HD12	1:B:286:LEU:N	2.15	0.43
1:C:3:PHE:O	1:C:4:SER:C	2.61	0.43
1:C:16:ILE:HD13	1:C:261:ILE:HD11	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:36:ILE:O	1:C:40:THR:OG1	2.36	0.43
1:C:234:ILE:C	1:C:234:ILE:CD1	2.91	0.43
1:C:257:ILE:O	1:C:261:ILE:HG13	2.19	0.43
1:C:406:LYS:HB3	1:C:433:VAL:O	2.18	0.43
1:D:41:PHE:CE1	1:D:256:VAL:HG21	2.54	0.43
1:D:315:ASP:OD2	1:D:324:LYS:HD3	2.19	0.43
1:A:211:ASP:OD1	1:A:213:ARG:HB2	2.19	0.43
1:B:297:GLU:C	1:B:299:ALA:H	2.27	0.43
1:B:360:PHE:N	1:B:360:PHE:CD2	2.84	0.43
1:C:303:TYR:CD1	1:C:303:TYR:C	2.97	0.43
1:D:10:ILE:C	1:D:12:GLU:N	2.75	0.43
1:D:283:ILE:H	1:D:283:ILE:CD1	2.30	0.43
1:D:375:LEU:C	1:D:377:ASN:N	2.76	0.43
1:A:279:ILE:O	1:A:333:VAL:HG13	2.19	0.43
1:A:292:GLU:CD	1:A:292:GLU:H	2.27	0.43
1:A:303:TYR:O	1:A:304:GLU:C	2.61	0.43
1:A:351:LEU:O	1:A:359:LYS:HG3	2.19	0.43
1:A:378:ILE:O	1:A:379:MET:C	2.61	0.43
1:B:36:ILE:HD13	1:B:36:ILE:O	2.18	0.43
1:B:40:THR:HG22	1:B:41:PHE:CD1	2.54	0.43
1:A:66:LEU:O	1:A:67:LEU:C	2.60	0.42
1:A:84:VAL:HG11	1:B:82:TYR:CD2	2.54	0.42
1:A:281:VAL:HB	1:A:312:VAL:HG12	2.01	0.42
1:B:292:GLU:CD	1:B:292:GLU:H	2.27	0.42
1:C:190:ARG:HH21	1:C:216:GLN:NE2	2.15	0.42
1:C:208:ILE:CD1	1:C:415:VAL:HG12	2.49	0.42
1:C:248:THR:O	1:C:248:THR:HG23	2.18	0.42
1:A:60:MET:HA	1:A:99:ARG:HH11	1.83	0.42
1:B:10:ILE:HD11	1:B:270:LEU:CB	2.33	0.42
1:B:91:GLN:HG2	1:B:93:ASP:H	1.84	0.42
1:C:292:GLU:CD	1:C:292:GLU:H	2.27	0.42
1:D:23:ILE:O	1:D:26:CYS:HB2	2.19	0.42
1:D:222:ASN:C	1:D:222:ASN:ND2	2.77	0.42
1:A:74:ILE:O	1:A:74:ILE:CG2	2.67	0.42
1:A:140:PRO:C	1:A:142:ILE:N	2.75	0.42
1:A:253:SER:C	1:A:255:ARG:N	2.76	0.42
1:A:405:ILE:HD13	1:A:451:ILE:HD12	2.02	0.42
1:B:10:ILE:O	1:B:12:GLU:N	2.52	0.42
1:B:105:PRO:HG2	1:B:106:ILE:H	1.84	0.42
1:B:125:TYR:HB2	1:B:153:ALA:HA	2.01	0.42
1:B:271:ILE:HG12	1:B:354:ARG:HH12	1.76	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:350:THR:CA	1:B:361:GLN:HG2	2.48	0.42
1:C:33:GLY:HA2	1:C:36:ILE:CG2	2.49	0.42
1:C:57:LEU:HD23	1:D:148:MET:HB3	1.99	0.42
1:C:71:ALA:HA	1:C:75:LYS:CE	2.31	0.42
1:C:84:VAL:HG21	1:D:98:LEU:HD11	2.00	0.42
1:C:269:GLY:O	1:C:270:LEU:O	2.37	0.42
1:C:403:ASP:HA	1:C:406:LYS:HD3	1.99	0.42
1:D:321:PRO:HG3	2:D:469:HOH:O	2.18	0.42
1:C:60:MET:HG3	1:C:99:ARG:HG2	1.99	0.42
1:C:92:LEU:O	1:C:94:VAL:N	2.52	0.42
1:D:63:PRO:HG2	1:D:66:LEU:HD13	2.01	0.42
1:D:174:TYR:O	1:D:175:LYS:C	2.62	0.42
1:D:433:VAL:O	1:D:434:GLU:C	2.63	0.42
1:A:362:VAL:HG22	1:A:363:ASP:N	2.34	0.42
1:B:66:LEU:HB3	1:B:104:THR:CG2	2.48	0.42
1:B:99:ARG:HH21	1:B:129:ASN:H	1.66	0.42
1:C:99:ARG:HH21	1:C:129:ASN:H	1.67	0.42
1:C:206:ASP:CG	1:C:438:LEU:HD22	2.44	0.42
1:C:211:ASP:OD1	1:C:213:ARG:HB2	2.20	0.42
1:C:379:MET:O	1:C:380:GLU:C	2.62	0.42
1:D:177:PHE:CZ	1:D:181:LEU:HD11	2.55	0.42
1:A:3:PHE:O	1:A:4:SER:C	2.62	0.42
1:A:279:ILE:HD13	1:A:313:HIS:HB3	2.01	0.42
1:B:192:GLU:O	1:B:194:ASP:N	2.53	0.42
1:C:101:THR:CG2	1:C:102:SER:H	2.14	0.42
1:C:256:VAL:O	1:C:259:SER:N	2.53	0.42
1:D:297:GLU:C	1:D:299:ALA:H	2.27	0.42
1:D:379:MET:HE3	1:D:383:LYS:HB2	2.00	0.42
1:D:398:GLU:OE1	1:D:399:ASP:N	2.52	0.42
1:A:92:LEU:O	1:A:94:VAL:N	2.52	0.42
1:A:105:PRO:O	1:A:109:MET:HG2	2.19	0.42
1:A:107:TYR:N	1:A:107:TYR:CD2	2.87	0.42
1:A:127:ILE:HA	1:A:151:LYS:HA	2.01	0.42
1:A:405:ILE:HA	1:A:408:ILE:CG2	2.47	0.42
1:B:152:GLU:O	1:B:152:GLU:HG3	2.19	0.42
1:C:37:ARG:HA	1:C:40:THR:HB	2.02	0.42
1:C:356:THR:OG1	1:C:358:GLU:HG2	2.19	0.42
1:D:34:PHE:CE2	1:D:37:ARG:NH1	2.87	0.42
1:A:64:GLU:O	1:A:65:ASP:C	2.63	0.42
1:A:101:THR:CG2	1:A:102:SER:H	2.12	0.42
1:A:104:THR:N	1:A:105:PRO:HD2	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:367:LEU:O	1:B:368:MET:C	2.63	0.42
1:C:2:GLU:HG3	1:C:3:PHE:N	2.35	0.42
1:C:418:VAL:O	1:C:419:PRO:C	2.63	0.42
1:D:39:TYR:CD2	1:D:311:ARG:NH1	2.87	0.42
1:D:190:ARG:HH22	1:D:206:ASP:CG	2.28	0.42
1:D:292:GLU:O	1:D:293:ASP:C	2.63	0.42
1:A:283:ILE:HB	1:A:314:ILE:HG12	2.01	0.42
1:B:351:LEU:HD22	1:B:351:LEU:N	2.35	0.42
1:C:14:ALA:O	1:C:15:GLU:HB2	2.19	0.42
1:C:402:PRO:O	1:C:406:LYS:HG2	2.20	0.42
1:D:191:PRO:HB3	1:D:425:TYR:CE2	2.55	0.42
1:A:36:ILE:O	1:A:40:THR:OG1	2.37	0.42
1:A:56:ALA:CA	1:B:34:PHE:HD1	2.32	0.42
1:B:416:ILE:HD13	1:B:416:ILE:HA	1.89	0.42
1:C:58:PHE:CD1	1:C:126:GLN:NE2	2.83	0.42
1:C:284:VAL:HG11	1:C:325:PHE:HE1	1.84	0.42
1:C:335:LEU:HD12	1:C:352:PHE:O	2.20	0.42
1:C:437:ILE:HG22	1:C:439:GLY:N	2.34	0.42
1:D:270:LEU:HG	1:D:272:LEU:HD23	2.00	0.42
1:D:355:ASP:OD2	1:D:355:ASP:N	2.53	0.42
1:D:385:ARG:HH11	1:D:385:ARG:HG3	1.85	0.42
1:D:421:LYS:O	1:D:422:GLU:C	2.63	0.42
1:A:37:ARG:HA	1:A:40:THR:HB	2.02	0.41
1:A:104:THR:HB	1:A:105:PRO:HD3	2.01	0.41
1:A:277:ALA:C	1:A:279:ILE:H	2.27	0.41
1:C:56:ALA:HA	1:D:34:PHE:HD1	1.85	0.41
1:A:112:LEU:O	1:A:113:TRP:HD1	2.03	0.41
1:A:151:LYS:O	1:A:151:LYS:HE2	2.19	0.41
1:C:99:ARG:HA	1:C:100:PRO:HD2	1.95	0.41
1:D:277:ALA:C	1:D:279:ILE:N	2.77	0.41
1:A:21:TYR:CD2	1:B:59:PRO:HG2	2.55	0.41
1:A:103:GLU:HB2	1:A:107:TYR:CE1	2.55	0.41
1:B:190:ARG:HH22	1:B:206:ASP:CG	2.29	0.41
1:C:66:LEU:HD12	1:C:66:LEU:N	2.36	0.41
1:C:134:GLU:OE1	1:C:134:GLU:HA	2.19	0.41
1:C:405:ILE:HA	1:C:408:ILE:CG2	2.47	0.41
1:C:424:ILE:C	1:C:424:ILE:CD1	2.93	0.41
1:D:82:TYR:OH	1:D:145:ARG:NH1	2.51	0.41
1:A:57:LEU:HD23	1:B:148:MET:HB3	2.01	0.41
1:A:103:GLU:HG2	1:A:104:THR:N	2.36	0.41
1:A:107:TYR:HB3	1:A:233:ILE:HD11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:34:PHE:CE2	1:B:37:ARG:NH1	2.88	0.41
1:B:178:PHE:CD2	1:B:217:ILE:HD12	2.55	0.41
1:B:351:LEU:HB2	1:B:360:PHE:CE2	2.54	0.41
1:C:64:GLU:O	1:C:65:ASP:C	2.63	0.41
1:C:405:ILE:HD13	1:C:451:ILE:HD12	2.03	0.41
1:D:415:VAL:HG23	1:D:452:ALA:HB2	2.02	0.41
1:D:416:ILE:HD13	1:D:416:ILE:HA	1.87	0.41
1:A:140:PRO:C	1:A:142:ILE:H	2.29	0.41
1:A:229:LYS:O	1:A:231:PHE:N	2.54	0.41
1:B:106:ILE:O	1:B:106:ILE:HG22	2.20	0.41
1:B:139:ARG:HB2	1:B:143:ARG:H	1.84	0.41
1:C:60:MET:HA	1:C:99:ARG:HH11	1.84	0.41
1:C:170:ALA:O	1:C:173:ILE:N	2.53	0.41
1:C:171:ILE:O	1:C:175:LYS:HB2	2.20	0.41
1:C:282:VAL:HG11	1:C:328:TRP:CD1	2.56	0.41
1:C:378:ILE:O	1:C:379:MET:C	2.62	0.41
1:D:139:ARG:HB2	1:D:143:ARG:H	1.84	0.41
1:D:254:ASP:O	1:D:255:ARG:C	2.63	0.41
1:D:310:PHE:CZ	1:D:372:GLU:HA	2.56	0.41
1:A:110:MET:HE1	1:A:156:ALA:HB2	2.03	0.41
1:A:196:PHE:O	1:A:197:PRO:C	2.63	0.41
1:A:206:ASP:CG	1:A:438:LEU:HD22	2.46	0.41
1:A:421:LYS:O	1:A:422:GLU:C	2.63	0.41
1:B:36:ILE:HD13	1:B:36:ILE:C	2.45	0.41
1:C:67:LEU:HD11	1:C:77:PHE:CE2	2.50	0.41
1:C:287:ILE:HG13	1:C:287:ILE:O	2.21	0.41
1:A:190:ARG:HH21	1:A:216:GLN:NE2	2.17	0.41
1:B:45:ARG:HE	1:B:127:ILE:HD12	1.85	0.41
1:B:174:TYR:O	1:B:175:LYS:C	2.63	0.41
1:B:303:TYR:O	1:B:304:GLU:C	2.64	0.41
1:B:325:PHE:HD1	1:B:336:ARG:HD3	1.81	0.41
1:C:229:LYS:O	1:C:231:PHE:N	2.54	0.41
1:C:274:PRO:HD2	1:C:275:ILE:CD1	2.51	0.41
1:A:127:ILE:HG12	1:A:151:LYS:HG3	2.03	0.41
1:B:102:SER:HB3	1:B:152:GLU:CD	2.44	0.41
1:B:293:ASP:O	1:B:294:ILE:C	2.62	0.41
1:C:55:GLU:HB3	2:C:477:HOH:O	2.20	0.41
1:C:103:GLU:HG2	1:C:104:THR:N	2.36	0.41
1:D:14:ALA:O	1:D:15:GLU:HB2	2.20	0.41
1:D:103:GLU:C	1:D:105:PRO:HD2	2.45	0.41
1:D:125:TYR:HB2	1:D:153:ALA:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:192:GLU:O	1:D:194:ASP:N	2.54	0.41
1:A:16:ILE:HD13	1:A:261:ILE:HD11	2.03	0.41
1:A:43:ILE:O	1:A:47:LEU:HG	2.20	0.41
1:A:129:ASN:O	1:A:129:ASN:CG	2.64	0.41
1:A:353:ARG:NH2	1:A:377:ASN:OD1	2.54	0.41
1:A:401:ASN:CG	1:A:404:GLU:HB2	2.45	0.41
1:B:124:ILE:O	1:B:154:HIS:N	2.54	0.41
1:B:174:TYR:O	1:B:177:PHE:HB3	2.21	0.41
1:B:186:LEU:HD21	1:B:441:THR:OG1	2.20	0.41
1:B:223:LEU:HD13	1:B:227:PHE:HD2	1.86	0.41
1:B:310:PHE:CZ	1:B:372:GLU:HA	2.56	0.41
1:B:355:ASP:OD2	1:B:355:ASP:N	2.54	0.41
1:B:415:VAL:HG23	1:B:452:ALA:HB2	2.02	0.41
1:C:16:ILE:HG21	1:C:261:ILE:HD11	2.03	0.41
1:C:24:LYS:NZ	1:C:137:HIS:CD2	2.89	0.41
1:C:74:ILE:O	1:C:74:ILE:CG2	2.69	0.41
1:C:189:LYS:O	1:C:190:ARG:C	2.63	0.41
1:C:270:LEU:HB3	1:C:332:GLY:HA3	2.02	0.41
1:D:190:ARG:HB2	1:D:202:THR:O	2.21	0.41
1:D:293:ASP:O	1:D:294:ILE:C	2.63	0.41
1:D:367:LEU:O	1:D:368:MET:C	2.64	0.41
1:D:428:GLU:O	1:D:429:LEU:C	2.64	0.41
1:A:436:THR:O	1:A:436:THR:HG22	2.20	0.41
1:C:99:ARG:CZ	1:C:128:VAL:HB	2.51	0.41
1:C:257:ILE:HA	1:C:260:ILE:HD12	2.03	0.41
1:D:64:GLU:C	1:D:64:GLU:OE2	2.63	0.41
1:D:163:ALA:O	1:D:166:GLN:N	2.52	0.41
1:D:256:VAL:HG23	1:D:257:ILE:N	2.34	0.41
1:D:328:TRP:HA	1:D:328:TRP:CE3	2.55	0.41
1:A:424:ILE:C	1:A:424:ILE:CD1	2.94	0.40
1:B:222:ASN:ND2	1:B:224:GLY:H	2.19	0.40
1:B:329:GLU:HG2	1:B:354:ARG:NE	2.36	0.40
1:C:21:TYR:CG	1:D:59:PRO:HG2	2.56	0.40
1:C:422:GLU:O	1:C:423:GLU:C	2.64	0.40
1:D:24:LYS:O	1:D:25:GLY:C	2.64	0.40
1:D:34:PHE:C	1:D:34:PHE:CD2	2.99	0.40
1:D:36:ILE:HD13	1:D:36:ILE:O	2.20	0.40
1:D:152:GLU:HG3	1:D:152:GLU:O	2.21	0.40
1:A:256:VAL:O	1:A:259:SER:N	2.55	0.40
1:A:287:ILE:O	1:A:287:ILE:HG13	2.21	0.40
1:B:37:ARG:O	1:B:37:ARG:HG2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:170:ALA:O	1:B:171:ILE:C	2.65	0.40
1:B:191:PRO:HB3	1:B:425:TYR:CE2	2.56	0.40
1:C:60:MET:SD	1:C:131:PHE:HE1	2.44	0.40
1:C:115:LYS:O	1:C:235:PHE:HA	2.21	0.40
1:D:189:LYS:O	1:D:190:ARG:O	2.39	0.40
1:D:228:SER:OG	1:D:245:ALA:O	2.30	0.40
1:A:0:MET:HE3	1:A:0:MET:O	2.22	0.40
1:A:10:ILE:CD1	1:A:270:LEU:N	2.75	0.40
1:B:24:LYS:O	1:B:25:GLY:C	2.65	0.40
1:B:32:TYR:CE1	1:B:278:PRO:HB2	2.57	0.40
1:B:379:MET:HE3	1:B:383:LYS:HB2	2.02	0.40
1:C:140:PRO:C	1:C:142:ILE:H	2.30	0.40
1:C:190:ARG:HH12	1:C:438:LEU:HD22	1.85	0.40
1:C:205:PHE:CG	1:C:218:ALA:HB3	2.56	0.40
1:C:253:SER:C	1:C:255:ARG:N	2.78	0.40
1:D:202:THR:O	1:D:202:THR:HG22	2.21	0.40
1:D:208:ILE:HD11	1:D:415:VAL:HG12	2.03	0.40
1:D:397:LEU:HD13	1:D:416:ILE:HG23	2.02	0.40
1:D:405:ILE:O	1:D:408:ILE:N	2.54	0.40
1:A:66:LEU:H	1:A:66:LEU:CD1	2.32	0.40
1:A:422:GLU:O	1:A:423:GLU:C	2.65	0.40
1:C:191:PRO:HB2	1:C:193:TRP:CE3	2.56	0.40
1:C:351:LEU:O	1:C:359:LYS:HG3	2.21	0.40
1:C:432:LYS:HD2	1:C:432:LYS:HA	1.91	0.40
1:D:157:HIS:HD1	1:D:162:GLU:HG2	1.87	0.40
1:D:360:PHE:HD2	1:D:360:PHE:N	2.19	0.40
1:A:24:LYS:HZ3	1:A:137:HIS:CD2	2.40	0.40
1:A:324:LYS:O	1:A:325:PHE:C	2.64	0.40
1:C:139:ARG:HH11	1:C:139:ARG:HG2	1.87	0.40
1:C:140:PRO:C	1:C:142:ILE:N	2.78	0.40
1:C:276:VAL:O	1:C:278:PRO:HD3	2.22	0.40
1:C:395:THR:HG21	1:C:408:ILE:HD11	2.03	0.40
1:D:10:ILE:O	1:D:12:GLU:N	2.55	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:323:ARG:NH1	1:C:323:ARG:NH1[2_646]	1.95	0.25
1:A:293:ASP:OD1	1:D:392:ASN:OD1[1_554]	2.10	0.10

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	454/459 (99%)	331 (73%)	84 (18%)	39 (9%)	0	3
1	B	454/459 (99%)	313 (69%)	104 (23%)	37 (8%)	1	4
1	C	454/459 (99%)	330 (73%)	85 (19%)	39 (9%)	0	3
1	D	454/459 (99%)	312 (69%)	107 (24%)	35 (8%)	1	5
All	All	1816/1836 (99%)	1286 (71%)	380 (21%)	150 (8%)	0	4

All (150) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	36	ILE
1	A	74	ILE
1	A	75	LYS
1	A	76	GLY
1	A	102	SER
1	A	262	ALA
1	A	263	ILE
1	A	270	LEU
1	A	272	LEU
1	A	317	ARG
1	A	354	ARG
1	B	102	SER
1	B	316	ASP
1	B	446	ASN
1	C	36	ILE
1	C	74	ILE
1	C	75	LYS
1	C	76	GLY
1	C	102	SER
1	C	262	ALA
1	C	263	ILE
1	C	270	LEU

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Mol	Chain	Res	Type
1	C	272	LEU
1	C	317	ARG
1	C	354	ARG
1	D	93	ASP
1	D	102	SER
1	D	190	ARG
1	D	316	ASP
1	D	446	ASN
1	A	65	ASP
1	A	271	ILE
1	A	303	TYR
1	A	423	GLU
1	B	22	PRO
1	B	27	GLY
1	B	76	GLY
1	B	93	ASP
1	B	190	ARG
1	B	248	THR
1	B	317	ARG
1	C	65	ASP
1	C	230	THR
1	C	271	ILE
1	C	303	TYR
1	C	423	GLU
1	D	22	PRO
1	D	27	GLY
1	D	76	GLY
1	D	95	LYS
1	D	193	TRP
1	D	248	THR
1	D	317	ARG
1	D	334	PRO
1	A	4	SER
1	A	11	LEU
1	A	22	PRO
1	A	24	LYS
1	A	31	PRO
1	A	123	LYS
1	A	132	ARG
1	A	133	TYR
1	A	197	PRO
1	A	230	THR

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Mol	Chain	Res	Type
1	A	411	GLU
1	B	65	ASP
1	B	95	LYS
1	B	188	SER
1	B	193	TRP
1	B	267	GLU
1	B	296	MET
1	B	307	LYS
1	B	334	PRO
1	B	368	MET
1	B	411	GLU
1	C	4	SER
1	C	11	LEU
1	C	22	PRO
1	C	24	LYS
1	C	123	LYS
1	C	132	ARG
1	C	133	TYR
1	C	197	PRO
1	C	241	ASP
1	C	411	GLU
1	C	436	THR
1	D	65	ASP
1	D	188	SER
1	D	267	GLU
1	D	296	MET
1	D	368	MET
1	D	411	GLU
1	A	3	PHE
1	A	192	GLU
1	A	241	ASP
1	A	436	THR
1	B	7	TYR
1	B	50	GLU
1	B	67	LEU
1	B	100	PRO
1	B	136	LYS
1	B	400	ILE
1	C	3	PHE
1	C	31	PRO
1	C	100	PRO
1	C	192	GLU

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Mol	Chain	Res	Type
1	D	7	TYR
1	D	100	PRO
1	D	189	LYS
1	D	307	LYS
1	D	400	ILE
1	D	403	ASP
1	A	100	PRO
1	A	248	THR
1	A	341	PRO
1	A	367	LEU
1	A	400	ILE
1	B	189	LYS
1	B	403	ASP
1	C	141	LEU
1	C	341	PRO
1	C	367	LEU
1	C	400	ILE
1	D	50	GLU
1	D	67	LEU
1	D	136	LYS
1	A	77	PHE
1	C	77	PHE
1	A	23	ILE
1	A	142	ILE
1	B	25	GLY
1	B	171	ILE
1	B	405	ILE
1	C	23	ILE
1	D	25	GLY
1	D	405	ILE
1	A	319	ILE
1	B	74	ILE
1	B	371	VAL
1	C	142	ILE
1	D	74	ILE
1	D	171	ILE
1	D	371	VAL
1	B	142	ILE
1	C	319	ILE
1	D	142	ILE
1	D	370	VAL
1	B	128	VAL

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Mol	Chain	Res	Type
1	B	197	PRO
1	B	370	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	412/414 (100%)	367 (89%)	45 (11%)	6	26
1	B	412/414 (100%)	369 (90%)	43 (10%)	7	28
1	C	412/414 (100%)	365 (89%)	47 (11%)	5	24
1	D	412/414 (100%)	369 (90%)	43 (10%)	7	28
All	All	1648/1656 (100%)	1470 (89%)	178 (11%)	6	27

All (178) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	LEU
1	A	28	VAL
1	A	31	PRO
1	A	36	ILE
1	A	94	VAL
1	A	103	GLU
1	A	114	VAL
1	A	122	ILE
1	A	132	ARG
1	A	136	LYS
1	A	137	HIS
1	A	140	PRO
1	A	211	ASP
1	A	213	ARG
1	A	216	GLN
1	A	239	THR
1	A	250	TYR
1	A	257	ILE
1	A	270	LEU

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Mol	Chain	Res	Type
1	A	271	ILE
1	A	275	ILE
1	A	315	ASP
1	A	323	ARG
1	A	351	LEU
1	A	354	ARG
1	A	360	PHE
1	A	369	GLU
1	A	373	LYS
1	A	382	ILE
1	A	389	LYS
1	A	392	ASN
1	A	393	PHE
1	A	396	ILE
1	A	398	GLU
1	A	401	ASN
1	A	413	ARG
1	A	417	LEU
1	A	424	ILE
1	A	426	ASN
1	A	436	THR
1	A	442	GLU
1	A	446	ASN
1	A	447	LYS
1	A	448	TYR
1	A	454	THR
1	B	1	LEU
1	B	26	CYS
1	B	28	VAL
1	B	31	PRO
1	B	36	ILE
1	B	77	PHE
1	B	78	GLU
1	B	104	THR
1	B	112	LEU
1	B	124	ILE
1	B	164	GLU
1	B	186	LEU
1	B	192	GLU
1	B	197	PRO
1	B	222	ASN
1	B	247	GLN

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Mol	Chain	Res	Type
1	B	248	THR
1	B	256	VAL
1	B	257	ILE
1	B	267	GLU
1	B	272	LEU
1	B	275	ILE
1	B	276	VAL
1	B	278	PRO
1	B	283	ILE
1	B	286	LEU
1	B	321	PRO
1	B	327	ASP
1	B	335	LEU
1	B	339	VAL
1	B	354	ARG
1	B	360	PHE
1	B	372	GLU
1	B	373	LYS
1	B	376	ASN
1	B	396	ILE
1	B	398	GLU
1	B	424	ILE
1	B	437	ILE
1	B	441	THR
1	B	442	GLU
1	B	447	LYS
1	B	449	ILE
1	C	1	LEU
1	C	10	ILE
1	C	28	VAL
1	C	31	PRO
1	C	36	ILE
1	C	94	VAL
1	C	103	GLU
1	C	114	VAL
1	C	122	ILE
1	C	132	ARG
1	C	136	LYS
1	C	137	HIS
1	C	140	PRO
1	C	211	ASP
1	C	213	ARG

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Mol	Chain	Res	Type
1	C	216	GLN
1	C	222	ASN
1	C	239	THR
1	C	250	TYR
1	C	257	ILE
1	C	270	LEU
1	C	271	ILE
1	C	275	ILE
1	C	315	ASP
1	C	323	ARG
1	C	351	LEU
1	C	354	ARG
1	C	360	PHE
1	C	369	GLU
1	C	373	LYS
1	C	382	ILE
1	C	389	LYS
1	C	392	ASN
1	C	393	PHE
1	C	396	ILE
1	C	398	GLU
1	C	401	ASN
1	C	413	ARG
1	C	417	LEU
1	C	424	ILE
1	C	426	ASN
1	C	436	THR
1	C	442	GLU
1	C	446	ASN
1	C	447	LYS
1	C	448	TYR
1	C	454	THR
1	D	1	LEU
1	D	26	CYS
1	D	28	VAL
1	D	31	PRO
1	D	36	ILE
1	D	77	PHE
1	D	78	GLU
1	D	104	THR
1	D	112	LEU
1	D	124	ILE

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Mol	Chain	Res	Type
1	D	164	GLU
1	D	186	LEU
1	D	192	GLU
1	D	197	PRO
1	D	222	ASN
1	D	247	GLN
1	D	248	THR
1	D	256	VAL
1	D	257	ILE
1	D	267	GLU
1	D	272	LEU
1	D	275	ILE
1	D	276	VAL
1	D	278	PRO
1	D	283	ILE
1	D	286	LEU
1	D	321	PRO
1	D	327	ASP
1	D	335	LEU
1	D	339	VAL
1	D	354	ARG
1	D	360	PHE
1	D	372	GLU
1	D	373	LYS
1	D	376	ASN
1	D	396	ILE
1	D	398	GLU
1	D	424	ILE
1	D	437	ILE
1	D	441	THR
1	D	442	GLU
1	D	447	LYS
1	D	449	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (51) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	46	ASN
1	A	126	GLN
1	A	137	HIS
1	A	216	GLN
1	A	222	ASN

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Mol	Chain	Res	Type
1	A	225	GLN
1	A	226	ASN
1	A	247	GLN
1	A	264	HIS
1	A	313	HIS
1	A	366	GLN
1	A	381	ASN
1	A	384	ASN
1	A	401	ASN
1	B	46	ASN
1	B	91	GLN
1	B	126	GLN
1	B	216	GLN
1	B	222	ASN
1	B	225	GLN
1	B	226	ASN
1	B	313	HIS
1	B	366	GLN
1	B	384	ASN
1	B	401	ASN
1	B	446	ASN
1	C	46	ASN
1	C	126	GLN
1	C	137	HIS
1	C	216	GLN
1	C	222	ASN
1	C	225	GLN
1	C	226	ASN
1	C	247	GLN
1	C	264	HIS
1	C	366	GLN
1	C	381	ASN
1	C	384	ASN
1	C	401	ASN
1	D	46	ASN
1	D	91	GLN
1	D	126	GLN
1	D	216	GLN
1	D	222	ASN
1	D	225	GLN
1	D	226	ASN
1	D	313	HIS

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Mol	Chain	Res	Type
1	D	366	GLN
1	D	384	ASN
1	D	401	ASN
1	D	446	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 [i](#)

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	456/459 (99%)	-0.63	0 100 100	10, 49, 112, 140	0
1	B	456/459 (99%)	-0.41	0 100 100	17, 69, 129, 144	0
1	C	456/459 (99%)	-0.63	0 100 100	11, 49, 111, 140	0
1	D	456/459 (99%)	-0.43	0 100 100	16, 69, 129, 144	0
All	All	1824/1836 (99%)	-0.53	0 100 100	10, 58, 122, 144	0

There are no RSRZ outliers to report.

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.