



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 05:11 PM UTC

PDB ID : 1X0U / pdb_00001x0u
Title : Crystal Structure of the carboxyl transferase subunit of putative PCC of *Sulfolobus tokodaii*
Authors : Kakuta, Y.; Sueda, S.; Kondo, H.
Deposited on : 2005-03-29
Resolution : 2.20 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

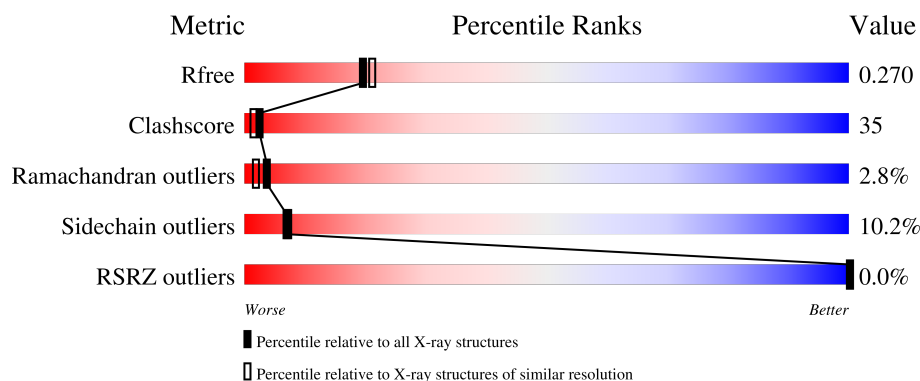
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	522	55% 36% 8% ..
1	B	522	58% 32% 8% ..
1	C	522	52% 36% 11% ..
1	D	522	55% 34% 9% ..
1	E	522	57% 35% 7% ..

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Mol	Chain	Length	Quality of chain
1	F	522	 A horizontal bar chart showing the quality of the chain. The bar is divided into three segments: green (60%), yellow (30%), and orange (9%). The orange segment is further divided into a red segment (2%) and a grey segment (7%). The percentages 60%, 30%, and 9% are labeled below the green, yellow, and orange segments respectively. The red segment is labeled with '2%' and the grey segment with '7%'.

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 25335 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 hypothetical methylmalonyl-CoA decarboxylase alpha subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	518	Total	C	N	O	S	0	0	0
			4002	2560	683	746	13			
1	B	518	Total	C	N	O	S	0	0	0
			4002	2560	683	746	13			
1	C	518	Total	C	N	O	S	0	0	0
			4002	2560	683	746	13			
1	D	518	Total	C	N	O	S	0	0	0
			4002	2560	683	746	13			
1	E	518	Total	C	N	O	S	0	0	0
			4002	2560	683	746	13			
1	F	518	Total	C	N	O	S	0	0	0
			4002	2560	683	746	13			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	ALA	SER	conflict	UNP Q974R9
B	2	ALA	SER	conflict	UNP Q974R9
C	2	ALA	SER	conflict	UNP Q974R9
D	2	ALA	SER	conflict	UNP Q974R9
E	2	ALA	SER	conflict	UNP Q974R9
F	2	ALA	SER	conflict	UNP Q974R9

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	216	Total	O	0	0
			216	216		
2	B	214	Total	O	0	0
			214	214		
2	C	205	Total	O	0	0
			205	205		

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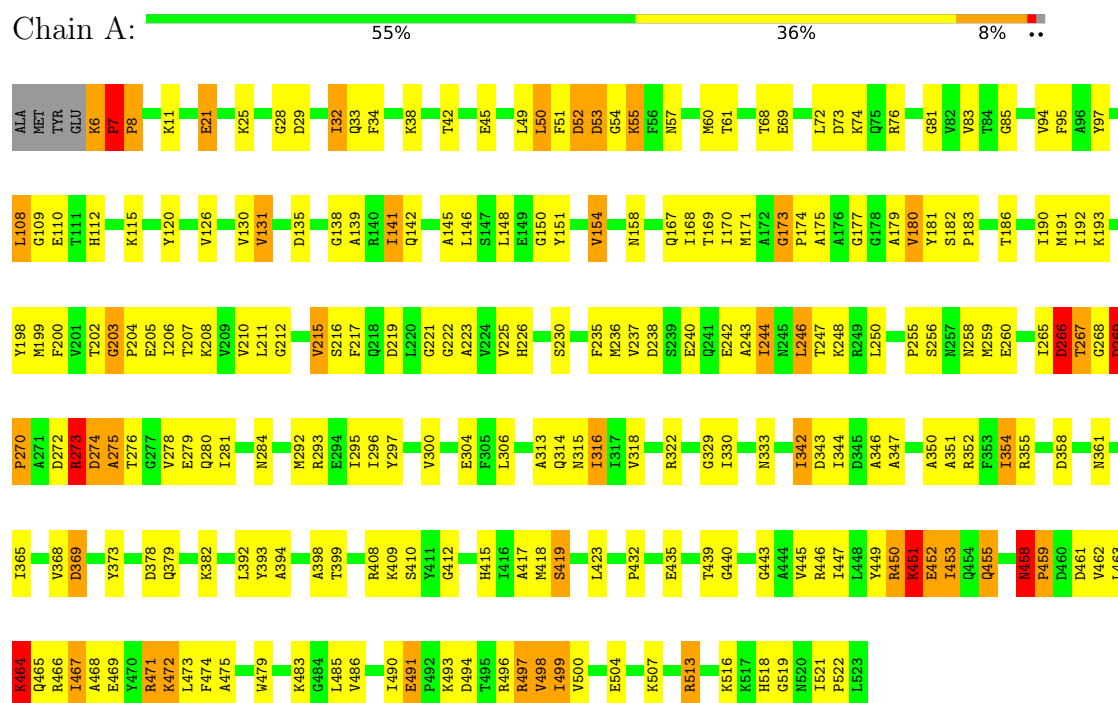
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	235	Total 235	O 235	0	0
2	E	230	Total 230	O 230	0	0
2	F	223	Total 223	O 223	0	0

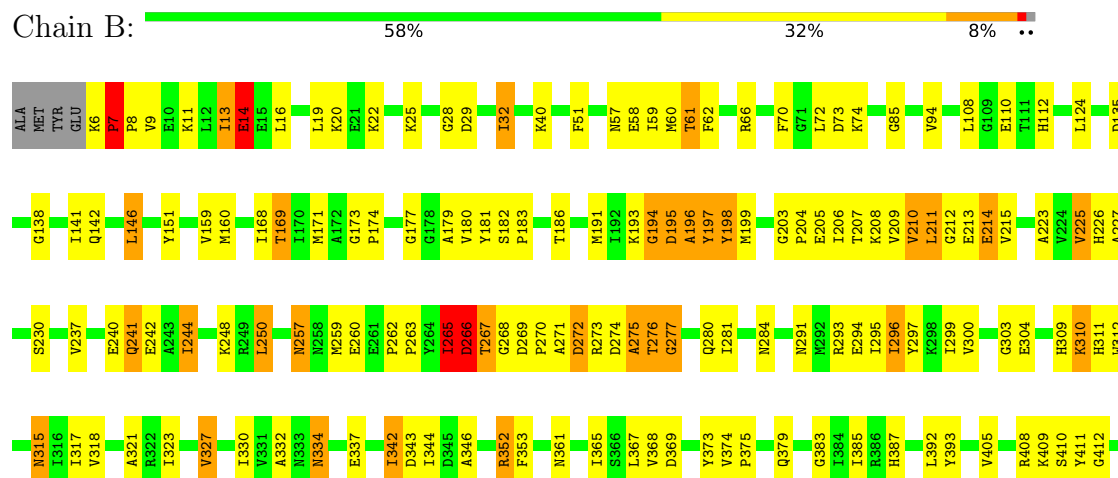
3 Residue-property plots

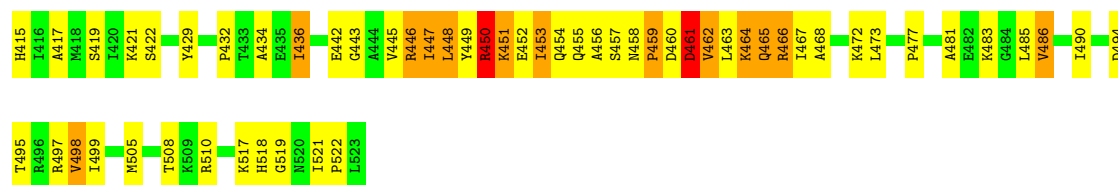
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: hypothetical methylmalonyl-CoA decarboxylase alpha subunit



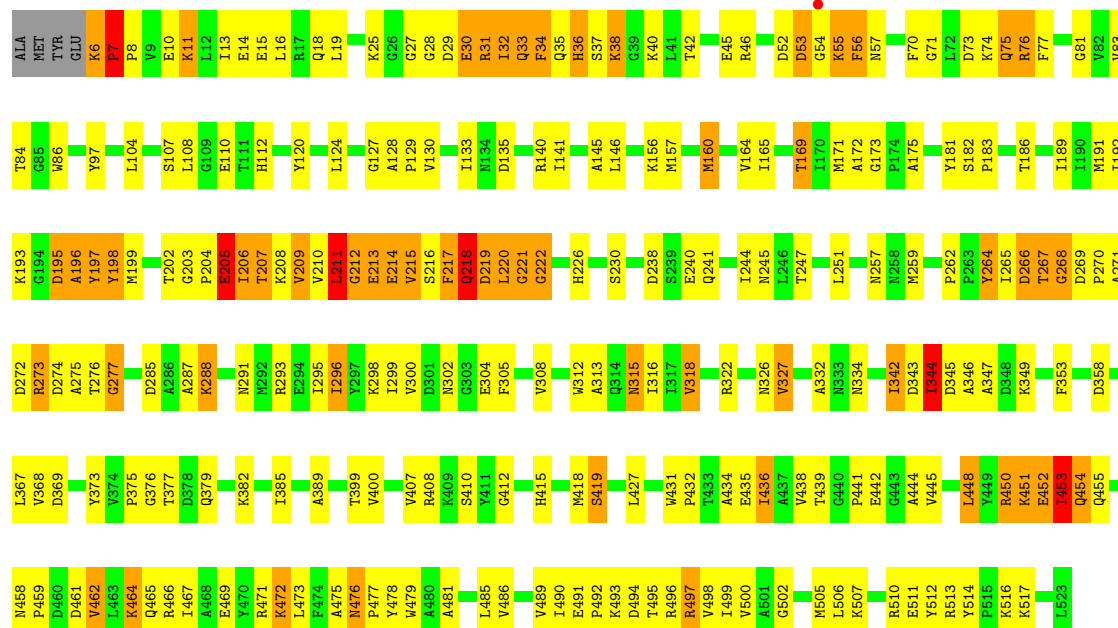
- Molecule 1: hypothetical methylmalonyl-CoA decarboxylase alpha subunit





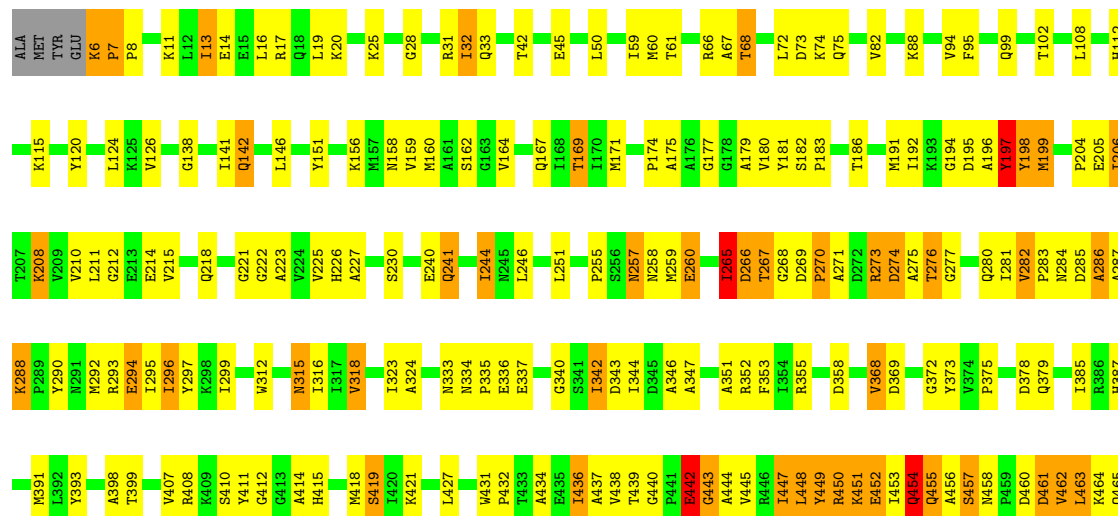
- Molecule 1: hypothetical methylmalonyl-CoA decarboxylase alpha subunit

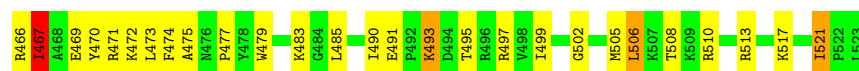
Chain C: 52% 36% 11% ..



- Molecule 1: hypothetical methylmalonyl-CoA decarboxylase alpha subunit

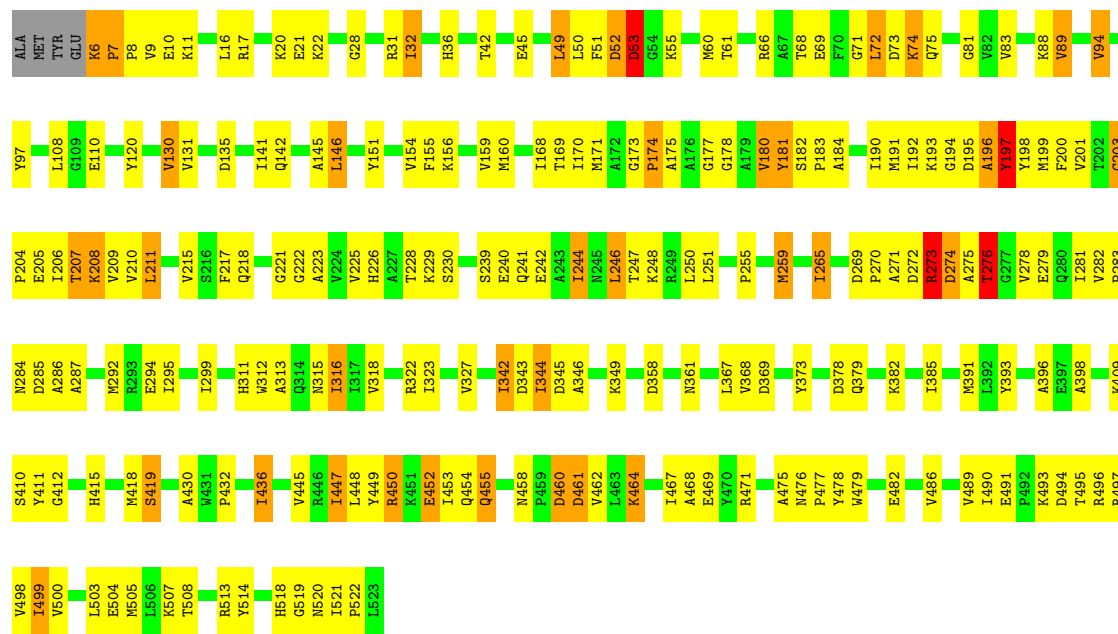
Chain D: 55% 34% 9% ..





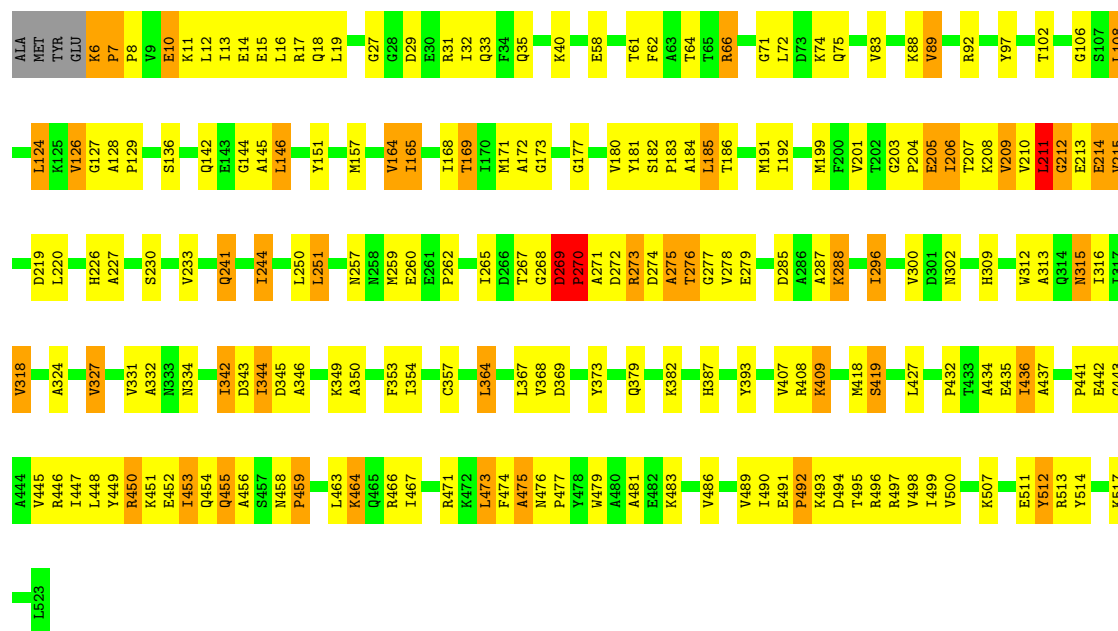
- Molecule 1: hypothetical methylmalonyl-CoA decarboxylase alpha subunit

Chain E: 57% 35% 7% ..



- Molecule 1: hypothetical methylmalonyl-CoA decarboxylase alpha subunit

Chain F: 60% 30% 9% ..



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	99.61Å 181.47Å 112.70Å 90.00° 116.21° 90.00°	Depositor
Resolution (Å)	48.03 – 2.20 48.03 – 2.20	Depositor EDS
% Data completeness (in resolution range)	92.4 (48.03-2.20) 92.6 (48.03-2.20)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.61 (at 2.20Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.228 , 0.271 0.227 , 0.270	Depositor DCC
R_{free} test set	9045 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	16.7	Xtriage
Anisotropy	1.205	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 16.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.479 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	25335	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.73% 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	0.48	0/4086	1.03	23/5531 (0.4%)
1	B	0.48	0/4086	1.01	24/5531 (0.4%)
1	C	0.47	0/4086	1.02	30/5531 (0.5%)
1	D	0.46	0/4086	1.00	16/5531 (0.3%)
1	E	0.49	0/4086	0.99	12/5531 (0.2%)
1	F	0.45	0/4086	0.98	15/5531 (0.3%)
All	All	0.47	0/24516	1.00	120/33186 (0.4%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (120) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	197	TYR	N-CA-C	12.57	124.40	108.19
1	A	453	ILE	N-CA-C	-11.32	99.88	111.88
1	A	7	PRO	N-CA-C	11.13	124.28	110.70
1	B	368	VAL	N-CA-C	10.29	122.58	108.17
1	C	368	VAL	N-CA-C	10.14	122.36	108.17
1	E	368	VAL	N-CA-C	9.82	122.41	108.36
1	D	368	VAL	N-CA-C	9.81	122.39	108.36
1	A	181	TYR	N-CA-C	9.80	122.05	111.36
1	F	368	VAL	N-CA-C	9.27	122.53	108.71
1	E	181	TYR	N-CA-C	9.18	121.37	111.36
1	B	7	PRO	N-CA-C	8.69	121.30	110.70
1	D	447	ILE	N-CA-C	-8.53	104.43	112.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	368	VAL	N-CA-C	8.46	120.80	108.53
1	C	53	ASP	N-CA-C	8.42	128.74	110.80
1	C	196	ALA	N-CA-C	-8.36	97.08	108.86
1	F	7	PRO	N-CA-C	8.24	120.75	110.70
1	C	7	PRO	N-CA-C	8.19	120.69	110.70
1	C	34	PHE	N-CA-C	-7.90	99.70	110.68
1	D	199	MET	N-CA-C	7.82	121.26	108.99
1	A	451	LYS	N-CA-C	-7.73	98.11	109.63
1	B	195	ASP	N-CA-C	-7.69	103.64	112.87
1	D	517	LYS	N-CA-C	-7.65	103.02	111.36
1	F	181	TYR	N-CA-C	7.62	119.67	111.36
1	C	197	TYR	N-CA-C	7.59	126.97	110.80
1	C	181	TYR	N-CA-C	7.58	120.61	111.82
1	D	7	PRO	N-CA-C	7.47	119.81	110.70
1	B	517	LYS	N-CA-C	-7.32	103.38	111.36
1	B	272	ASP	N-CA-C	7.29	116.87	108.49
1	D	181	TYR	N-CA-C	7.26	120.24	111.82
1	B	181	TYR	N-CA-C	7.18	120.15	111.82
1	F	450	ARG	N-CA-C	-7.07	100.59	110.35
1	C	164	VAL	N-CA-C	-7.05	106.19	112.12
1	A	300	VAL	N-CA-C	7.04	117.72	110.05
1	A	464	LYS	N-CA-C	-7.02	104.87	113.50
1	C	30	GLU	N-CA-C	-7.00	100.84	111.56
1	D	282	VAL	CA-C-N	6.87	127.80	120.11
1	D	282	VAL	C-N-CA	6.87	127.80	120.11
1	C	209	VAL	N-CA-C	-6.85	104.62	111.88
1	F	300	VAL	N-CA-C	6.83	117.49	110.05
1	C	52	ASP	N-CA-C	-6.79	102.96	111.11
1	B	198	TYR	N-CA-C	6.72	117.45	108.38
1	D	454	GLN	N-CA-C	-6.71	96.51	110.80
1	C	203	GLY	CA-C-N	6.67	126.36	119.56
1	C	203	GLY	C-N-CA	6.67	126.36	119.56
1	A	55	LYS	N-CA-C	6.50	118.66	107.93
1	C	198	TYR	N-CA-C	6.50	118.09	108.60
1	C	273	ARG	N-CA-C	6.39	118.23	108.07
1	F	271	ALA	N-CA-C	6.37	119.46	109.96
1	B	266	ASP	N-CA-C	6.37	124.36	110.80
1	C	489	VAL	N-CA-C	-6.35	99.33	108.53
1	C	222	GLY	N-CA-C	6.33	122.31	111.98
1	A	50	LEU	N-CA-C	6.22	117.73	111.07
1	E	461	ASP	N-CA-C	-6.21	105.66	113.18
1	B	203	GLY	CA-C-N	6.21	125.77	119.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	203	GLY	C-N-CA	6.21	125.77	119.19
1	B	448	LEU	N-CA-C	-6.14	104.85	112.90
1	D	467	ILE	N-CA-C	-6.14	103.96	112.50
1	F	211	LEU	N-CA-C	6.13	117.94	109.54
1	B	265	ILE	N-CA-C	6.11	122.05	109.34
1	A	314	GLN	N-CA-C	-6.04	106.00	113.19
1	E	203	GLY	CA-C-N	5.98	125.69	119.05
1	E	203	GLY	C-N-CA	5.98	125.69	119.05
1	C	218	GLN	N-CA-C	5.91	118.57	110.24
1	E	255	PRO	N-CA-C	-5.90	102.34	111.13
1	B	284	ASN	N-CA-C	-5.89	104.99	111.82
1	D	164	VAL	N-CA-C	-5.88	106.50	111.56
1	A	314	GLN	CA-C-N	5.83	128.37	120.38
1	A	314	GLN	C-N-CA	5.83	128.37	120.38
1	E	72	LEU	N-CA-C	-5.80	105.98	114.39
1	C	268	GLY	N-CA-C	-5.78	104.28	112.37
1	F	344	ILE	N-CA-C	-5.74	105.14	110.53
1	E	411	TYR	N-CA-C	5.72	118.80	109.59
1	F	269	ASP	N-CA-C	5.70	122.41	109.81
1	B	361	ASN	N-CA-C	5.69	119.52	112.24
1	C	73	ASP	N-CA-C	-5.69	106.18	113.23
1	B	14	GLU	N-CA-C	-5.68	105.17	111.36
1	C	517	LYS	N-CA-C	-5.60	105.27	111.71
1	F	164	VAL	N-CA-C	-5.53	107.42	111.90
1	A	281	ILE	N-CA-C	5.52	115.72	110.53
1	D	443	GLY	N-CA-C	-5.49	106.97	113.99
1	B	450	ARG	N-CA-C	-5.48	105.69	112.38
1	C	36	HIS	N-CA-C	5.46	119.58	113.02
1	E	7	PRO	N-CA-C	5.46	117.36	110.70
1	F	517	LYS	N-CA-C	-5.46	105.33	111.28
1	F	334	ASN	CA-C-N	5.45	125.12	119.56
1	F	334	ASN	C-N-CA	5.45	125.12	119.56
1	C	221	GLY	N-CA-C	-5.39	100.41	113.18
1	D	265	ILE	N-CA-C	5.37	120.50	109.34
1	F	489	VAL	N-CA-C	-5.31	100.80	108.71
1	B	461	ASP	CB-CA-C	-5.29	108.82	116.54
1	A	255	PRO	N-CA-C	-5.28	103.26	111.13
1	B	411	TYR	N-CA-C	5.27	118.33	109.95
1	C	334	ASN	CA-C-N	5.26	124.93	119.56
1	C	334	ASN	C-N-CA	5.26	124.93	119.56
1	E	361	ASN	N-CA-C	5.26	118.98	112.24
1	A	329	GLY	N-CA-C	-5.26	101.34	110.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	421	LYS	N-CA-C	5.23	116.67	111.07
1	A	8	PRO	N-CA-C	5.22	119.78	111.26
1	C	344	ILE	N-CA-C	-5.22	105.45	110.72
1	C	300	VAL	N-CA-C	5.21	116.70	109.45
1	A	471	ARG	N-CA-C	5.21	117.03	111.36
1	E	398	ALA	N-CA-C	5.18	117.74	110.23
1	A	173	GLY	CA-C-N	5.16	126.29	119.84
1	A	173	GLY	C-N-CA	5.16	126.29	119.84
1	A	203	GLY	CA-C-N	5.15	124.77	119.05
1	A	203	GLY	C-N-CA	5.15	124.77	119.05
1	D	66	ARG	N-CA-C	-5.12	107.08	113.38
1	D	449	TYR	N-CA-C	5.12	116.86	108.52
1	B	51	PHE	N-CA-C	5.10	118.03	110.48
1	B	334	ASN	CA-C-N	5.09	124.81	119.82
1	B	334	ASN	C-N-CA	5.09	124.81	119.82
1	C	478	TYR	N-CA-C	5.07	118.72	112.54
1	B	263	PRO	N-CA-C	5.05	119.25	111.21
1	E	447	ILE	N-CA-C	-5.05	105.48	112.50
1	A	361	ASN	N-CA-C	5.04	118.55	111.74
1	B	421	LYS	N-CA-C	5.04	117.16	111.11
1	F	409	LYS	N-CA-C	5.04	117.35	110.55
1	C	205	GLU	N-CA-C	5.04	116.77	111.28
1	A	491	GLU	N-CA-C	-5.01	103.33	109.65
1	C	81	GLY	N-CA-C	5.01	122.23	115.32

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	269	ASP	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4002	0	4019	309	0
1	B	4002	0	4019	283	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	4002	0	4019	355	0
1	D	4002	0	4019	294	0
1	E	4002	0	4019	279	0
1	F	4002	0	4019	263	0
2	A	216	0	0	5	0
2	B	214	0	0	4	0
2	C	205	0	0	8	0
2	D	235	0	0	9	0
2	E	230	0	0	9	0
2	F	223	0	0	8	0
All	All	25335	0	24114	1676	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 35.

All (1676) 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:E:273:ARG:HB3	1:E:497:ARG:HG3	1.21	1.18
1:A:275:ALA:HA	1:A:493:LYS:HD2	1.25	1.16
1:B:466:ARG:NH2	1:B:468:ALA:H	1.46	1.12
1:F:273:ARG:HD3	1:F:493:LYS:HD2	1.32	1.11
1:B:466:ARG:HG2	1:B:467:ILE:H	1.13	1.09
1:A:273:ARG:HG3	1:A:497:ARG:HG3	1.13	1.07
1:E:74:LYS:HE3	1:E:75:GLN:H	1.19	1.06
1:E:198:TYR:HD2	1:E:222:GLY:HA2	1.17	1.06
1:B:273:ARG:HG3	1:B:497:ARG:HH22	1.15	1.06
1:B:463:LEU:HD12	1:B:466:ARG:HE	1.16	1.05
1:A:284:ASN:HD21	1:B:7:PRO:HB2	1.16	1.05
1:E:198:TYR:CD2	1:E:222:GLY:HA2	1.92	1.04
1:F:273:ARG:HB3	1:F:497:ARG:HH12	1.19	1.04
1:B:180:VAL:HG23	1:B:199:MET:HE2	1.40	1.03
1:A:273:ARG:NE	1:A:497:ARG:HD3	1.73	1.03
1:F:490:ILE:HD12	1:F:498:VAL:HG21	1.40	1.03
1:E:171:MET:HG2	1:E:191:MET:HE3	1.37	1.03
1:F:205:GLU:HA	1:F:208:LYS:HE2	1.39	1.01
1:A:205:GLU:HG2	1:A:206:ILE:HD12	1.39	1.01
1:B:458:ASN:HD22	1:B:462:VAL:HG21	1.24	1.01
1:F:6:LYS:HD2	1:F:8:PRO:HD2	1.43	1.01
1:C:453:ILE:HA	1:C:462:VAL:HG11	1.42	1.00
1:F:455:GLN:HA	1:F:455:GLN:HE21	1.27	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:315:ASN:H	1:D:315:ASN:HD22	1.01	0.97
1:D:50:LEU:HA	1:D:244:ILE:HD11	1.45	0.97
1:D:198:TYR:CD2	1:D:222:GLY:HA2	1.99	0.97
1:F:315:ASN:HD21	1:F:343:ASP:HB2	1.28	0.97
1:D:142:GLN:H	1:D:142:GLN:HE21	1.13	0.96
1:C:344:ILE:HD12	1:C:379:GLN:HE22	1.28	0.96
1:A:284:ASN:ND2	1:B:7:PRO:HB2	1.79	0.96
1:D:521:ILE:HD12	1:D:521:ILE:H	1.31	0.95
1:D:265:ILE:HG22	1:D:266:ASP:N	1.81	0.95
1:D:171:MET:HG2	1:D:191:MET:HE2	1.45	0.94
1:B:171:MET:HG2	1:B:191:MET:HE3	1.49	0.94
1:D:208:LYS:HE3	1:D:208:LYS:HA	1.48	0.94
1:B:451:LYS:HA	1:B:451:LYS:HZ3	1.29	0.94
1:B:451:LYS:HA	1:B:451:LYS:NZ	1.82	0.94
1:E:494:ASP:HB3	1:E:497:ARG:HH11	1.30	0.94
1:A:207:THR:HG22	1:D:375:PRO:HB2	1.50	0.93
1:C:192:ILE:HG21	1:C:195:ASP:HB2	1.47	0.93
1:F:434:ALA:HB3	1:F:477:PRO:HG3	1.51	0.93
1:D:493:LYS:H	1:D:493:LYS:CD	1.83	0.92
1:D:273:ARG:HG3	1:D:497:ARG:CZ	1.99	0.92
1:C:375:PRO:HB2	1:F:207:THR:HG22	1.50	0.92
1:E:6:LYS:HD2	1:E:7:PRO:HD3	1.49	0.92
1:F:445:VAL:HG21	1:F:467:ILE:HA	1.50	0.92
1:A:273:ARG:CZ	1:A:497:ARG:HD3	1.99	0.92
1:D:142:GLN:H	1:D:142:GLN:NE2	1.67	0.92
1:C:315:ASN:HD21	1:C:343:ASP:HB2	1.31	0.92
1:C:273:ARG:HH21	1:C:274:ASP:H	1.01	0.92
1:B:375:PRO:HB2	1:E:207:THR:HG22	1.51	0.91
1:F:257:ASN:HD22	1:F:259:MET:H	1.17	0.91
1:E:391:MET:HE1	1:E:418:MET:HE1	1.51	0.91
1:A:211:LEU:HD23	1:D:375:PRO:HG2	1.52	0.91
1:B:210:VAL:HG12	1:B:211:LEU:HD13	1.50	0.91
1:A:273:ARG:HG3	1:A:497:ARG:CG	1.99	0.91
1:A:95:PHE:CZ	1:C:505:MET:HE3	2.06	0.90
1:C:215:VAL:HG21	1:C:220:LEU:HD21	1.50	0.90
1:C:32:ILE:O	1:C:35:GLN:HB3	1.69	0.90
1:E:194:GLY:N	1:E:198:TYR:OH	2.05	0.90
1:D:276:THR:HG22	1:D:277:GLY:H	1.35	0.90
1:D:315:ASN:H	1:D:315:ASN:ND2	1.68	0.90
1:B:466:ARG:HG2	1:B:467:ILE:N	1.87	0.89
1:A:451:LYS:H	1:A:451:LYS:HD2	1.35	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:451:LYS:HE3	1:C:452:GLU:HG3	1.54	0.88
1:A:494:ASP:HB3	1:A:497:ARG:HH12	1.39	0.88
1:C:257:ASN:HD22	1:C:259:MET:H	1.19	0.87
1:A:273:ARG:HB3	1:A:496:ARG:HB3	1.53	0.87
1:F:331:VAL:HG21	1:F:354:ILE:HD11	1.57	0.87
1:B:463:LEU:HB3	1:B:466:ARG:CZ	2.04	0.87
1:C:265:ILE:HG22	1:C:322:ARG:NH2	1.89	0.87
1:E:273:ARG:HG3	1:E:494:ASP:HA	1.57	0.87
1:B:466:ARG:HH22	1:B:468:ALA:H	1.15	0.87
1:D:126:VAL:HG11	1:E:505:MET:HE2	1.57	0.86
1:E:273:ARG:HH21	1:E:497:ARG:HD2	1.41	0.86
1:B:273:ARG:HG3	1:B:497:ARG:NH2	1.90	0.86
1:C:30:GLU:HG2	1:C:31:ARG:HH11	1.40	0.86
1:D:265:ILE:HG22	1:D:266:ASP:H	1.37	0.86
1:A:50:LEU:HA	1:A:244:ILE:HD13	1.58	0.85
1:A:51:PHE:O	1:A:53:ASP:N	2.09	0.85
1:C:273:ARG:NH1	1:C:494:ASP:OD2	2.08	0.85
1:C:441:PRO:HG3	1:C:471:ARG:NH2	1.91	0.85
1:F:273:ARG:HD2	1:F:275:ALA:H	1.42	0.85
1:C:490:ILE:HD11	1:C:494:ASP:OD1	1.77	0.85
1:C:458:ASN:HB3	1:C:461:ASP:HB3	1.58	0.84
1:B:385:ILE:HG23	1:E:180:VAL:HG13	1.57	0.84
1:B:466:ARG:CG	1:B:467:ILE:H	1.89	0.84
1:E:494:ASP:HB3	1:E:497:ARG:NH1	1.92	0.84
1:A:275:ALA:HA	1:A:493:LYS:CD	2.08	0.84
1:A:451:LYS:C	1:A:453:ILE:H	1.84	0.84
1:E:191:MET:CE	1:E:198:TYR:HB3	2.08	0.84
1:D:73:ASP:OD1	1:D:74:LYS:HG3	1.78	0.83
1:E:17:ARG:O	1:E:21:GLU:HG2	1.78	0.83
1:C:128:ALA:O	1:C:165:ILE:HD13	1.77	0.83
1:F:269:ASP:H	1:F:270:PRO:HD2	1.42	0.83
1:F:435:GLU:HG3	1:F:475:ALA:HB1	1.61	0.83
1:C:342:ILE:HD11	1:C:347:ALA:HB2	1.61	0.83
1:E:197:TYR:HD1	1:E:197:TYR:H	1.24	0.82
1:C:264:TYR:HD2	1:C:326:ASN:ND2	1.77	0.82
1:C:31:ARG:CZ	1:C:31:ARG:HA	2.09	0.82
1:A:180:VAL:HG13	1:D:385:ILE:HG23	1.60	0.82
1:C:195:ASP:HB3	1:C:240:GLU:HG3	1.60	0.82
1:B:445:VAL:HG21	1:B:467:ILE:HG23	1.62	0.82
1:C:74:LYS:HD3	1:C:75:GLN:N	1.94	0.82
1:C:29:ASP:HA	1:C:32:ILE:HD11	1.60	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:259:MET:HA	1:E:259:MET:HE2	1.62	0.82
1:A:273:ARG:HG2	1:A:494:ASP:HA	1.62	0.81
1:A:316:ILE:HD12	1:A:346:ALA:HB1	1.63	0.81
1:D:273:ARG:HG3	1:D:497:ARG:NH2	1.95	0.81
1:A:141:ILE:H	1:A:141:ILE:HD12	1.46	0.81
1:A:265:ILE:HG23	1:A:266:ASP:N	1.93	0.81
1:E:74:LYS:CE	1:E:75:GLN:H	1.93	0.81
1:E:292:MET:HE3	1:E:295:ILE:HB	1.61	0.81
1:E:449:TYR:H	1:E:450:ARG:HH11	1.28	0.81
1:E:449:TYR:N	1:E:450:ARG:HH11	1.79	0.81
1:D:466:ARG:HH11	1:D:469:GLU:CG	1.95	0.80
1:D:241:GLN:H	1:D:241:GLN:NE2	1.79	0.80
1:F:315:ASN:ND2	1:F:343:ASP:HB2	1.96	0.80
1:A:490:ILE:HD12	1:A:491:GLU:H	1.46	0.80
1:A:497:ARG:NH1	1:A:497:ARG:HB2	1.96	0.80
1:B:454:GLN:HE21	1:B:455:GLN:HG3	1.46	0.80
1:A:95:PHE:HZ	1:C:505:MET:HE3	1.43	0.79
1:B:463:LEU:O	1:B:466:ARG:NH2	2.15	0.79
1:F:490:ILE:CD1	1:F:498:VAL:HG21	2.13	0.79
1:D:393:TYR:CZ	1:D:521:ILE:HG13	2.18	0.79
1:C:445:VAL:HG21	1:C:467:ILE:HA	1.65	0.79
1:C:29:ASP:O	1:C:33:GLN:HB2	1.81	0.78
1:E:74:LYS:HZ1	1:E:75:GLN:HB3	1.48	0.78
1:D:436:ILE:O	1:D:436:ILE:HG13	1.83	0.78
1:E:171:MET:CG	1:E:191:MET:HE3	2.14	0.78
1:E:378:ASP:O	1:E:382:LYS:HG2	1.84	0.78
1:B:463:LEU:CD1	1:B:466:ARG:HE	1.94	0.78
1:B:458:ASN:ND2	1:B:462:VAL:HG21	1.98	0.78
1:B:210:VAL:CG1	1:B:211:LEU:HD13	2.14	0.78
1:A:146:LEU:HD22	1:D:485:LEU:HD11	1.64	0.78
1:B:262:PRO:HB2	1:B:327:VAL:HG11	1.66	0.78
1:C:273:ARG:HH12	1:C:493:LYS:HG3	1.49	0.78
1:B:352:ARG:HD3	1:E:520:ASN:HD21	1.47	0.77
1:C:28:GLY:O	1:C:32:ILE:HD13	1.83	0.77
1:C:382:LYS:HE3	1:F:382:LYS:NZ	1.99	0.77
1:E:74:LYS:HE3	1:E:75:GLN:N	1.96	0.77
1:E:450:ARG:O	1:E:453:ILE:HG12	1.84	0.77
1:C:269:ASP:C	1:C:271:ALA:H	1.92	0.77
1:F:74:LYS:HD3	1:F:74:LYS:C	2.10	0.77
1:C:192:ILE:HB	1:C:196:ALA:HB3	1.66	0.77
1:B:450:ARG:HH12	1:B:453:ILE:HD13	1.50	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:198:TYR:HB2	1:E:221:GLY:O	1.84	0.77
1:B:174:PRO:HB3	1:B:197:TYR:CD1	2.19	0.77
1:F:171:MET:HG2	1:F:191:MET:HE2	1.67	0.77
1:E:51:PHE:O	1:E:53:ASP:N	2.17	0.77
1:C:54:GLY:O	1:C:55:LYS:HG2	1.84	0.76
1:F:455:GLN:HA	1:F:455:GLN:NE2	2.00	0.76
1:D:171:MET:CG	1:D:191:MET:HE2	2.16	0.76
1:D:198:TYR:HE2	1:D:218:GLN:NE2	1.83	0.76
1:C:273:ARG:NH2	1:C:274:ASP:H	1.81	0.76
1:B:463:LEU:HD12	1:B:466:ARG:NE	1.98	0.76
1:E:196:ALA:O	1:E:197:TYR:O	2.03	0.76
1:B:466:ARG:H	1:B:466:ARG:HD3	1.50	0.76
1:C:192:ILE:HB	1:C:196:ALA:CB	2.16	0.76
1:D:466:ARG:HH11	1:D:469:GLU:HG3	1.50	0.76
1:B:241:GLN:H	1:B:241:GLN:HE21	1.34	0.76
1:A:351:ALA:HA	1:A:354:ILE:CD1	2.15	0.75
1:C:434:ALA:HB3	1:C:477:PRO:HG3	1.68	0.75
1:D:241:GLN:H	1:D:241:GLN:HE21	1.29	0.75
1:C:74:LYS:HD3	1:C:74:LYS:C	2.11	0.75
1:C:410:SER:OG	1:C:415:HIS:HD2	1.69	0.75
1:C:211:LEU:HG	1:C:212:GLY:H	1.51	0.75
1:A:267:THR:HG22	1:A:268:GLY:H	1.52	0.75
1:E:69:GLU:O	1:E:72:LEU:HD23	1.87	0.75
1:B:463:LEU:HB3	1:B:466:ARG:NH1	1.99	0.75
1:A:171:MET:HG2	1:A:199:MET:HE2	1.67	0.75
1:C:315:ASN:ND2	1:C:343:ASP:HB2	2.02	0.75
1:D:315:ASN:HD22	1:D:315:ASN:N	1.82	0.74
1:A:462:VAL:HA	1:A:465:GLN:CD	2.12	0.74
1:C:29:ASP:HA	1:C:32:ILE:CD1	2.16	0.74
1:F:463:LEU:O	1:F:467:ILE:HB	1.86	0.74
1:B:269:ASP:N	1:B:270:PRO:HD2	2.02	0.74
1:D:191:MET:HE1	1:D:199:MET:SD	2.27	0.74
1:D:495:THR:O	1:D:499:ILE:HG12	1.88	0.74
1:B:463:LEU:O	1:B:465:GLN:N	2.20	0.74
1:C:197:TYR:CZ	1:C:218:GLN:HB2	2.22	0.74
1:E:191:MET:HE1	1:E:199:MET:HG2	1.69	0.74
1:A:485:LEU:HD11	1:D:146:LEU:HD22	1.69	0.74
1:E:391:MET:HE1	1:E:418:MET:CE	2.18	0.73
1:A:445:VAL:HG21	1:A:467:ILE:HG22	1.69	0.73
1:C:441:PRO:HG3	1:C:471:ARG:HH21	1.50	0.73
1:B:40:LYS:CE	1:B:197:TYR:HE2	2.01	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:264:TYR:CD2	1:C:326:ASN:ND2	2.56	0.73
1:E:315:ASN:HD21	1:E:343:ASP:HB2	1.52	0.73
1:F:269:ASP:HB2	1:F:496:ARG:NH2	2.03	0.73
1:C:273:ARG:HH21	1:C:274:ASP:N	1.83	0.73
1:B:374:VAL:HG13	1:B:379:GLN:HG3	1.70	0.73
1:B:466:ARG:NH1	1:B:467:ILE:HG13	2.03	0.73
1:C:492:PRO:O	1:C:495:THR:HG23	1.88	0.73
1:E:259:MET:HA	1:E:259:MET:CE	2.17	0.73
1:A:237:VAL:HG21	1:A:242:GLU:HB3	1.71	0.73
1:D:464:LYS:HA	1:D:467:ILE:CG1	2.19	0.73
1:B:466:ARG:HH22	1:B:468:ALA:N	1.86	0.72
1:E:50:LEU:HA	1:E:244:ILE:HD13	1.71	0.72
1:A:342:ILE:HD12	1:A:343:ASP:H	1.51	0.72
1:A:265:ILE:HG12	1:A:266:ASP:H	1.54	0.72
1:D:174:PRO:HB3	1:D:197:TYR:CD2	2.24	0.72
1:D:198:TYR:CE2	1:D:222:GLY:HA2	2.24	0.72
1:D:393:TYR:CE2	1:D:521:ILE:HG13	2.24	0.72
1:F:127:GLY:HA2	1:F:165:ILE:HD11	1.70	0.72
1:A:69:GLU:O	1:A:72:LEU:HD23	1.88	0.72
1:A:458:ASN:N	1:A:458:ASN:HD22	1.87	0.72
1:C:28:GLY:C	1:C:30:GLU:H	1.96	0.72
1:F:209:VAL:HG12	1:F:210:VAL:HG23	1.72	0.72
1:A:351:ALA:HA	1:A:354:ILE:HD11	1.71	0.72
1:A:450:ARG:HA	1:A:450:ARG:CZ	2.20	0.71
1:B:28:GLY:O	1:B:32:ILE:HG23	1.89	0.71
1:D:95:PHE:CZ	1:E:505:MET:HE3	2.24	0.71
1:B:171:MET:CG	1:B:191:MET:HE3	2.20	0.71
1:B:450:ARG:CZ	1:B:453:ILE:HG21	2.20	0.71
1:B:257:ASN:ND2	1:B:260:GLU:HG3	2.06	0.71
1:D:222:GLY:O	1:D:225:VAL:HG22	1.91	0.71
1:E:342:ILE:HD12	1:E:343:ASP:H	1.55	0.71
1:A:451:LYS:N	1:A:451:LYS:HZ3	1.88	0.71
1:B:262:PRO:HB2	1:B:327:VAL:CG1	2.20	0.71
1:C:192:ILE:HD13	1:C:196:ALA:HB2	1.72	0.71
1:C:274:ASP:OD2	1:C:276:THR:HG22	1.90	0.71
1:B:466:ARG:NH2	1:B:468:ALA:N	2.31	0.71
1:E:455:GLN:O	1:E:455:GLN:HG2	1.89	0.71
1:A:145:ALA:HB1	1:D:436:ILE:HD11	1.71	0.71
1:A:496:ARG:O	1:A:499:ILE:HG22	1.90	0.71
1:A:399:THR:HG23	1:A:513:ARG:HE	1.54	0.71
1:D:493:LYS:H	1:D:493:LYS:HD2	1.56	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:472:LYS:O	1:D:472:LYS:HD3	1.91	0.71
1:A:293:ARG:O	1:A:296:ILE:HG12	1.91	0.70
1:D:521:ILE:H	1:D:521:ILE:CD1	2.03	0.70
1:E:6:LYS:HA	1:E:11:LYS:HG2	1.73	0.70
1:B:241:GLN:O	1:B:244:ILE:HD13	1.92	0.70
1:B:257:ASN:HD22	1:B:259:MET:H	1.40	0.70
1:B:466:ARG:CZ	1:B:468:ALA:H	2.04	0.70
1:C:490:ILE:HD12	1:C:491:GLU:H	1.56	0.70
1:C:127:GLY:HA2	1:C:165:ILE:HD11	1.73	0.70
1:D:142:GLN:HE21	1:D:142:GLN:N	1.89	0.70
1:A:7:PRO:HG2	1:A:8:PRO:CD	2.22	0.70
1:B:25:LYS:HE3	1:B:29:ASP:OD2	1.91	0.70
1:A:494:ASP:HB3	1:A:497:ARG:NH1	2.06	0.70
1:C:343:ASP:H	1:C:346:ALA:HB3	1.56	0.70
1:C:399:THR:HG21	1:C:513:ARG:HD3	1.73	0.70
1:A:206:ILE:HD12	1:A:206:ILE:H	1.56	0.70
1:D:286:ALA:HA	1:D:408:ARG:NH2	2.07	0.70
1:E:273:ARG:HH21	1:E:497:ARG:CD	2.05	0.70
1:D:192:ILE:O	1:D:198:TYR:HE1	1.75	0.69
1:E:315:ASN:ND2	1:E:343:ASP:HB2	2.06	0.69
1:E:450:ARG:C	1:E:452:GLU:H	2.00	0.69
1:E:490:ILE:HD12	1:E:491:GLU:H	1.55	0.69
1:A:469:GLU:HA	1:A:472:LYS:HE3	1.72	0.69
1:D:169:THR:HG21	1:D:183:PRO:HA	1.73	0.69
1:D:505:MET:O	1:F:126:VAL:HG21	1.93	0.69
1:F:490:ILE:HG12	1:F:491:GLU:N	2.07	0.69
1:A:292:MET:HE3	1:A:295:ILE:HB	1.75	0.69
1:C:375:PRO:HB3	1:F:206:ILE:HD11	1.73	0.69
1:D:210:VAL:HG12	1:D:211:LEU:HD22	1.74	0.69
1:D:50:LEU:HA	1:D:244:ILE:CD1	2.20	0.69
1:E:450:ARG:NH2	1:E:450:ARG:HB2	2.07	0.69
1:F:58:GLU:HG2	1:F:61:THR:HG22	1.74	0.69
1:B:385:ILE:HD12	1:E:180:VAL:HG11	1.75	0.69
1:B:450:ARG:NH1	1:B:453:ILE:HG21	2.07	0.69
1:C:207:THR:O	1:C:211:LEU:HD22	1.93	0.69
1:C:265:ILE:HG22	1:C:322:ARG:CZ	2.22	0.69
1:F:106:GLY:O	1:F:136:SER:HB2	1.92	0.69
1:A:141:ILE:HD12	1:A:141:ILE:N	2.06	0.69
1:A:169:THR:HG21	1:A:183:PRO:HA	1.73	0.69
1:B:385:ILE:HG23	1:E:180:VAL:CG1	2.23	0.69
1:D:368:VAL:O	1:D:407:VAL:HG12	1.91	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:191:MET:HE1	1:E:198:TYR:HB3	1.73	0.69
1:A:273:ARG:CG	1:A:497:ARG:HG3	2.08	0.69
1:D:273:ARG:H	1:D:497:ARG:CG	2.06	0.68
1:E:199:MET:O	1:E:226:HIS:HE1	1.76	0.68
1:F:203:GLY:HA3	1:F:205:GLU:OE2	1.93	0.68
1:D:195:ASP:C	1:D:197:TYR:H	2.00	0.68
1:D:269:ASP:N	1:D:270:PRO:HD2	2.08	0.68
1:D:483:LYS:HD2	1:F:66:ARG:HH21	1.56	0.68
1:E:74:LYS:NZ	1:E:75:GLN:HB3	2.07	0.68
1:A:469:GLU:HA	1:A:472:LYS:CE	2.22	0.68
1:B:495:THR:O	1:B:499:ILE:HG12	1.92	0.68
1:E:222:GLY:O	1:E:225:VAL:HG22	1.92	0.68
1:A:222:GLY:O	1:A:225:VAL:HG22	1.94	0.68
1:A:273:ARG:HE	1:A:497:ARG:HD3	1.56	0.68
1:B:180:VAL:CG2	1:B:199:MET:HE2	2.20	0.68
1:E:410:SER:OG	1:E:415:HIS:HD2	1.76	0.68
1:F:191:MET:HE1	1:F:199:MET:SD	2.33	0.68
1:F:205:GLU:CD	1:F:205:GLU:H	2.02	0.68
1:B:450:ARG:NH1	1:B:453:ILE:HD13	2.09	0.68
1:C:104:LEU:O	1:C:107:SER:HB2	1.94	0.68
1:F:285:ASP:CG	1:F:288:LYS:HD3	2.18	0.68
1:A:354:ILE:CG1	1:A:394:ALA:HB1	2.24	0.68
1:C:452:GLU:C	1:C:454:GLN:H	2.01	0.68
1:F:490:ILE:HD11	1:F:494:ASP:CB	2.23	0.68
1:C:6:LYS:HA	1:C:6:LYS:HE3	1.76	0.68
1:A:497:ARG:HB2	1:A:497:ARG:CZ	2.24	0.67
1:E:198:TYR:HE2	1:E:218:GLN:OE1	1.76	0.67
1:A:193:LYS:HD3	1:A:236:MET:SD	2.34	0.67
1:D:449:TYR:O	1:D:450:ARG:HG3	1.93	0.67
1:E:447:ILE:C	1:E:447:ILE:HD12	2.19	0.67
1:F:441:PRO:HG3	1:F:471:ARG:NH2	2.10	0.67
1:B:508:THR:O	1:B:510:ARG:HD3	1.95	0.67
1:C:31:ARG:N	1:C:31:ARG:NE	2.43	0.67
1:C:344:ILE:HD12	1:C:379:GLN:NE2	2.06	0.67
1:D:240:GLU:O	1:D:244:ILE:HG22	1.95	0.67
1:B:447:ILE:HD11	1:E:141:ILE:HD12	1.77	0.67
1:E:191:MET:HE2	1:E:198:TYR:HB3	1.75	0.67
1:B:9:VAL:O	1:B:13:ILE:HG23	1.95	0.67
1:E:478:TYR:O	1:E:482:GLU:HG3	1.93	0.67
1:F:128:ALA:O	1:F:165:ILE:HG21	1.95	0.67
1:A:243:ALA:O	1:A:247:THR:HG23	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:476:ASN:HD22	1:C:476:ASN:C	2.03	0.67
1:F:10:GLU:CD	1:F:10:GLU:H	2.03	0.67
1:F:29:ASP:HA	1:F:32:ILE:HG12	1.75	0.67
1:C:7:PRO:HG2	1:C:8:PRO:HD3	1.76	0.67
1:B:194:GLY:C	1:B:196:ALA:H	2.01	0.67
1:B:468:ALA:O	1:B:472:LYS:HG2	1.95	0.67
1:D:445:VAL:HG21	1:D:467:ILE:HD12	1.76	0.67
1:A:273:ARG:C	1:A:273:ARG:HD2	2.20	0.67
1:A:518:HIS:HE1	1:D:358:ASP:OD1	1.78	0.67
1:B:180:VAL:HG23	1:B:199:MET:CE	2.22	0.67
1:A:145:ALA:CB	1:D:436:ILE:HD11	2.25	0.66
1:A:410:SER:OG	1:A:415:HIS:HD2	1.78	0.66
1:D:452:GLU:H	1:D:452:GLU:CD	2.01	0.66
1:C:199:MET:O	1:C:226:HIS:HE1	1.79	0.66
1:C:215:VAL:CG2	1:C:220:LEU:HD21	2.22	0.66
1:C:344:ILE:HG23	1:C:379:GLN:OE1	1.94	0.66
1:E:316:ILE:HD12	1:E:346:ALA:HB1	1.77	0.66
1:D:208:LYS:HD2	1:D:214:GLU:HG2	1.77	0.66
1:D:451:LYS:HE2	1:D:451:LYS:N	2.09	0.66
1:E:448:LEU:C	1:E:450:ARG:HE	2.01	0.66
1:E:273:ARG:CB	1:E:497:ARG:HG3	2.11	0.66
1:B:269:ASP:N	1:B:270:PRO:CD	2.57	0.66
1:C:215:VAL:HB	1:C:220:LEU:HD11	1.78	0.66
1:C:265:ILE:O	1:C:265:ILE:HG23	1.96	0.66
1:E:276:THR:HG22	1:E:279:GLU:OE2	1.96	0.66
1:F:316:ILE:HG22	2:F:527:HOH:O	1.94	0.66
1:C:28:GLY:C	1:C:30:GLU:N	2.51	0.66
1:B:466:ARG:HH12	1:B:468:ALA:HB2	1.61	0.66
1:E:195:ASP:O	1:E:197:TYR:N	2.29	0.66
1:F:273:ARG:HE	1:F:275:ALA:HB2	1.61	0.66
1:C:273:ARG:NH2	1:C:274:ASP:O	2.29	0.65
1:F:74:LYS:HD3	1:F:75:GLN:N	2.11	0.65
1:A:490:ILE:CD1	1:A:491:GLU:H	2.09	0.65
1:C:31:ARG:O	1:C:34:PHE:HB3	1.97	0.65
1:C:192:ILE:HG21	1:C:195:ASP:CB	2.22	0.65
1:C:211:LEU:CG	1:C:212:GLY:H	2.08	0.65
1:D:206:ILE:HD13	1:D:206:ILE:O	1.96	0.65
1:C:6:LYS:NZ	1:C:11:LYS:HG2	2.12	0.65
1:D:191:MET:SD	1:D:198:TYR:HB3	2.37	0.65
1:D:450:ARG:HB3	1:D:451:LYS:HZ3	1.59	0.65
1:E:182:SER:HB3	1:E:183:PRO:HD3	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:269:ASP:C	1:A:270:PRO:O	2.40	0.65
1:A:378:ASP:OD1	1:A:382:LYS:HE2	1.97	0.65
1:A:497:ARG:HA	1:A:500:VAL:HG12	1.79	0.65
1:E:206:ILE:HD12	1:E:206:ILE:H	1.61	0.65
1:F:269:ASP:OD1	1:F:324:ALA:HA	1.96	0.65
1:A:169:THR:HG23	1:A:186:THR:OG1	1.96	0.65
1:A:451:LYS:C	1:A:453:ILE:N	2.50	0.65
1:B:385:ILE:HD12	1:E:180:VAL:CG1	2.26	0.65
1:D:197:TYR:N	1:D:197:TYR:CD1	2.65	0.65
1:E:316:ILE:HG23	1:E:346:ALA:HB1	1.79	0.65
1:F:490:ILE:HD11	1:F:494:ASP:HB2	1.79	0.65
1:A:240:GLU:O	1:A:244:ILE:HG23	1.97	0.65
1:C:42:THR:OG1	1:C:45:GLU:HG3	1.97	0.65
1:D:273:ARG:H	1:D:497:ARG:HG3	1.61	0.65
1:A:141:ILE:H	1:A:141:ILE:CD1	2.10	0.65
1:A:170:ILE:HD11	1:A:247:THR:HG21	1.78	0.65
1:A:462:VAL:HA	1:A:465:GLN:CG	2.27	0.65
1:C:160:MET:HE3	1:C:160:MET:HA	1.79	0.65
1:C:431:TRP:HE1	1:C:495:THR:CG2	2.10	0.65
1:F:6:LYS:HZ3	1:F:8:PRO:C	2.05	0.65
1:C:145:ALA:HB2	1:F:436:ILE:HD11	1.79	0.65
1:C:129:PRO:HA	1:C:165:ILE:HG23	1.78	0.64
1:C:369:ASP:OD1	1:C:408:ARG:HB3	1.98	0.64
1:C:264:TYR:HD2	1:C:326:ASN:HD22	1.44	0.64
1:D:493:LYS:H	1:D:493:LYS:HD3	1.58	0.64
1:C:30:GLU:HB3	1:C:31:ARG:HE	1.62	0.64
1:D:464:LYS:HA	1:D:467:ILE:HG12	1.78	0.64
1:E:203:GLY:O	1:E:207:THR:HG23	1.97	0.64
1:A:7:PRO:HG2	1:A:8:PRO:HD3	1.80	0.64
1:A:355:ARG:HH12	1:D:521:ILE:HD13	1.62	0.64
1:E:89:VAL:HG21	1:E:251:LEU:HD13	1.80	0.64
1:A:151:TYR:O	1:A:154:VAL:HG13	1.98	0.64
1:B:40:LYS:NZ	1:B:197:TYR:HE2	1.95	0.64
1:C:315:ASN:HD21	1:C:343:ASP:CB	2.10	0.64
1:C:481:ALA:HA	1:C:486:VAL:HG22	1.79	0.64
1:F:27:GLY:O	1:F:31:ARG:HD3	1.98	0.64
1:D:95:PHE:HZ	1:E:505:MET:HE3	1.61	0.64
1:B:160:MET:HE2	1:E:514:TYR:HE2	1.63	0.64
1:B:194:GLY:C	1:B:196:ALA:N	2.52	0.64
1:C:271:ALA:HB1	1:C:500:VAL:HG21	1.80	0.64
1:D:182:SER:HB3	1:D:183:PRO:HD3	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:199:MET:O	1:D:226:HIS:HE1	1.80	0.64
1:D:464:LYS:C	1:D:467:ILE:HG12	2.22	0.64
1:E:464:LYS:O	1:E:467:ILE:HG12	1.96	0.64
1:A:354:ILE:HD11	1:A:394:ALA:CB	2.27	0.64
1:D:508:THR:O	1:D:510:ARG:HD3	1.98	0.64
1:E:120:TYR:CE2	1:E:130:VAL:HG11	2.33	0.64
1:A:284:ASN:HD21	1:B:7:PRO:CB	2.02	0.64
1:B:205:GLU:H	1:B:205:GLU:CD	2.06	0.64
1:C:241:GLN:O	1:C:244:ILE:HG13	1.97	0.64
1:E:225:VAL:HA	1:E:229:LYS:HD3	1.80	0.64
1:F:343:ASP:H	1:F:346:ALA:HB3	1.62	0.64
1:C:197:TYR:CE2	1:C:218:GLN:HB2	2.32	0.64
1:C:461:ASP:CG	1:C:462:VAL:N	2.56	0.64
1:A:6:LYS:HZ1	1:A:8:PRO:HG2	1.63	0.63
1:B:447:ILE:HD11	1:E:141:ILE:CD1	2.28	0.63
1:C:38:LYS:HD2	1:C:40:LYS:H	1.62	0.63
1:C:172:ALA:HA	1:C:196:ALA:HB1	1.80	0.63
1:D:7:PRO:HB2	1:E:284:ASN:HB3	1.78	0.63
1:E:228:THR:OG1	1:E:229:LYS:HD2	1.98	0.63
1:D:158:ASN:HA	1:D:167:GLN:HE22	1.63	0.63
1:E:6:LYS:HD2	1:E:7:PRO:CD	2.27	0.63
1:C:451:LYS:HE2	1:C:452:GLU:H	1.63	0.63
1:C:25:LYS:HD2	1:C:32:ILE:HD11	1.78	0.63
1:D:6:LYS:NZ	1:D:6:LYS:HB3	2.13	0.63
1:E:273:ARG:HD3	1:E:497:ARG:CD	2.29	0.63
1:B:450:ARG:HH12	1:B:453:ILE:CD1	2.11	0.63
1:C:32:ILE:O	1:C:35:GLN:CB	2.44	0.63
1:A:449:TYR:H	1:A:450:ARG:HH11	1.46	0.63
1:F:257:ASN:ND2	1:F:259:MET:H	1.95	0.63
1:A:354:ILE:HD11	1:A:394:ALA:HB3	1.79	0.63
1:C:510:ARG:HH11	1:C:510:ARG:HG2	1.61	0.63
1:D:198:TYR:CE1	1:D:223:ALA:HB2	2.34	0.63
1:E:315:ASN:HD21	1:E:343:ASP:CB	2.10	0.63
1:F:432:PRO:HD3	1:F:490:ILE:O	1.99	0.63
1:F:464:LYS:O	1:F:467:ILE:HG22	1.98	0.63
1:C:435:GLU:HG3	1:C:475:ALA:HB1	1.80	0.63
1:D:483:LYS:HB3	1:F:66:ARG:HH22	1.63	0.63
1:E:228:THR:HG22	1:E:311:HIS:HB3	1.80	0.63
1:F:450:ARG:C	1:F:452:GLU:H	2.07	0.62
1:A:450:ARG:O	1:A:453:ILE:HG22	1.99	0.62
1:C:442:GLU:HB2	1:C:467:ILE:HD11	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:479:TRP:CH2	1:D:146:LEU:HD23	2.34	0.62
1:D:204:PRO:HB3	1:D:215:VAL:HG13	1.81	0.62
1:D:266:ASP:O	1:D:267:THR:C	2.41	0.62
1:F:171:MET:HE3	1:F:172:ALA:N	2.15	0.62
1:F:269:ASP:N	1:F:270:PRO:HD2	2.12	0.62
1:B:191:MET:CE	1:B:199:MET:HG3	2.29	0.62
1:B:446:ARG:HB3	1:B:446:ARG:CZ	2.29	0.62
1:C:55:LYS:NZ	1:C:55:LYS:HB3	2.14	0.62
1:F:58:GLU:CG	1:F:61:THR:HG22	2.30	0.62
1:A:265:ILE:HG22	1:A:322:ARG:HD3	1.81	0.62
1:D:126:VAL:CG1	1:E:505:MET:HE2	2.28	0.62
1:B:110:GLU:OE1	1:B:146:LEU:HG	1.99	0.62
1:D:461:ASP:C	1:D:461:ASP:OD2	2.42	0.62
1:D:451:LYS:HE2	1:D:451:LYS:H	1.62	0.62
1:A:205:GLU:HG2	1:A:206:ILE:CD1	2.21	0.62
1:A:450:ARG:HA	1:A:450:ARG:NH2	2.14	0.62
1:B:204:PRO:HD2	1:B:205:GLU:OE1	1.99	0.62
1:B:40:LYS:HD2	1:B:197:TYR:CE2	2.35	0.62
1:A:203:GLY:O	1:A:207:THR:HG23	2.00	0.61
1:A:344:ILE:HG13	1:A:379:GLN:OE1	2.00	0.61
1:A:333:ASN:HD22	1:A:369:ASP:H	1.45	0.61
1:A:466:ARG:HD2	1:A:469:GLU:OE1	2.00	0.61
1:B:385:ILE:HG12	2:B:549:HOH:O	2.00	0.61
1:C:267:THR:HG22	1:C:267:THR:O	2.00	0.61
1:C:295:ILE:O	1:C:299:ILE:HG13	1.99	0.61
1:B:7:PRO:HG2	1:B:8:PRO:HD3	1.82	0.61
1:C:197:TYR:HB2	2:C:525:HOH:O	2.01	0.61
1:C:445:VAL:CG1	1:C:466:ARG:HB3	2.30	0.61
1:D:194:GLY:N	1:D:198:TYR:OH	2.25	0.61
1:F:171:MET:HE2	1:F:173:GLY:H	1.64	0.61
1:F:241:GLN:O	1:F:244:ILE:HG13	1.99	0.61
1:C:244:ILE:HD12	1:C:245:ASN:N	2.15	0.61
1:D:277:GLY:HA2	1:D:280:GLN:HG3	1.82	0.61
1:C:57:ASN:HB3	1:C:86:TRP:CH2	2.35	0.61
1:A:447:ILE:C	1:A:450:ARG:HE	2.09	0.61
1:D:460:ASP:O	1:D:463:LEU:HB3	2.01	0.61
1:A:158:ASN:HA	1:A:167:GLN:HE22	1.65	0.61
1:A:451:LYS:H	1:A:451:LYS:CD	2.11	0.61
1:A:466:ARG:O	1:A:469:GLU:HG2	2.00	0.61
1:E:6:LYS:N	1:E:7:PRO:CD	2.64	0.61
1:F:452:GLU:O	1:F:452:GLU:HG2	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:32:ILE:HG12	1:C:33:GLN:N	2.15	0.60
1:D:316:ILE:CD1	1:D:346:ALA:HB1	2.31	0.60
1:E:316:ILE:HG22	2:E:527:HOH:O	2.00	0.60
1:B:182:SER:HB3	1:B:183:PRO:HD3	1.82	0.60
1:D:296:ILE:HD13	1:D:297:TYR:N	2.16	0.60
1:D:410:SER:OG	1:D:415:HIS:HD2	1.85	0.60
1:E:283:PRO:C	1:E:285:ASP:H	2.09	0.60
1:B:463:LEU:HB3	1:B:466:ARG:NE	2.16	0.60
1:B:466:ARG:HD3	1:B:466:ARG:N	2.16	0.60
1:B:169:THR:HG22	1:B:186:THR:OG1	2.00	0.60
1:D:450:ARG:HA	1:D:454:GLN:HG3	1.83	0.60
1:C:495:THR:O	1:C:499:ILE:HG12	2.01	0.60
1:A:221:GLY:HA2	1:A:225:VAL:HG21	1.83	0.60
1:E:521:ILE:HG13	1:E:522:PRO:HD2	1.83	0.60
1:F:129:PRO:HA	1:F:165:ILE:CG2	2.31	0.60
1:B:6:LYS:HE2	1:B:6:LYS:HA	1.83	0.60
1:C:344:ILE:HD13	1:C:344:ILE:H	1.67	0.60
1:E:74:LYS:HE3	1:E:74:LYS:H	1.66	0.60
1:B:141:ILE:HG13	1:E:447:ILE:HG12	1.84	0.60
1:B:432:PRO:HG3	1:C:16:LEU:HD22	1.82	0.60
1:C:451:LYS:HD2	1:C:452:GLU:N	2.17	0.60
1:D:197:TYR:N	1:D:197:TYR:HD1	2.00	0.60
1:E:198:TYR:CE2	1:E:218:GLN:OE1	2.54	0.60
1:A:273:ARG:NH1	1:A:497:ARG:HD3	2.16	0.60
1:C:273:ARG:NH2	1:C:273:ARG:HG3	2.16	0.60
1:E:197:TYR:N	1:E:197:TYR:CD1	2.64	0.60
1:B:205:GLU:O	1:B:209:VAL:HG23	2.02	0.60
1:E:198:TYR:CD2	1:E:222:GLY:CA	2.76	0.60
1:A:54:GLY:C	1:A:55:LYS:HG2	2.27	0.59
1:B:6:LYS:HG3	1:B:11:LYS:HD3	1.82	0.59
1:B:237:VAL:HG22	1:B:242:GLU:OE2	2.01	0.59
1:C:273:ARG:HH21	1:C:273:ARG:HG3	1.66	0.59
1:A:6:LYS:NZ	1:A:8:PRO:HG2	2.17	0.59
1:A:318:VAL:HA	1:A:330:ILE:O	2.01	0.59
1:B:135:ASP:HA	1:B:173:GLY:HA3	1.84	0.59
1:D:195:ASP:O	1:D:197:TYR:N	2.26	0.59
1:D:226:HIS:HD2	1:D:230:SER:OG	1.85	0.59
1:A:273:ARG:C	1:A:273:ARG:HH21	2.09	0.59
1:C:497:ARG:HG2	1:C:497:ARG:HH11	1.67	0.59
1:D:198:TYR:CE2	1:D:218:GLN:NE2	2.62	0.59
1:D:340:GLY:HA3	2:D:700:HOH:O	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:237:VAL:HG21	1:A:242:GLU:CB	2.32	0.59
1:F:262:PRO:HB2	1:F:327:VAL:HG13	1.83	0.59
1:B:463:LEU:C	1:B:465:GLN:H	2.11	0.59
1:C:6:LYS:HZ3	1:C:11:LYS:HG2	1.66	0.59
1:E:342:ILE:HD12	1:E:343:ASP:N	2.17	0.59
1:C:444:ALA:O	1:C:448:LEU:HB2	2.02	0.59
1:D:455:GLN:HE21	1:D:455:GLN:HA	1.68	0.59
1:E:316:ILE:HD12	1:E:346:ALA:CB	2.33	0.59
1:B:432:PRO:HD3	1:B:490:ILE:O	2.01	0.59
1:B:463:LEU:O	1:B:466:ARG:HD3	2.02	0.59
1:C:31:ARG:HG3	1:C:31:ARG:HH21	1.66	0.59
1:C:197:TYR:CZ	1:C:218:GLN:CB	2.85	0.59
1:D:460:ASP:O	1:D:463:LEU:HD12	2.03	0.59
1:F:445:VAL:HG13	1:F:449:TYR:CD1	2.37	0.59
1:F:452:GLU:OE2	1:F:466:ARG:NH2	2.31	0.59
1:B:385:ILE:HD13	1:E:201:VAL:HG23	1.85	0.59
1:C:465:GLN:O	1:C:466:ARG:HD2	2.03	0.58
1:D:285:ASP:OD1	1:D:287:ALA:HB3	2.03	0.58
1:A:342:ILE:HD12	1:A:343:ASP:N	2.18	0.58
1:B:453:ILE:CG1	1:B:454:GLN:N	2.65	0.58
1:C:11:LYS:HE3	1:C:11:LYS:HA	1.85	0.58
1:C:107:SER:OG	1:C:140:ARG:HA	2.03	0.58
1:C:266:ASP:O	1:C:268:GLY:N	2.35	0.58
1:E:199:MET:O	1:E:226:HIS:CE1	2.56	0.58
1:E:206:ILE:HD12	1:E:206:ILE:N	2.18	0.58
1:C:208:LYS:HA	1:C:211:LEU:CD2	2.33	0.58
1:D:265:ILE:CG2	1:D:266:ASP:N	2.54	0.58
1:A:439:THR:HG22	1:A:440:GLY:H	1.69	0.58
1:B:291:ASN:HD21	1:B:293:ARG:HB2	1.68	0.58
1:C:157:MET:HE2	1:C:157:MET:HA	1.84	0.58
1:C:182:SER:HB3	1:C:183:PRO:HD3	1.85	0.58
1:C:215:VAL:HB	1:C:220:LEU:CG	2.34	0.58
1:C:450:ARG:CZ	1:C:450:ARG:HA	2.33	0.58
1:A:120:TYR:CE2	1:A:130:VAL:HG11	2.38	0.58
1:C:266:ASP:C	1:C:268:GLY:H	2.09	0.58
1:D:316:ILE:HG13	1:D:346:ALA:HB1	1.85	0.58
1:E:198:TYR:CD2	1:E:223:ALA:N	2.71	0.58
1:A:206:ILE:HD12	1:A:206:ILE:N	2.17	0.58
1:A:316:ILE:HD12	1:A:346:ALA:CB	2.32	0.58
1:C:34:PHE:CZ	1:C:38:LYS:HB2	2.39	0.58
1:C:215:VAL:CG1	1:C:220:LEU:HG	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:333:ASN:OD1	1:D:418:MET:HE2	2.04	0.58
1:D:444:ALA:O	1:D:448:LEU:HB2	2.04	0.58
1:E:193:LYS:HA	1:E:198:TYR:OH	2.03	0.58
1:A:479:TRP:CZ3	1:D:146:LEU:HD23	2.38	0.58
1:B:208:LYS:HD2	1:B:213:GLU:N	2.18	0.58
1:F:169:THR:HG22	1:F:186:THR:OG1	2.03	0.58
1:F:215:VAL:HG23	1:F:219:ASP:HB2	1.86	0.58
1:A:350:ALA:O	1:A:354:ILE:HD13	2.03	0.58
1:A:458:ASN:N	1:A:458:ASN:ND2	2.50	0.58
1:B:173:GLY:O	1:B:197:TYR:HB3	2.04	0.58
1:B:454:GLN:NE2	1:B:455:GLN:HG3	2.15	0.58
1:E:499:ILE:C	1:E:499:ILE:HD13	2.28	0.58
1:A:28:GLY:O	1:A:32:ILE:HG23	2.04	0.58
1:B:191:MET:HE1	1:B:199:MET:HG3	1.86	0.58
1:C:10:GLU:O	1:C:14:GLU:HG3	2.04	0.58
1:A:207:THR:O	1:A:211:LEU:HB2	2.04	0.57
1:E:273:ARG:HH21	1:E:497:ARG:CG	2.17	0.57
1:B:458:ASN:HB3	1:B:462:VAL:CG2	2.34	0.57
1:C:34:PHE:O	1:C:38:LYS:HG2	2.04	0.57
1:C:71:GLY:O	1:C:74:LYS:HB3	2.04	0.57
1:C:257:ASN:ND2	1:C:259:MET:HB2	2.19	0.57
1:A:148:LEU:HD11	1:D:438:VAL:HA	1.86	0.57
1:A:182:SER:HB3	1:A:183:PRO:HD3	1.86	0.57
1:A:497:ARG:CG	1:A:497:ARG:HH11	2.16	0.57
1:D:293:ARG:HA	1:D:296:ILE:HG23	1.87	0.57
1:F:471:ARG:O	1:F:475:ALA:HB3	2.04	0.57
1:A:313:ALA:C	1:A:315:ASN:H	2.11	0.57
1:A:315:ASN:ND2	1:A:343:ASP:HB2	2.18	0.57
1:D:195:ASP:O	1:D:197:TYR:HD1	1.88	0.57
1:E:273:ARG:NH2	1:E:497:ARG:HD2	2.17	0.57
1:E:316:ILE:CG2	1:E:346:ALA:HB1	2.34	0.57
1:A:399:THR:CG2	1:A:513:ARG:HE	2.18	0.57
1:C:344:ILE:HD13	1:C:345:ASP:H	1.69	0.57
1:C:458:ASN:O	1:C:461:ASP:OD1	2.22	0.57
1:E:490:ILE:CD1	1:E:491:GLU:H	2.17	0.57
1:F:191:MET:CE	1:F:199:MET:SD	2.93	0.57
1:B:138:GLY:HA2	1:B:179:ALA:HB2	1.87	0.57
1:B:466:ARG:NE	1:B:467:ILE:HG12	2.20	0.57
1:C:435:GLU:CG	1:C:475:ALA:HB1	2.34	0.57
1:E:71:GLY:C	1:E:74:LYS:HE2	2.28	0.57
1:F:8:PRO:HG2	1:F:11:LYS:HB3	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:204:PRO:HB3	1:B:215:VAL:HG13	1.86	0.57
1:B:344:ILE:H	1:B:379:GLN:HE22	1.53	0.57
1:B:410:SER:OG	1:B:415:HIS:HD2	1.88	0.57
1:A:499:ILE:HD13	1:A:499:ILE:O	2.05	0.57
1:C:269:ASP:C	1:C:271:ALA:N	2.62	0.57
1:C:369:ASP:CG	1:C:408:ARG:HB3	2.30	0.57
1:D:246:LEU:O	1:D:246:LEU:HD23	2.04	0.57
1:F:357:CYS:CB	1:F:364:LEU:HD11	2.35	0.57
1:F:441:PRO:HG3	1:F:471:ARG:HH21	1.69	0.57
1:A:145:ALA:HB3	1:D:479:TRP:HZ3	1.69	0.57
1:A:237:VAL:HG22	1:A:238:ASP:N	2.20	0.57
1:A:458:ASN:OD1	1:A:462:VAL:HG13	2.04	0.57
1:C:171:MET:HE2	1:C:173:GLY:O	2.05	0.57
1:C:266:ASP:C	1:C:268:GLY:N	2.62	0.57
1:D:344:ILE:HG23	1:D:387:HIS:CG	2.39	0.57
1:A:120:TYR:HE2	1:A:167:GLN:HE21	1.52	0.56
1:B:70:PHE:CE2	1:E:448:LEU:HD21	2.40	0.56
1:C:291:ASN:ND2	1:C:293:ARG:H	2.02	0.56
1:E:448:LEU:HD12	1:E:449:TYR:H	1.69	0.56
1:A:126:VAL:HG21	1:C:505:MET:HE2	1.87	0.56
1:D:316:ILE:HG12	2:D:550:HOH:O	2.06	0.56
1:D:456:ALA:O	1:D:457:SER:C	2.47	0.56
1:D:464:LYS:CA	1:D:467:ILE:HG12	2.33	0.56
1:F:127:GLY:CA	1:F:165:ILE:HD11	2.35	0.56
1:F:269:ASP:O	1:F:270:PRO:O	2.23	0.56
1:A:72:LEU:HD21	1:A:142:GLN:HB3	1.88	0.56
1:A:274:ASP:OD2	1:A:274:ASP:N	2.36	0.56
1:A:292:MET:HE3	1:A:292:MET:O	2.05	0.56
1:C:211:LEU:HG	1:C:213:GLU:OE2	2.06	0.56
1:C:461:ASP:CG	1:C:462:VAL:H	2.13	0.56
1:D:156:LYS:O	1:D:160:MET:HG2	2.05	0.56
1:E:108:LEU:HD22	1:E:151:TYR:CD2	2.40	0.56
1:E:436:ILE:HD13	1:E:436:ILE:H	1.70	0.56
1:F:128:ALA:O	1:F:165:ILE:HD13	2.05	0.56
1:B:450:ARG:HA	1:B:450:ARG:NE	2.21	0.56
1:D:6:LYS:HD3	1:D:11:LYS:CD	2.35	0.56
1:D:463:LEU:HD13	1:D:464:LYS:N	2.21	0.56
1:E:496:ARG:O	1:E:500:VAL:HG23	2.06	0.56
1:D:32:ILE:HG13	1:D:33:GLN:N	2.19	0.56
1:D:198:TYR:HE2	1:D:218:GLN:CD	2.12	0.56
1:D:276:THR:HG22	1:D:277:GLY:N	2.14	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:422:SER:O	1:E:156:LYS:HE2	2.05	0.56
1:D:273:ARG:H	1:D:497:ARG:HD3	1.70	0.56
1:D:458:ASN:HB2	1:D:461:ASP:HB3	1.87	0.56
1:E:194:GLY:H	1:E:198:TYR:HH	1.47	0.56
1:E:265:ILE:HG22	1:E:322:ARG:CZ	2.35	0.56
1:B:241:GLN:H	1:B:241:GLN:NE2	2.00	0.56
1:C:31:ARG:NE	1:C:31:ARG:CA	2.69	0.56
1:C:75:GLN:NE2	1:C:75:GLN:C	2.64	0.56
1:C:451:LYS:CE	1:C:452:GLU:HG3	2.32	0.56
1:C:464:LYS:HA	1:C:467:ILE:HG22	1.87	0.56
1:D:198:TYR:HB2	1:D:221:GLY:O	2.05	0.56
1:D:295:ILE:O	1:D:299:ILE:HG13	2.06	0.56
1:F:35:GLN:NE2	1:F:40:LYS:HE2	2.21	0.56
1:F:262:PRO:HB2	1:F:327:VAL:CG1	2.36	0.56
1:A:316:ILE:HG23	1:A:346:ALA:HB1	1.88	0.56
1:C:75:GLN:C	1:C:75:GLN:HE21	2.14	0.56
1:C:172:ALA:HA	1:C:196:ALA:CB	2.35	0.56
1:D:191:MET:CE	1:D:199:MET:SD	2.94	0.56
1:D:274:ASP:OD1	1:D:275:ALA:N	2.39	0.56
1:F:453:ILE:HG22	1:F:454:GLN:OE1	2.04	0.56
1:C:13:ILE:HD12	1:C:14:GLU:N	2.20	0.56
1:C:215:VAL:HB	1:C:220:LEU:CD1	2.34	0.56
1:C:272:ASP:O	1:C:273:ARG:HB2	2.06	0.56
1:C:382:LYS:HE3	1:F:382:LYS:HZ2	1.69	0.56
1:C:453:ILE:O	1:C:459:PRO:HA	2.06	0.56
1:D:28:GLY:O	1:D:32:ILE:HG23	2.06	0.56
1:D:269:ASP:C	1:D:271:ALA:H	2.14	0.56
1:D:344:ILE:HG23	1:D:387:HIS:CD2	2.41	0.56
1:A:146:LEU:HD23	1:D:479:TRP:CH2	2.40	0.55
1:B:281:ILE:HD13	1:B:294:GLU:HB3	1.87	0.55
1:B:385:ILE:CD1	1:E:180:VAL:HG11	2.36	0.55
1:B:450:ARG:HH22	1:B:453:ILE:HD13	1.71	0.55
1:D:13:ILE:HG13	1:D:14:GLU:N	2.20	0.55
1:D:273:ARG:NH1	1:D:276:THR:OG1	2.39	0.55
1:E:206:ILE:O	1:E:210:VAL:HG12	2.06	0.55
1:A:465:GLN:NE2	1:A:466:ARG:HG2	2.22	0.55
1:C:30:GLU:HG2	1:C:31:ARG:NH1	2.18	0.55
1:C:169:THR:HG23	1:C:189:ILE:HG12	1.88	0.55
1:F:257:ASN:ND2	1:F:259:MET:HB2	2.21	0.55
1:F:316:ILE:HD11	1:F:349:LYS:HD3	1.88	0.55
1:F:436:ILE:HD12	1:F:437:ALA:N	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:285:ASP:OD1	1:D:288:LYS:HE3	2.06	0.55
1:E:239:SER:OG	1:E:242:GLU:HG3	2.07	0.55
1:F:88:LYS:HA	1:F:92:ARG:O	2.05	0.55
1:A:237:VAL:CG2	1:A:242:GLU:HB3	2.35	0.55
1:C:110:GLU:OE1	1:C:146:LEU:HD22	2.05	0.55
1:A:72:LEU:HD21	1:A:142:GLN:CB	2.37	0.55
1:D:273:ARG:H	1:D:497:ARG:CD	2.20	0.55
1:D:343:ASP:OD1	1:D:344:ILE:N	2.39	0.55
1:A:73:ASP:OD2	1:A:74:LYS:HG2	2.05	0.55
1:B:177:GLY:O	1:B:180:VAL:HG12	2.06	0.55
1:D:284:ASN:OD1	1:D:285:ASP:N	2.33	0.55
1:D:292:MET:HE1	1:D:407:VAL:HG11	1.89	0.55
1:E:271:ALA:HB3	2:E:579:HOH:O	2.06	0.55
1:E:342:ILE:HD12	1:E:346:ALA:HB3	1.89	0.55
1:F:350:ALA:O	1:F:354:ILE:HG12	2.06	0.55
1:B:273:ARG:CG	1:B:497:ARG:HH12	2.19	0.55
1:C:287:ALA:C	1:C:288:LYS:HE3	2.31	0.55
1:D:99:GLN:HE21	1:D:112:HIS:CE1	2.25	0.55
1:D:169:THR:CG2	1:D:186:THR:OG1	2.54	0.55
1:D:342:ILE:HD12	1:D:391:MET:SD	2.46	0.55
1:D:479:TRP:O	1:D:483:LYS:HG2	2.07	0.55
1:F:182:SER:HB3	1:F:183:PRO:HD3	1.89	0.55
1:B:275:ALA:O	1:B:276:THR:C	2.50	0.55
1:C:316:ILE:HG12	1:C:346:ALA:HB1	1.88	0.55
1:D:483:LYS:HB2	1:D:485:LEU:HG	1.87	0.55
1:F:273:ARG:NE	1:F:275:ALA:HB2	2.22	0.55
1:C:454:GLN:OE1	1:C:455:GLN:HG2	2.07	0.55
1:E:6:LYS:N	1:E:7:PRO:HD2	2.20	0.55
1:F:455:GLN:HE21	1:F:455:GLN:CA	2.03	0.55
1:A:490:ILE:CG1	1:A:491:GLU:N	2.69	0.55
1:B:193:LYS:HA	1:B:223:ALA:HB3	1.88	0.55
1:B:450:ARG:O	1:B:450:ARG:HD3	2.07	0.55
1:C:344:ILE:H	1:C:344:ILE:CD1	2.20	0.55
1:C:476:ASN:C	1:C:476:ASN:ND2	2.65	0.55
1:E:270:PRO:HG2	1:E:496:ARG:NH2	2.21	0.55
1:F:495:THR:O	1:F:499:ILE:HG12	2.07	0.55
1:B:40:LYS:HZ2	1:B:197:TYR:HE2	1.49	0.54
1:D:449:TYR:HE1	1:D:469:GLU:OE2	1.90	0.54
1:A:6:LYS:HA	1:A:6:LYS:HE2	1.88	0.54
1:A:483:LYS:CB	1:D:146:LEU:HD21	2.38	0.54
1:C:31:ARG:CZ	1:C:31:ARG:CA	2.83	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:491:GLU:OE1	1:F:17:ARG:HD3	2.08	0.54
1:F:342:ILE:HG23	1:F:373:TYR:CD2	2.41	0.54
1:A:490:ILE:HG13	1:A:491:GLU:N	2.22	0.54
1:C:120:TYR:CZ	1:C:130:VAL:HG11	2.42	0.54
1:B:343:ASP:HB3	1:B:374:VAL:CG1	2.37	0.54
1:E:17:ARG:HD3	1:F:491:GLU:OE2	2.07	0.54
1:E:276:THR:HG22	1:E:279:GLU:CD	2.33	0.54
1:C:205:GLU:HA	1:C:208:LYS:HG2	1.90	0.54
1:D:195:ASP:C	1:D:197:TYR:N	2.61	0.54
1:F:58:GLU:OE2	1:F:83:VAL:HG13	2.08	0.54
1:A:443:GLY:O	1:A:447:ILE:HG12	2.07	0.54
1:D:7:PRO:N	1:D:8:PRO:HD2	2.23	0.54
1:E:240:GLU:O	1:E:244:ILE:HG23	2.07	0.54
1:E:273:ARG:HD3	1:E:497:ARG:HD2	1.88	0.54
1:E:450:ARG:HB2	1:E:450:ARG:CZ	2.38	0.54
1:A:351:ALA:HA	1:A:354:ILE:HD13	1.88	0.54
1:A:418:MET:O	1:A:419:SER:HB3	2.08	0.54
1:C:288:LYS:HE3	1:C:288:LYS:N	2.22	0.54
1:C:514:TYR:CZ	1:F:124:LEU:HD21	2.43	0.54
1:E:170:ILE:HD11	1:E:247:THR:OG1	2.08	0.54
1:F:269:ASP:HB2	1:F:496:ARG:HH22	1.70	0.54
1:F:435:GLU:CG	1:F:475:ALA:HB1	2.36	0.54
1:A:42:THR:OG1	1:A:45:GLU:HG3	2.07	0.54
1:A:95:PHE:CE1	1:C:505:MET:HE3	2.43	0.54
1:B:210:VAL:HG12	1:B:211:LEU:N	2.22	0.54
1:A:447:ILE:HD12	1:D:141:ILE:HG13	1.90	0.54
1:A:462:VAL:HA	1:A:465:GLN:NE2	2.22	0.54
1:C:344:ILE:HD13	1:C:344:ILE:N	2.21	0.54
1:F:369:ASP:OD1	1:F:409:LYS:HG2	2.07	0.54
1:B:168:ILE:CD1	1:B:250:LEU:HD13	2.38	0.53
1:B:174:PRO:HB3	1:B:197:TYR:CE1	2.42	0.53
1:C:451:LYS:CE	1:C:452:GLU:H	2.20	0.53
1:D:277:GLY:HA2	1:D:280:GLN:CG	2.38	0.53
1:C:169:THR:HG22	1:C:186:THR:OG1	2.08	0.53
1:E:274:ASP:OD2	1:E:275:ALA:N	2.41	0.53
1:B:483:LYS:HB2	1:B:485:LEU:HG	1.90	0.53
1:C:389:ALA:HB1	1:F:185:LEU:HD13	1.89	0.53
1:D:269:ASP:O	1:D:271:ALA:N	2.39	0.53
1:E:180:VAL:HG22	1:E:199:MET:HB2	1.91	0.53
1:F:6:LYS:HE2	1:F:12:LEU:CD2	2.38	0.53
1:F:490:ILE:HD11	1:F:494:ASP:HB3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:235:PHE:CE2	1:A:306:LEU:HD21	2.43	0.53
1:A:237:VAL:HG23	2:A:733:HOH:O	2.08	0.53
1:B:463:LEU:CB	1:B:466:ARG:NE	2.71	0.53
1:C:215:VAL:HB	1:C:220:LEU:HG	1.90	0.53
1:D:108:LEU:HD22	1:D:151:TYR:CD2	2.43	0.53
1:F:273:ARG:HD2	1:F:275:ALA:N	2.18	0.53
1:A:138:GLY:HA2	1:A:179:ALA:HB2	1.91	0.53
1:A:175:ALA:O	1:A:199:MET:HA	2.09	0.53
1:B:463:LEU:HA	1:B:466:ARG:CD	2.39	0.53
1:B:518:HIS:HE1	1:E:358:ASP:OD2	1.91	0.53
1:C:496:ARG:O	1:C:500:VAL:HG23	2.08	0.53
1:D:244:ILE:HD12	1:D:244:ILE:O	2.09	0.53
1:E:265:ILE:HG23	1:E:265:ILE:O	2.08	0.53
1:F:31:ARG:HB3	1:F:102:THR:HB	1.90	0.53
1:A:158:ASN:HD22	1:A:167:GLN:NE2	2.07	0.53
1:B:466:ARG:H	1:B:466:ARG:HH21	1.56	0.53
1:C:510:ARG:HG2	1:C:510:ARG:NH1	2.23	0.53
1:D:192:ILE:O	1:D:198:TYR:CE1	2.61	0.53
1:E:448:LEU:HG	1:E:449:TYR:CD1	2.43	0.53
1:A:446:ARG:C	1:A:450:ARG:NH1	2.66	0.53
1:A:451:LYS:HD2	1:A:451:LYS:N	2.15	0.53
1:B:268:GLY:C	1:B:270:PRO:HD2	2.34	0.53
1:C:452:GLU:C	1:C:454:GLN:N	2.67	0.53
1:A:226:HIS:HA	1:A:230:SER:HG	1.74	0.53
1:B:171:MET:HE3	1:B:199:MET:HE3	1.89	0.53
1:C:436:ILE:HD13	1:C:436:ILE:O	2.09	0.53
1:F:192:ILE:HD12	1:F:192:ILE:N	2.24	0.53
1:A:439:THR:HG22	1:A:440:GLY:N	2.23	0.53
1:A:451:LYS:O	1:A:453:ILE:N	2.42	0.53
1:A:497:ARG:HG3	1:A:497:ARG:HH11	1.73	0.53
1:C:257:ASN:ND2	1:C:259:MET:H	1.98	0.53
1:E:275:ALA:O	1:E:276:THR:O	2.27	0.53
1:E:467:ILE:HG13	1:E:468:ALA:N	2.22	0.53
1:F:168:ILE:HD12	1:F:251:LEU:HD13	1.89	0.53
1:A:458:ASN:HD21	1:A:462:VAL:HG11	1.73	0.53
1:B:463:LEU:O	1:B:466:ARG:CZ	2.56	0.53
1:C:445:VAL:HG11	1:C:466:ARG:HB3	1.91	0.53
1:D:378:ASP:HB3	2:D:663:HOH:O	2.08	0.53
1:E:7:PRO:N	1:E:8:PRO:HD2	2.23	0.53
1:E:210:VAL:O	1:E:211:LEU:HD13	2.08	0.53
1:F:211:LEU:HD23	1:F:211:LEU:N	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:146:LEU:HD21	1:D:483:LYS:HB3	1.91	0.52
1:B:108:LEU:HD22	1:B:151:TYR:CD2	2.44	0.52
1:C:11:LYS:HE3	1:C:14:GLU:OE1	2.09	0.52
1:C:308:VAL:HB	1:C:318:VAL:HG12	1.90	0.52
1:B:73:ASP:OD2	1:B:74:LYS:HG3	2.10	0.52
1:E:169:THR:HG21	1:E:183:PRO:HB3	1.91	0.52
1:E:450:ARG:C	1:E:452:GLU:N	2.67	0.52
1:E:494:ASP:CB	1:E:497:ARG:HH11	2.14	0.52
1:A:453:ILE:O	1:A:453:ILE:HG23	2.09	0.52
1:C:410:SER:OG	1:C:415:HIS:CD2	2.56	0.52
1:C:490:ILE:CD1	1:C:491:GLU:H	2.21	0.52
1:D:471:ARG:HA	1:D:475:ALA:CB	2.40	0.52
1:E:490:ILE:HG13	1:E:491:GLU:N	2.25	0.52
1:A:369:ASP:HA	1:A:409:LYS:O	2.10	0.52
1:A:449:TYR:N	1:A:450:ARG:HH11	2.06	0.52
1:B:276:THR:HG22	1:B:276:THR:O	2.09	0.52
1:B:375:PRO:HG3	1:E:210:VAL:CG1	2.39	0.52
1:C:431:TRP:HE1	1:C:495:THR:HG22	1.74	0.52
1:D:285:ASP:C	1:D:287:ALA:H	2.18	0.52
1:F:275:ALA:C	1:F:277:GLY:N	2.65	0.52
1:B:445:VAL:CG2	1:B:467:ILE:HG23	2.38	0.52
1:C:296:ILE:HD11	1:C:305:PHE:HB2	1.91	0.52
1:D:205:GLU:CD	1:D:205:GLU:H	2.17	0.52
1:D:412:GLY:O	1:D:415:HIS:HB3	2.10	0.52
1:E:273:ARG:HG3	1:E:493:LYS:O	2.10	0.52
1:E:507:LYS:HG3	1:E:508:THR:N	2.23	0.52
1:F:14:GLU:O	1:F:18:GLN:HG3	2.10	0.52
1:A:269:ASP:HB2	1:A:270:PRO:CA	2.39	0.52
1:D:443:GLY:O	1:D:447:ILE:HG23	2.10	0.52
1:E:464:LYS:O	1:E:464:LYS:HD2	2.09	0.52
1:F:6:LYS:HE2	1:F:12:LEU:HG	1.91	0.52
1:B:257:ASN:HD21	1:B:260:GLU:HG3	1.73	0.52
1:B:415:HIS:NE2	1:B:436:ILE:HD12	2.25	0.52
1:D:6:LYS:C	1:D:8:PRO:HD2	2.35	0.52
1:E:292:MET:HE2	1:E:367:LEU:HD13	1.90	0.52
1:F:208:LYS:HA	1:F:213:GLU:O	2.10	0.52
1:A:450:ARG:HA	1:A:450:ARG:NE	2.23	0.52
1:B:450:ARG:NH2	1:B:453:ILE:HD13	2.25	0.52
1:B:466:ARG:HH22	1:B:468:ALA:HB3	1.73	0.52
1:C:205:GLU:HA	1:C:208:LYS:HE2	1.92	0.52
1:E:108:LEU:HD22	1:E:151:TYR:CE2	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:13:ILE:O	1:F:17:ARG:HG3	2.10	0.52
1:C:56:PHE:HB2	1:C:86:TRP:O	2.10	0.52
1:C:432:PRO:HD3	1:C:490:ILE:O	2.10	0.52
1:A:200:PHE:CE2	1:A:203:GLY:HA2	2.45	0.52
1:B:318:VAL:HA	1:B:330:ILE:O	2.09	0.52
1:B:458:ASN:HB3	1:B:462:VAL:HG21	1.91	0.52
1:D:177:GLY:O	1:D:180:VAL:HG22	2.10	0.52
1:D:466:ARG:NE	1:D:469:GLU:OE2	2.35	0.52
1:D:470:TYR:O	1:D:474:PHE:N	2.43	0.52
1:A:208:LYS:O	1:A:212:GLY:HA2	2.10	0.51
1:B:463:LEU:HA	1:B:466:ARG:HD2	1.91	0.51
1:C:6:LYS:HE3	1:C:6:LYS:CA	2.40	0.51
1:C:226:HIS:HA	1:C:230:SER:HG	1.75	0.51
1:C:445:VAL:HG13	1:C:466:ARG:HB3	1.92	0.51
1:C:452:GLU:O	1:C:454:GLN:N	2.43	0.51
1:D:466:ARG:NH1	1:D:469:GLU:HB2	2.25	0.51
1:E:445:VAL:O	1:E:448:LEU:O	2.28	0.51
1:A:244:ILE:CD1	1:A:248:LYS:HE3	2.40	0.51
1:B:40:LYS:NZ	1:B:197:TYR:CE2	2.72	0.51
1:C:264:TYR:HB3	2:C:560:HOH:O	2.11	0.51
1:C:514:TYR:CE1	1:F:124:LEU:HD21	2.45	0.51
1:E:31:ARG:HG3	1:E:31:ARG:HH11	1.73	0.51
1:E:192:ILE:O	1:E:198:TYR:HE1	1.93	0.51
1:A:455:GLN:HG3	1:A:455:GLN:O	2.09	0.51
1:C:342:ILE:HG12	1:C:373:TYR:CE2	2.46	0.51
1:D:315:ASN:ND2	1:D:315:ASN:N	2.44	0.51
1:D:493:LYS:CD	1:D:493:LYS:N	2.61	0.51
1:E:177:GLY:O	1:E:180:VAL:HB	2.10	0.51
1:E:210:VAL:O	1:E:210:VAL:HG22	2.10	0.51
1:C:316:ILE:HD12	1:C:316:ILE:O	2.11	0.51
1:C:453:ILE:HG13	1:C:462:VAL:HG21	1.92	0.51
1:C:512:TYR:O	1:C:513:ARG:HG3	2.10	0.51
1:F:35:GLN:CD	1:F:40:LYS:HG3	2.35	0.51
1:F:215:VAL:HG23	1:F:219:ASP:CB	2.41	0.51
1:F:342:ILE:HD12	1:F:346:ALA:HB3	1.92	0.51
1:F:418:MET:O	1:F:419:SER:HB3	2.11	0.51
1:A:280:GLN:HA	1:A:280:GLN:NE2	2.26	0.51
1:A:466:ARG:HA	1:A:469:GLU:HG2	1.92	0.51
1:A:469:GLU:HA	1:A:472:LYS:CD	2.40	0.51
1:B:442:GLU:O	1:B:446:ARG:HB2	2.10	0.51
1:C:145:ALA:HB3	1:F:479:TRP:HZ3	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:169:THR:CG2	1:C:189:ILE:HG12	2.41	0.51
1:F:62:PHE:O	1:F:64:THR:HG23	2.11	0.51
1:F:435:GLU:HG3	1:F:475:ALA:CB	2.35	0.51
1:A:168:ILE:HD13	1:A:250:LEU:HD23	1.92	0.51
1:A:450:ARG:NE	1:A:450:ARG:CA	2.74	0.51
1:A:451:LYS:HB3	1:A:451:LYS:NZ	2.25	0.51
1:E:460:ASP:N	1:E:460:ASP:OD2	2.43	0.51
1:F:58:GLU:CD	1:F:61:THR:HG22	2.36	0.51
1:B:466:ARG:HH22	1:B:468:ALA:CB	2.24	0.51
1:C:462:VAL:O	1:C:466:ARG:HB2	2.11	0.51
1:F:511:GLU:C	1:F:512:TYR:CD1	2.89	0.51
1:B:206:ILE:O	1:B:210:VAL:HB	2.11	0.51
1:C:8:PRO:HG2	1:C:11:LYS:HB3	1.93	0.51
1:C:135:ASP:HA	1:C:173:GLY:HA3	1.91	0.51
1:D:99:GLN:HE21	1:D:112:HIS:HE1	1.57	0.51
1:E:168:ILE:HD13	1:E:250:LEU:HD23	1.93	0.51
1:E:396:ALA:O	1:E:513:ARG:NH1	2.44	0.51
1:F:273:ARG:HB2	1:F:493:LYS:HB2	1.93	0.51
1:B:7:PRO:HG2	1:B:8:PRO:CD	2.40	0.51
1:B:518:HIS:HD2	1:B:519:GLY:O	1.94	0.51
1:C:296:ILE:C	1:C:296:ILE:HD12	2.36	0.51
1:C:418:MET:O	1:C:419:SER:HB3	2.10	0.51
1:F:6:LYS:HE2	1:F:12:LEU:HD21	1.92	0.51
1:C:316:ILE:HD11	1:C:349:LYS:HD3	1.92	0.51
1:C:342:ILE:HD12	1:C:343:ASP:N	2.26	0.51
1:E:499:ILE:HD13	1:E:499:ILE:O	2.11	0.51
1:C:197:TYR:CE1	1:C:218:GLN:HB3	2.46	0.50
1:C:431:TRP:HE1	1:C:495:THR:HG21	1.76	0.50
1:D:316:ILE:CG1	1:D:346:ALA:HB1	2.42	0.50
1:E:192:ILE:O	1:E:198:TYR:CE1	2.64	0.50
1:F:191:MET:HE3	1:F:233:VAL:CG2	2.41	0.50
1:A:6:LYS:HZ3	1:A:8:PRO:CD	2.23	0.50
1:B:32:ILE:HD12	1:B:32:ILE:C	2.35	0.50
1:B:169:THR:CG2	1:B:186:THR:OG1	2.59	0.50
1:C:202:THR:HG21	1:C:206:ILE:CD1	2.41	0.50
1:E:175:ALA:O	1:E:199:MET:HA	2.11	0.50
1:E:205:GLU:CD	1:E:205:GLU:H	2.18	0.50
1:E:292:MET:CE	1:E:295:ILE:HB	2.38	0.50
1:F:481:ALA:HA	1:F:486:VAL:HG22	1.91	0.50
1:A:494:ASP:O	1:A:498:VAL:HG13	2.12	0.50
1:C:127:GLY:CA	1:C:165:ILE:HD11	2.40	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:313:ALA:HB2	1:C:345:ASP:HB3	1.92	0.50
1:D:471:ARG:HA	1:D:475:ALA:HB2	1.93	0.50
1:F:288:LYS:HD2	1:F:288:LYS:N	2.27	0.50
1:B:40:LYS:CD	1:B:197:TYR:HE2	2.24	0.50
1:B:342:ILE:HG13	1:B:343:ASP:N	2.26	0.50
1:B:344:ILE:HG23	1:B:387:HIS:CG	2.46	0.50
1:C:15:GLU:O	1:C:19:LEU:HD13	2.11	0.50
1:C:199:MET:O	1:C:226:HIS:CE1	2.64	0.50
1:C:512:TYR:CD2	1:C:513:ARG:N	2.80	0.50
1:D:191:MET:SD	1:D:198:TYR:CD1	3.05	0.50
1:E:418:MET:O	1:E:419:SER:HB3	2.10	0.50
1:A:313:ALA:C	1:A:315:ASN:N	2.69	0.50
1:B:485:LEU:HD11	1:E:146:LEU:HD12	1.94	0.50
1:D:434:ALA:HB3	1:D:477:PRO:HG3	1.93	0.50
1:F:344:ILE:HG13	1:F:379:GLN:OE1	2.12	0.50
1:A:315:ASN:HD21	1:A:343:ASP:HB2	1.74	0.50
1:A:467:ILE:HG13	1:A:468:ALA:N	2.25	0.50
1:F:126:VAL:O	1:F:126:VAL:HG13	2.12	0.50
1:B:277:GLY:HA2	1:B:280:GLN:CG	2.42	0.50
1:B:332:ALA:CB	1:B:367:LEU:HB2	2.42	0.50
1:D:318:VAL:HG13	1:D:353:PHE:CG	2.47	0.50
1:E:55:LYS:HD2	1:E:88:LYS:HB2	1.94	0.50
1:E:197:TYR:O	1:E:198:TYR:CD1	2.65	0.50
1:E:208:LYS:HD2	1:E:208:LYS:O	2.12	0.50
1:F:309:HIS:HB3	1:F:349:LYS:HE3	1.92	0.50
1:F:450:ARG:C	1:F:452:GLU:N	2.70	0.50
1:A:226:HIS:HA	1:A:230:SER:OG	2.11	0.50
1:B:375:PRO:HG3	1:E:210:VAL:HG11	1.94	0.50
1:C:13:ILE:HD12	1:C:13:ILE:C	2.37	0.50
1:D:266:ASP:O	1:D:266:ASP:CG	2.54	0.50
1:D:452:GLU:CD	1:D:452:GLU:N	2.69	0.50
1:E:89:VAL:CG2	1:E:89:VAL:O	2.60	0.50
1:E:490:ILE:CG1	1:E:491:GLU:N	2.74	0.50
1:F:342:ILE:HD12	1:F:343:ASP:H	1.76	0.50
1:B:8:PRO:HG2	1:B:11:LYS:HB2	1.93	0.50
1:F:157:MET:HA	1:F:157:MET:HE2	1.93	0.50
1:A:449:TYR:C	1:A:450:ARG:NH1	2.70	0.49
1:C:471:ARG:O	1:C:475:ALA:HB3	2.12	0.49
1:C:490:ILE:HG13	1:C:494:ASP:HB2	1.93	0.49
1:D:241:GLN:O	1:D:244:ILE:HG23	2.12	0.49
1:B:159:VAL:HG21	1:E:396:ALA:HB3	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:214:GLU:N	1:C:214:GLU:CD	2.70	0.49
1:A:51:PHE:O	1:A:52:ASP:C	2.55	0.49
1:A:145:ALA:HB3	1:D:479:TRP:CZ3	2.46	0.49
1:C:217:PHE:CG	1:C:218:GLN:N	2.76	0.49
1:C:471:ARG:HA	1:C:475:ALA:CB	2.42	0.49
1:D:265:ILE:CG2	1:D:266:ASP:H	2.08	0.49
1:D:463:LEU:HD13	1:D:463:LEU:C	2.37	0.49
1:F:443:GLY:O	1:F:447:ILE:HD13	2.11	0.49
1:B:461:ASP:O	1:B:462:VAL:C	2.54	0.49
1:B:485:LEU:HD11	1:E:146:LEU:CD1	2.43	0.49
1:C:14:GLU:O	1:C:18:GLN:HG3	2.12	0.49
1:D:453:ILE:HD13	1:D:462:VAL:HB	1.94	0.49
1:A:273:ARG:O	1:A:273:ARG:NH2	2.43	0.49
1:A:447:ILE:HA	1:A:450:ARG:NE	2.26	0.49
1:B:453:ILE:HG12	1:B:454:GLN:N	2.27	0.49
1:B:466:ARG:CZ	1:B:467:ILE:CG1	2.91	0.49
1:D:138:GLY:HA2	1:D:179:ALA:HB2	1.94	0.49
1:D:447:ILE:HD12	1:D:447:ILE:C	2.36	0.49
1:E:226:HIS:HA	1:E:230:SER:OG	2.12	0.49
1:A:272:ASP:O	1:A:273:ARG:O	2.30	0.49
1:B:266:ASP:O	1:B:267:THR:C	2.56	0.49
1:D:68:THR:O	1:D:73:ASP:HB3	2.13	0.49
1:D:461:ASP:O	1:D:465:GLN:HB2	2.13	0.49
1:F:180:VAL:C	1:F:183:PRO:HD2	2.37	0.49
1:A:6:LYS:HE2	1:A:6:LYS:CA	2.43	0.49
1:A:190:ILE:HD12	1:A:247:THR:HG22	1.93	0.49
1:A:469:GLU:HA	1:A:472:LYS:HD3	1.95	0.49
1:B:293:ARG:HA	1:B:296:ILE:HG23	1.95	0.49
1:B:436:ILE:HD11	1:E:145:ALA:HB1	1.93	0.49
1:B:447:ILE:CD1	1:E:141:ILE:HD12	2.43	0.49
1:C:6:LYS:CE	1:C:8:PRO:HD2	2.43	0.49
1:E:343:ASP:H	1:E:346:ALA:HB3	1.78	0.49
1:A:471:ARG:O	1:A:475:ALA:HB3	2.12	0.49
1:C:264:TYR:HE2	1:C:507:LYS:NZ	2.11	0.49
1:A:7:PRO:HG2	1:A:8:PRO:HD2	1.95	0.49
1:B:315:ASN:HA	1:B:337:GLU:HB2	1.95	0.49
1:E:73:ASP:OD1	1:E:74:LYS:HG3	2.13	0.49
1:E:83:VAL:O	1:E:97:TYR:HA	2.13	0.49
1:F:169:THR:CG2	1:F:186:THR:OG1	2.61	0.49
1:F:369:ASP:CG	1:F:408:ARG:HB3	2.38	0.49
1:A:473:LEU:HD23	1:A:474:PHE:CE2	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:494:ASP:CB	1:A:497:ARG:NH1	2.73	0.49
1:B:463:LEU:CD1	1:B:466:ARG:NE	2.69	0.49
1:C:343:ASP:CG	1:C:344:ILE:HD13	2.37	0.49
1:D:472:LYS:HD3	1:D:472:LYS:C	2.38	0.49
1:E:226:HIS:HA	1:E:230:SER:HG	1.78	0.49
1:A:191:MET:HE1	1:A:198:TYR:HA	1.94	0.48
1:A:292:MET:CE	1:A:295:ILE:HB	2.43	0.48
1:B:237:VAL:HG21	1:B:242:GLU:HB3	1.95	0.48
1:B:483:LYS:HB3	1:E:146:LEU:HD11	1.95	0.48
1:C:204:PRO:HD2	1:C:205:GLU:OE1	2.13	0.48
1:C:382:LYS:HE3	1:F:382:LYS:HZ1	1.77	0.48
1:C:385:ILE:HD13	1:F:199:MET:HE2	1.95	0.48
1:D:197:TYR:H	1:D:197:TYR:HD1	1.59	0.48
1:D:269:ASP:H	1:D:270:PRO:HD2	1.75	0.48
1:E:292:MET:HE3	1:E:292:MET:O	2.13	0.48
1:F:270:PRO:HA	2:F:688:HOH:O	2.12	0.48
1:A:83:VAL:O	1:A:97:TYR:HA	2.13	0.48
1:B:66:ARG:NH2	1:D:146:LEU:HG	2.27	0.48
1:C:145:ALA:CB	1:F:436:ILE:HD11	2.41	0.48
1:E:455:GLN:O	1:E:455:GLN:CG	2.60	0.48
1:A:354:ILE:HG12	1:A:355:ARG:N	2.28	0.48
1:C:264:TYR:N	1:C:264:TYR:CD1	2.81	0.48
1:E:344:ILE:HG13	1:E:379:GLN:OE1	2.14	0.48
1:F:309:HIS:CB	1:F:349:LYS:HE3	2.43	0.48
1:F:456:ALA:C	1:F:458:ASN:H	2.21	0.48
1:A:73:ASP:CG	1:A:74:LYS:HE3	2.38	0.48
1:A:497:ARG:NH1	1:A:497:ARG:CB	2.72	0.48
1:B:169:THR:HG21	1:B:183:PRO:HA	1.96	0.48
1:C:191:MET:HE1	1:C:198:TYR:HA	1.95	0.48
1:D:458:ASN:O	1:D:462:VAL:HG22	2.13	0.48
2:D:574:HOH:O	1:F:17:ARG:HG2	2.14	0.48
1:E:7:PRO:N	1:E:8:PRO:CD	2.76	0.48
1:F:168:ILE:CD1	1:F:251:LEU:HD13	2.44	0.48
1:A:60:MET:O	1:A:115:LYS:HE3	2.13	0.48
1:D:108:LEU:HD22	1:D:151:TYR:CE2	2.48	0.48
1:F:226:HIS:HA	1:F:230:SER:OG	2.13	0.48
1:A:192:ILE:HD12	1:A:192:ILE:N	2.28	0.48
1:B:40:LYS:HD2	1:B:197:TYR:HE2	1.76	0.48
1:B:352:ARG:CD	1:E:520:ASN:HD21	2.21	0.48
1:C:270:PRO:HG2	1:C:496:ARG:NH2	2.28	0.48
1:C:438:VAL:HG13	1:C:439:THR:HG22	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:451:LYS:HE3	1:C:452:GLU:CG	2.36	0.48
1:D:315:ASN:HA	1:D:337:GLU:HB2	1.96	0.48
1:D:442:GLU:HA	1:D:445:VAL:HG22	1.96	0.48
1:E:208:LYS:O	1:E:211:LEU:O	2.31	0.48
1:E:496:ARG:O	1:E:499:ILE:HG22	2.14	0.48
1:F:10:GLU:O	1:F:13:ILE:HG12	2.14	0.48
1:A:244:ILE:HD12	1:A:244:ILE:O	2.13	0.48
1:A:466:ARG:HH21	1:A:469:GLU:CD	2.21	0.48
1:E:74:LYS:HE3	1:E:74:LYS:N	2.29	0.48
1:E:313:ALA:HB2	1:E:345:ASP:HB3	1.95	0.48
1:A:469:GLU:O	1:A:472:LYS:HD3	2.13	0.48
1:B:16:LEU:C	1:B:16:LEU:HD13	2.39	0.48
1:D:439:THR:HG22	1:D:440:GLY:N	2.28	0.48
1:D:466:ARG:HA	1:D:469:GLU:HB3	1.96	0.48
1:E:206:ILE:H	1:E:206:ILE:CD1	2.26	0.48
1:E:272:ASP:HB3	1:E:273:ARG:NH1	2.28	0.48
1:E:285:ASP:OD1	1:E:286:ALA:N	2.47	0.48
1:A:131:VAL:HA	1:A:168:ILE:O	2.13	0.48
1:A:150:GLY:O	1:A:154:VAL:HG12	2.14	0.48
1:B:446:ARG:HB3	1:B:446:ARG:NH2	2.28	0.48
1:C:124:LEU:HD13	1:F:514:TYR:CE2	2.48	0.48
1:C:226:HIS:HD2	1:C:230:SER:OG	1.97	0.48
1:C:412:GLY:O	1:C:415:HIS:HB3	2.14	0.48
1:D:269:ASP:N	1:D:270:PRO:CD	2.77	0.48
1:E:17:ARG:HG2	2:F:621:HOH:O	2.13	0.48
1:F:316:ILE:HD11	1:F:349:LYS:CD	2.43	0.48
1:A:244:ILE:HD11	1:A:248:LYS:HE3	1.96	0.48
1:A:378:ASP:CG	1:A:382:LYS:HE2	2.39	0.48
1:F:511:GLU:HG3	1:F:512:TYR:H	1.79	0.48
1:A:126:VAL:CG2	1:C:505:MET:HE2	2.43	0.47
1:A:306:LEU:HD23	1:A:306:LEU:C	2.39	0.47
1:A:315:ASN:ND2	1:A:343:ASP:CB	2.76	0.47
1:C:210:VAL:HG12	1:C:210:VAL:O	2.13	0.47
1:C:344:ILE:CD1	1:C:379:GLN:HE22	2.13	0.47
1:D:344:ILE:HG13	1:D:379:GLN:NE2	2.29	0.47
1:E:42:THR:OG1	1:E:45:GLU:HG3	2.13	0.47
1:E:191:MET:HE2	1:E:198:TYR:CB	2.43	0.47
1:A:393:TYR:HA	1:D:159:VAL:HG21	1.96	0.47
1:B:315:ASN:ND2	1:B:346:ALA:HB2	2.29	0.47
1:C:53:ASP:HB3	2:C:545:HOH:O	2.13	0.47
1:C:296:ILE:HD12	1:C:296:ILE:O	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:175:ALA:O	1:D:199:MET:HA	2.14	0.47
1:D:463:LEU:HD13	1:D:464:LYS:HB3	1.95	0.47
1:A:139:ALA:O	1:A:141:ILE:HD12	2.14	0.47
1:B:295:ILE:O	1:B:299:ILE:HG13	2.13	0.47
1:B:445:VAL:C	1:B:447:ILE:H	2.23	0.47
1:C:516:LYS:HE2	1:F:164:VAL:HG23	1.97	0.47
1:F:35:GLN:HG3	1:F:40:LYS:HG3	1.95	0.47
1:F:171:MET:HE2	1:F:173:GLY:N	2.29	0.47
1:F:227:ALA:O	1:F:312:TRP:HB2	2.14	0.47
1:F:315:ASN:HD21	1:F:343:ASP:CB	2.14	0.47
1:A:6:LYS:HE2	1:A:7:PRO:N	2.29	0.47
1:A:21:GLU:N	1:A:21:GLU:OE2	2.48	0.47
1:B:375:PRO:HB2	1:E:207:THR:CG2	2.35	0.47
1:C:171:MET:HB3	1:C:191:MET:HG3	1.96	0.47
1:C:342:ILE:HD12	1:C:343:ASP:H	1.78	0.47
1:D:432:PRO:HD3	1:D:490:ILE:O	2.15	0.47
1:E:66:ARG:NH2	1:F:483:LYS:O	2.44	0.47
1:E:269:ASP:C	1:E:271:ALA:H	2.22	0.47
1:F:344:ILE:HG23	1:F:387:HIS:CG	2.49	0.47
1:B:193:LYS:O	1:B:194:GLY:C	2.56	0.47
1:C:6:LYS:HZ3	1:C:11:LYS:CG	2.28	0.47
1:F:83:VAL:O	1:F:97:TYR:HA	2.14	0.47
1:F:204:PRO:HG3	1:F:220:LEU:HD22	1.96	0.47
1:A:54:GLY:O	1:A:55:LYS:HG2	2.15	0.47
1:A:458:ASN:HD21	1:A:462:VAL:CG1	2.28	0.47
1:D:197:TYR:C	1:D:198:TYR:CG	2.93	0.47
1:D:369:ASP:HB2	1:D:407:VAL:CG1	2.44	0.47
1:E:265:ILE:HG22	1:E:322:ARG:NH2	2.30	0.47
1:A:215:VAL:HG22	1:A:216:SER:O	2.15	0.47
1:A:215:VAL:HG23	1:A:219:ASP:HB2	1.97	0.47
1:A:237:VAL:CG2	1:A:242:GLU:CB	2.93	0.47
1:A:497:ARG:HA	1:A:500:VAL:CG1	2.43	0.47
1:B:466:ARG:CG	1:B:467:ILE:N	2.56	0.47
1:C:193:LYS:HE2	1:C:238:ASP:OD1	2.15	0.47
1:C:211:LEU:CG	1:C:212:GLY:N	2.77	0.47
1:E:316:ILE:HD11	1:E:349:LYS:HD3	1.95	0.47
1:F:316:ILE:HD12	1:F:316:ILE:C	2.39	0.47
1:A:108:LEU:HD22	1:A:151:TYR:CD2	2.49	0.47
1:A:446:ARG:O	1:A:446:ARG:HG2	2.14	0.47
1:C:34:PHE:CE1	1:C:38:LYS:HB2	2.50	0.47
1:C:358:ASP:HA	1:C:400:VAL:CG1	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:511:GLU:C	1:C:513:ARG:HH22	2.23	0.47
1:E:51:PHE:O	1:E:52:ASP:C	2.57	0.47
1:A:50:LEU:CA	1:A:244:ILE:HD13	2.38	0.47
1:A:265:ILE:HG22	1:A:322:ARG:CD	2.45	0.47
1:A:455:GLN:O	1:A:455:GLN:CG	2.61	0.47
1:C:318:VAL:HG13	1:C:353:PHE:CG	2.50	0.47
1:F:287:ALA:C	1:F:288:LYS:HD2	2.40	0.47
1:A:483:LYS:HB3	1:D:146:LEU:HD21	1.97	0.47
1:A:516:LYS:CE	1:D:162:SER:O	2.62	0.47
1:A:521:ILE:HG13	1:A:522:PRO:HD2	1.97	0.47
1:D:483:LYS:HD2	1:F:66:ARG:NH2	2.28	0.47
1:D:483:LYS:HB3	1:F:66:ARG:NH2	2.28	0.47
1:E:55:LYS:HG3	1:E:55:LYS:O	2.14	0.47
1:E:447:ILE:HD12	1:E:448:LEU:N	2.30	0.47
1:F:29:ASP:HA	1:F:32:ILE:CG1	2.43	0.47
1:F:273:ARG:O	1:F:274:ASP:OD2	2.33	0.47
1:A:204:PRO:HD2	1:A:205:GLU:OE1	2.15	0.46
1:A:354:ILE:HG12	1:A:394:ALA:HB1	1.95	0.46
1:B:494:ASP:O	1:B:498:VAL:HG12	2.14	0.46
1:D:407:VAL:HG13	1:D:408:ARG:N	2.30	0.46
1:E:499:ILE:HD11	1:E:503:LEU:HD11	1.96	0.46
1:E:504:GLU:O	1:E:507:LYS:HE3	2.14	0.46
1:F:29:ASP:O	1:F:33:GLN:HG3	2.15	0.46
1:A:499:ILE:HD13	1:A:499:ILE:C	2.41	0.46
1:F:205:GLU:HA	1:F:208:LYS:CE	2.29	0.46
1:A:446:ARG:C	1:A:450:ARG:CZ	2.89	0.46
1:A:464:LYS:NZ	1:A:464:LYS:HB3	2.30	0.46
1:B:193:LYS:O	1:B:194:GLY:O	2.33	0.46
1:A:494:ASP:CB	1:A:497:ARG:HH12	2.19	0.46
1:A:518:HIS:HD2	1:A:519:GLY:O	1.98	0.46
1:D:169:THR:HG22	1:D:186:THR:OG1	2.14	0.46
1:E:244:ILE:C	1:E:244:ILE:HD12	2.41	0.46
1:A:135:ASP:HA	1:A:173:GLY:HA3	1.98	0.46
1:A:204:PRO:HG2	1:A:217:PHE:CD1	2.50	0.46
1:C:464:LYS:C	1:C:466:ARG:H	2.24	0.46
1:C:469:GLU:O	1:C:473:LEU:HD13	2.15	0.46
1:F:496:ARG:O	1:F:500:VAL:HG23	2.15	0.46
1:C:192:ILE:CG2	1:C:195:ASP:HB2	2.33	0.46
1:C:274:ASP:OD2	1:C:275:ALA:N	2.48	0.46
1:D:208:LYS:HD2	1:D:214:GLU:CG	2.45	0.46
1:D:260:GLU:HG2	2:D:614:HOH:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:108:LEU:HD22	1:F:151:TYR:CD2	2.50	0.46
1:A:269:ASP:OD1	1:A:269:ASP:N	2.46	0.46
1:C:74:LYS:HD3	1:C:75:GLN:CA	2.46	0.46
1:C:472:LYS:HB3	1:C:473:LEU:HD12	1.98	0.46
1:D:120:TYR:O	1:D:124:LEU:HB2	2.15	0.46
1:E:49:LEU:HG	1:E:241:GLN:HE22	1.80	0.46
1:F:29:ASP:HA	1:F:32:ILE:CD1	2.45	0.46
1:F:171:MET:CG	1:F:191:MET:HE2	2.43	0.46
1:F:473:LEU:HD23	1:F:474:PHE:CD2	2.51	0.46
1:A:266:ASP:O	1:A:267:THR:O	2.33	0.46
1:A:342:ILE:HD11	1:A:347:ALA:HB2	1.98	0.46
1:B:297:TYR:O	1:B:303:GLY:HA2	2.16	0.46
1:C:175:ALA:O	1:C:199:MET:HA	2.16	0.46
1:C:418:MET:O	1:C:419:SER:CB	2.64	0.46
1:D:208:LYS:CE	1:D:212:GLY:HA2	2.45	0.46
1:F:275:ALA:O	1:F:277:GLY:N	2.49	0.46
1:B:269:ASP:O	1:B:271:ALA:N	2.42	0.46
1:B:296:ILE:HG13	1:B:297:TYR:N	2.19	0.46
1:B:446:ARG:CZ	1:B:446:ARG:CB	2.94	0.46
1:C:193:LYS:O	1:C:219:ASP:OD1	2.34	0.46
1:D:293:ARG:O	1:D:296:ILE:HD13	2.16	0.46
1:D:316:ILE:HD12	1:D:346:ALA:HB1	1.96	0.46
1:D:461:ASP:C	1:D:463:LEU:H	2.22	0.46
1:E:225:VAL:CG2	1:E:226:HIS:N	2.78	0.46
1:A:452:GLU:CD	1:A:452:GLU:O	2.59	0.46
1:C:171:MET:CE	1:C:173:GLY:H	2.28	0.46
1:C:217:PHE:H	1:C:217:PHE:HD2	1.63	0.46
1:D:334:ASN:ND2	1:D:336:GLU:H	2.13	0.46
1:E:281:ILE:HD12	1:E:294:GLU:OE2	2.15	0.46
1:E:393:TYR:CD2	1:E:521:ILE:HD12	2.50	0.46
1:F:72:LEU:HD11	1:F:142:GLN:HB2	1.97	0.46
1:F:180:VAL:HG21	1:F:201:VAL:HG12	1.98	0.46
1:A:447:ILE:CD1	1:D:141:ILE:HG13	2.46	0.45
1:B:72:LEU:HD11	1:B:142:GLN:HB2	1.98	0.45
1:B:168:ILE:HD13	1:B:250:LEU:HD13	1.97	0.45
1:B:208:LYS:HD2	1:B:212:GLY:C	2.42	0.45
1:B:273:ARG:HG2	1:B:497:ARG:HH12	1.82	0.45
1:B:343:ASP:HB3	1:B:374:VAL:HG12	1.97	0.45
1:B:450:ARG:CZ	1:B:453:ILE:HD13	2.46	0.45
1:B:466:ARG:CZ	1:B:467:ILE:HG12	2.46	0.45
1:C:107:SER:OG	1:C:140:ARG:CA	2.64	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:455:GLN:HE21	1:D:455:GLN:CA	2.27	0.45
1:F:6:LYS:HD2	1:F:8:PRO:CD	2.29	0.45
1:B:211:LEU:HB3	1:B:212:GLY:H	1.62	0.45
1:B:277:GLY:HA2	1:B:280:GLN:HG3	1.99	0.45
1:B:332:ALA:HB2	1:B:367:LEU:HB2	1.97	0.45
1:B:442:GLU:HA	1:B:467:ILE:CG2	2.46	0.45
1:D:257:ASN:HD22	1:D:259:MET:H	1.64	0.45
1:D:318:VAL:HG13	1:D:353:PHE:CD2	2.52	0.45
1:F:204:PRO:O	1:F:208:LYS:HG2	2.16	0.45
1:F:214:GLU:H	1:F:214:GLU:CD	2.24	0.45
1:B:442:GLU:HA	1:B:467:ILE:HG21	1.99	0.45
1:D:42:THR:OG1	1:D:45:GLU:HG3	2.16	0.45
1:D:50:LEU:HB2	1:D:244:ILE:HD13	1.99	0.45
1:E:81:GLY:HA3	2:E:558:HOH:O	2.16	0.45
1:F:6:LYS:NZ	1:F:8:PRO:C	2.74	0.45
1:F:450:ARG:C	1:F:451:LYS:HG2	2.41	0.45
1:A:225:VAL:HG23	1:A:226:HIS:N	2.30	0.45
1:C:332:ALA:HB2	1:C:367:LEU:HB2	1.99	0.45
1:E:71:GLY:O	1:E:74:LYS:NZ	2.48	0.45
1:E:174:PRO:HB2	1:E:197:TYR:CD2	2.51	0.45
1:E:225:VAL:HG23	1:E:226:HIS:N	2.30	0.45
1:E:270:PRO:C	1:E:496:ARG:HH21	2.24	0.45
1:E:504:GLU:O	1:E:507:LYS:HG2	2.17	0.45
1:F:192:ILE:HD12	1:F:192:ILE:H	1.81	0.45
1:B:196:ALA:O	1:B:197:TYR:CD1	2.69	0.45
1:C:83:VAL:O	1:C:97:TYR:HA	2.17	0.45
1:E:410:SER:OG	1:E:415:HIS:CD2	2.63	0.45
1:F:418:MET:O	1:F:419:SER:CB	2.64	0.45
1:A:449:TYR:C	1:A:450:ARG:CZ	2.89	0.45
1:B:393:TYR:HA	1:E:159:VAL:HG21	1.99	0.45
1:B:510:ARG:HE	1:B:510:ARG:HB2	1.57	0.45
1:C:34:PHE:CD2	1:C:38:LYS:NZ	2.84	0.45
1:C:490:ILE:CG1	1:C:491:GLU:N	2.80	0.45
1:D:273:ARG:N	1:D:497:ARG:HG3	2.28	0.45
1:E:60:MET:HA	2:F:603:HOH:O	2.17	0.45
1:E:135:ASP:HA	1:E:173:GLY:HA3	1.97	0.45
1:F:6:LYS:HE2	1:F:12:LEU:CG	2.46	0.45
1:A:126:VAL:HG11	1:C:505:MET:HE2	1.99	0.45
1:B:274:ASP:O	1:B:275:ALA:C	2.60	0.45
1:C:217:PHE:N	1:C:217:PHE:CD2	2.85	0.45
1:C:226:HIS:HA	1:C:230:SER:OG	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:438:VAL:HB	1:F:144:GLY:HA2	1.99	0.45
1:C:490:ILE:HG13	1:C:491:GLU:N	2.32	0.45
1:D:6:LYS:HB3	1:D:6:LYS:HZ2	1.81	0.45
1:D:342:ILE:HD11	1:D:347:ALA:HB2	1.98	0.45
1:E:6:LYS:HG2	2:E:705:HOH:O	2.16	0.45
1:E:89:VAL:HG13	1:E:94:VAL:HG13	1.99	0.45
1:F:6:LYS:HZ2	1:F:7:PRO:C	2.24	0.45
1:F:11:LYS:HZ3	1:F:15:GLU:HG3	1.82	0.45
1:A:483:LYS:HG3	1:D:146:LEU:HD21	1.97	0.45
1:A:496:ARG:HA	1:A:499:ILE:HG22	1.99	0.45
1:B:343:ASP:HB3	1:B:374:VAL:HG11	1.99	0.45
1:F:490:ILE:CG1	1:F:491:GLU:N	2.79	0.45
1:A:25:LYS:HE3	1:A:29:ASP:OD2	2.17	0.45
1:B:383:GLY:O	1:B:387:HIS:HD2	2.00	0.45
1:B:412:GLY:O	1:B:415:HIS:HB3	2.15	0.45
1:C:271:ALA:HB1	1:C:500:VAL:HG11	1.98	0.45
1:E:28:GLY:O	1:E:32:ILE:HG23	2.17	0.45
1:E:31:ARG:HG3	1:E:31:ARG:NH1	2.31	0.45
1:E:369:ASP:HA	1:E:409:LYS:O	2.17	0.45
1:A:497:ARG:CA	1:A:500:VAL:HG12	2.46	0.45
1:B:191:MET:HE3	1:B:199:MET:HG3	1.97	0.45
1:C:34:PHE:CE2	1:C:38:LYS:NZ	2.82	0.45
1:C:56:PHE:CG	1:C:57:ASN:N	2.83	0.45
1:D:273:ARG:N	1:D:497:ARG:HD3	2.32	0.45
1:D:290:TYR:CZ	1:D:335:PRO:HG2	2.52	0.45
1:E:110:GLU:HG3	2:E:697:HOH:O	2.17	0.45
1:F:273:ARG:HD2	1:F:275:ALA:HB2	1.98	0.45
1:F:316:ILE:HD12	1:F:316:ILE:O	2.17	0.45
1:A:72:LEU:O	1:A:76:ARG:NE	2.50	0.44
1:A:110:GLU:CD	1:A:146:LEU:HD12	2.42	0.44
1:A:273:ARG:HD2	1:A:274:ASP:N	2.31	0.44
1:A:490:ILE:HD11	1:A:494:ASP:OD2	2.16	0.44
1:B:257:ASN:HD21	1:B:260:GLU:CG	2.29	0.44
1:B:521:ILE:HG13	1:B:522:PRO:HD2	1.99	0.44
1:C:10:GLU:O	1:C:13:ILE:HG13	2.16	0.44
1:C:217:PHE:HD2	1:C:217:PHE:N	2.16	0.44
1:C:316:ILE:HD11	1:C:349:LYS:CD	2.47	0.44
1:C:342:ILE:HD12	1:C:346:ALA:HB3	1.99	0.44
1:E:156:LYS:O	1:E:160:MET:HG2	2.17	0.44
1:E:436:ILE:HD11	2:E:556:HOH:O	2.17	0.44
1:E:449:TYR:N	1:E:450:ARG:NH1	2.57	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:265:ILE:O	1:F:267:THR:HG23	2.16	0.44
1:A:461:ASP:O	1:A:465:GLN:HG2	2.17	0.44
1:B:456:ALA:C	1:B:458:ASN:H	2.25	0.44
1:C:209:VAL:HG12	1:C:209:VAL:O	2.18	0.44
1:D:369:ASP:CG	1:D:408:ARG:HB3	2.42	0.44
1:D:411:TYR:CD1	1:D:437:ALA:HB3	2.52	0.44
1:A:190:ILE:HD13	1:A:246:LEU:HD13	1.99	0.44
1:A:202:THR:HG21	1:D:375:PRO:HB3	1.99	0.44
1:A:272:ASP:HB3	1:A:273:ARG:HH22	1.83	0.44
1:B:57:ASN:O	1:B:85:GLY:HA3	2.17	0.44
1:B:173:GLY:HA2	1:B:197:TYR:CD2	2.53	0.44
1:B:466:ARG:CZ	1:B:467:ILE:HG13	2.47	0.44
1:C:220:LEU:HB3	1:C:221:GLY:H	1.68	0.44
1:C:431:TRP:NE1	1:C:495:THR:CG2	2.78	0.44
1:D:358:ASP:CG	1:D:398:ALA:HA	2.42	0.44
1:D:450:ARG:HB3	1:D:451:LYS:NZ	2.31	0.44
1:F:106:GLY:O	1:F:136:SER:CB	2.64	0.44
1:F:441:PRO:CG	1:F:471:ARG:HH21	2.30	0.44
1:F:512:TYR:O	1:F:513:ARG:HD3	2.17	0.44
1:A:81:GLY:HA3	2:A:533:HOH:O	2.18	0.44
1:A:158:ASN:HD22	1:A:167:GLN:HE22	1.64	0.44
1:A:450:ARG:CZ	1:A:450:ARG:CA	2.92	0.44
1:B:240:GLU:O	1:B:244:ILE:HG23	2.18	0.44
1:B:369:ASP:CG	1:B:408:ARG:HB3	2.43	0.44
1:C:75:GLN:HE21	1:C:76:ARG:N	2.15	0.44
1:C:473:LEU:HD12	1:C:473:LEU:N	2.33	0.44
1:D:208:LYS:HE3	1:D:208:LYS:CA	2.34	0.44
1:D:342:ILE:HD13	1:D:373:TYR:CE2	2.52	0.44
1:E:285:ASP:OD1	1:E:287:ALA:N	2.41	0.44
1:A:34:PHE:CZ	1:A:38:LYS:HE3	2.52	0.44
1:B:281:ILE:HD13	1:B:294:GLU:CB	2.48	0.44
1:B:342:ILE:HG12	1:B:373:TYR:CE2	2.53	0.44
1:B:393:TYR:OH	1:B:519:GLY:HA3	2.17	0.44
1:B:462:VAL:HG12	1:B:462:VAL:O	2.18	0.44
1:B:481:ALA:HA	1:B:486:VAL:HG22	1.98	0.44
1:C:497:ARG:HH11	1:C:497:ARG:CG	2.29	0.44
1:F:313:ALA:HB2	1:F:345:ASP:HB3	2.00	0.44
1:B:58:GLU:OE2	1:B:61:THR:HB	2.18	0.44
1:D:208:LYS:HA	1:D:208:LYS:CE	2.33	0.44
1:E:198:TYR:CE2	1:E:223:ALA:N	2.76	0.44
1:F:369:ASP:HA	1:F:409:LYS:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:490:ILE:HG13	1:A:491:GLU:O	2.18	0.44
1:B:405:VAL:HG21	1:B:499:ILE:HD11	2.00	0.44
1:C:28:GLY:O	1:C:31:ARG:N	2.51	0.44
1:C:485:LEU:HD11	1:F:146:LEU:HD12	2.00	0.44
1:D:225:VAL:HG13	2:D:738:HOH:O	2.17	0.44
1:D:466:ARG:O	1:D:469:GLU:HB3	2.18	0.44
1:D:493:LYS:HA	2:D:588:HOH:O	2.16	0.44
1:E:16:LEU:HD22	1:F:432:PRO:HG3	1.98	0.44
1:F:296:ILE:C	1:F:296:ILE:HD12	2.42	0.44
1:A:54:GLY:O	1:A:55:LYS:CG	2.66	0.44
1:B:273:ARG:HG3	1:B:497:ARG:CZ	2.47	0.44
1:C:34:PHE:CE1	1:C:38:LYS:CB	3.01	0.44
1:C:479:TRP:HZ3	1:F:145:ALA:HB3	1.82	0.44
1:E:89:VAL:O	1:E:89:VAL:HG23	2.16	0.44
1:F:474:PHE:O	1:F:476:ASN:N	2.45	0.44
1:B:281:ILE:CD1	1:B:294:GLU:HB3	2.48	0.44
1:B:466:ARG:NH1	1:B:467:ILE:CG1	2.79	0.44
1:C:160:MET:HA	1:C:160:MET:CE	2.45	0.44
1:C:160:MET:HG3	1:F:514:TYR:HD2	1.83	0.44
1:D:67:ALA:HB3	1:D:72:LEU:HD23	1.99	0.44
1:D:82:VAL:O	1:D:115:LYS:NZ	2.50	0.44
1:D:407:VAL:HG23	1:D:431:TRP:CE3	2.53	0.44
1:E:418:MET:O	1:E:419:SER:CB	2.66	0.44
1:F:467:ILE:O	1:F:471:ARG:HG3	2.18	0.44
1:A:76:ARG:HG2	1:A:76:ARG:HH21	1.83	0.43
1:A:432:PRO:HD3	1:A:490:ILE:O	2.18	0.43
1:B:7:PRO:N	1:B:8:PRO:HD2	2.32	0.43
1:B:466:ARG:N	1:B:466:ARG:HH21	2.15	0.43
1:C:197:TYR:CE2	1:C:219:ASP:OD1	2.70	0.43
1:C:276:THR:O	1:C:277:GLY:C	2.61	0.43
1:E:6:LYS:C	1:E:8:PRO:HD2	2.43	0.43
1:F:89:VAL:O	1:F:89:VAL:CG2	2.63	0.43
1:A:399:THR:CG2	1:A:513:ARG:NE	2.81	0.43
1:B:6:LYS:HG3	1:B:11:LYS:CD	2.47	0.43
1:B:19:LEU:O	1:B:22:LYS:HB3	2.17	0.43
1:B:244:ILE:O	1:B:248:LYS:HG3	2.19	0.43
1:B:265:ILE:O	1:B:266:ASP:HB2	2.18	0.43
1:B:460:ASP:OD1	1:B:460:ASP:O	2.36	0.43
1:C:182:SER:N	1:C:183:PRO:CD	2.81	0.43
1:C:431:TRP:NE1	1:C:495:THR:HG21	2.34	0.43
1:D:31:ARG:HB3	1:D:102:THR:HB	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:151:TYR:O	1:E:154:VAL:CG1	2.66	0.43
1:E:430:ALA:O	1:E:489:VAL:HA	2.17	0.43
1:F:257:ASN:HD21	1:F:259:MET:HB2	1.81	0.43
1:F:434:ALA:HB3	1:F:477:PRO:CG	2.35	0.43
1:B:14:GLU:HG3	2:B:722:HOH:O	2.17	0.43
1:C:451:LYS:O	1:C:454:GLN:HG3	2.17	0.43
1:C:513:ARG:HG2	2:C:698:HOH:O	2.18	0.43
1:D:241:GLN:NE2	1:D:241:GLN:N	2.57	0.43
1:D:369:ASP:HB2	1:D:407:VAL:HG13	2.00	0.43
1:E:342:ILE:HG23	1:E:373:TYR:CD2	2.53	0.43
1:E:504:GLU:HG2	1:E:507:LYS:HE3	2.00	0.43
1:F:257:ASN:HD21	1:F:260:GLU:HG3	1.84	0.43
1:A:169:THR:CG2	1:A:186:THR:OG1	2.66	0.43
1:C:205:GLU:OE1	1:C:205:GLU:N	2.47	0.43
1:F:29:ASP:CA	1:F:32:ILE:HG12	2.46	0.43
1:F:445:VAL:HG13	1:F:449:TYR:HD1	1.83	0.43
1:A:464:LYS:NZ	1:A:464:LYS:CB	2.80	0.43
1:B:20:LYS:HD2	1:B:62:PHE:HZ	1.84	0.43
1:C:312:TRP:O	1:C:313:ALA:C	2.60	0.43
1:C:316:ILE:CG1	1:C:346:ALA:HB1	2.49	0.43
1:C:512:TYR:C	1:C:513:ARG:HG3	2.42	0.43
1:B:195:ASP:O	1:B:196:ALA:C	2.61	0.43
1:B:241:GLN:HE21	1:B:241:GLN:N	2.09	0.43
1:D:16:LEU:HD11	1:D:20:LYS:HE3	1.99	0.43
1:D:493:LYS:HD2	1:D:493:LYS:N	2.28	0.43
1:E:16:LEU:HD11	1:E:20:LYS:HE3	1.99	0.43
1:E:412:GLY:O	1:E:415:HIS:HB3	2.19	0.43
1:F:11:LYS:NZ	1:F:15:GLU:HG3	2.33	0.43
1:F:490:ILE:CD1	1:F:498:VAL:CG2	2.93	0.43
1:A:7:PRO:CG	1:A:8:PRO:CD	2.95	0.43
1:B:180:VAL:HG22	1:E:385:ILE:HG23	2.00	0.43
1:C:208:LYS:HA	1:C:211:LEU:HD21	2.01	0.43
1:D:197:TYR:C	1:D:198:TYR:CD2	2.97	0.43
1:E:74:LYS:CE	1:E:74:LYS:H	2.30	0.43
1:F:7:PRO:HG2	1:F:8:PRO:HD3	2.01	0.43
1:F:182:SER:N	1:F:183:PRO:CD	2.82	0.43
1:F:316:ILE:HD11	1:F:349:LYS:CG	2.49	0.43
1:B:434:ALA:HB3	1:B:477:PRO:HB3	2.01	0.43
1:C:265:ILE:O	1:C:266:ASP:HB2	2.19	0.43
1:C:462:VAL:O	1:C:464:LYS:N	2.49	0.43
1:D:466:ARG:HH11	1:D:469:GLU:CB	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:214:GLU:O	1:F:215:VAL:O	2.37	0.43
1:F:275:ALA:C	1:F:277:GLY:H	2.26	0.43
1:B:318:VAL:HB	1:B:353:PHE:CD2	2.53	0.43
1:D:59:ILE:O	1:D:60:MET:C	2.62	0.43
1:D:75:GLN:HB3	2:D:745:HOH:O	2.19	0.43
1:E:273:ARG:CG	1:E:493:LYS:O	2.66	0.43
1:F:206:ILE:HG13	1:F:207:THR:N	2.32	0.43
1:F:473:LEU:CD2	1:F:474:PHE:CD2	3.02	0.43
1:B:291:ASN:ND2	1:B:293:ARG:HB2	2.34	0.43
1:B:458:ASN:ND2	1:B:462:VAL:HG11	2.34	0.43
1:C:257:ASN:HD22	1:C:259:MET:N	2.00	0.43
1:D:199:MET:O	1:D:221:GLY:HA3	2.18	0.43
1:D:344:ILE:HG13	1:D:379:GLN:HE22	1.84	0.43
1:E:282:VAL:HA	1:E:283:PRO:HD3	1.87	0.43
1:F:272:ASP:OD2	1:F:272:ASP:C	2.61	0.43
1:A:141:ILE:HD11	2:A:610:HOH:O	2.18	0.42
1:A:496:ARG:C	1:A:499:ILE:HG22	2.43	0.42
1:B:180:VAL:HG21	1:E:385:ILE:HD13	2.01	0.42
1:C:214:GLU:N	1:C:214:GLU:OE1	2.51	0.42
1:D:174:PRO:HB3	1:D:197:TYR:CE2	2.54	0.42
1:D:276:THR:HA	2:D:588:HOH:O	2.18	0.42
1:E:52:ASP:O	1:E:53:ASP:C	2.62	0.42
1:E:175:ALA:N	1:E:198:TYR:O	2.50	0.42
1:E:393:TYR:OH	1:E:519:GLY:HA3	2.19	0.42
1:E:432:PRO:HD3	1:E:490:ILE:O	2.19	0.42
1:F:276:THR:HA	1:F:279:GLU:OE2	2.19	0.42
1:A:296:ILE:HG13	1:A:297:TYR:N	2.33	0.42
1:C:30:GLU:CB	1:C:31:ARG:HE	2.30	0.42
1:C:215:VAL:CB	1:C:220:LEU:HG	2.48	0.42
1:C:516:LYS:HE2	1:F:164:VAL:CG2	2.48	0.42
1:D:275:ALA:O	1:D:276:THR:O	2.37	0.42
1:B:452:GLU:O	1:B:452:GLU:HG2	2.19	0.42
1:C:191:MET:CE	1:C:198:TYR:HA	2.49	0.42
1:C:247:THR:HG22	1:C:251:LEU:HD23	2.01	0.42
1:C:464:LYS:C	1:C:466:ARG:N	2.76	0.42
1:E:74:LYS:CE	1:E:75:GLN:N	2.67	0.42
1:E:449:TYR:N	1:E:450:ARG:HE	2.17	0.42
1:F:15:GLU:O	1:F:19:LEU:HD13	2.19	0.42
1:F:274:ASP:O	1:F:277:GLY:HA3	2.19	0.42
1:F:357:CYS:HB2	1:F:364:LEU:HD11	2.01	0.42
1:A:109:GLY:N	1:A:112:HIS:HB3	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:412:GLY:O	1:A:415:HIS:HB3	2.18	0.42
1:A:504:GLU:O	1:A:507:LYS:HG2	2.20	0.42
1:C:471:ARG:HA	1:C:475:ALA:HB2	2.00	0.42
1:D:277:GLY:O	1:D:280:GLN:HB2	2.19	0.42
1:D:502:GLY:O	1:D:506:LEU:HD22	2.19	0.42
1:E:32:ILE:HD12	1:E:36:HIS:CE1	2.54	0.42
1:E:244:ILE:HD12	1:E:244:ILE:O	2.20	0.42
1:E:476:ASN:HB2	1:E:477:PRO:HD2	2.01	0.42
1:A:54:GLY:O	1:A:55:LYS:CD	2.67	0.42
1:A:516:LYS:HA	1:D:258:ASN:HD21	1.84	0.42
1:C:29:ASP:HA	1:C:32:ILE:HD13	2.00	0.42
1:C:36:HIS:CE1	1:C:45:GLU:OE2	2.73	0.42
1:C:215:VAL:HG11	1:C:220:LEU:HG	2.01	0.42
1:D:418:MET:O	1:D:419:SER:HB3	2.19	0.42
1:D:439:THR:HG22	1:D:440:GLY:H	1.84	0.42
1:E:151:TYR:O	1:E:154:VAL:HG12	2.19	0.42
1:E:228:THR:OG1	1:E:229:LYS:CD	2.67	0.42
1:E:490:ILE:HG13	1:E:491:GLU:O	2.20	0.42
1:F:35:GLN:O	1:F:40:LYS:HG2	2.19	0.42
1:B:180:VAL:HG21	1:E:385:ILE:CD1	2.50	0.42
1:B:257:ASN:HD22	1:B:259:MET:N	2.12	0.42
1:B:334:ASN:ND2	2:B:618:HOH:O	2.51	0.42
1:C:6:LYS:NZ	1:C:8:PRO:HG2	2.34	0.42
1:C:502:GLY:O	1:C:506:LEU:HG	2.20	0.42
1:D:246:LEU:HD23	1:D:246:LEU:C	2.45	0.42
1:F:191:MET:HE3	1:F:191:MET:HB2	1.87	0.42
1:F:241:GLN:H	1:F:241:GLN:NE2	2.17	0.42
1:A:146:LEU:HD21	1:D:483:LYS:CB	2.50	0.42
1:A:193:LYS:HB3	1:A:223:ALA:HB3	2.01	0.42
1:A:272:ASP:C	1:A:273:ARG:NH2	2.78	0.42
1:B:369:ASP:HA	1:B:409:LYS:O	2.20	0.42
1:C:46:ARG:HH12	1:C:135:ASP:HB2	1.85	0.42
1:C:141:ILE:HG12	2:C:588:HOH:O	2.18	0.42
1:C:156:LYS:HE2	2:F:733:HOH:O	2.19	0.42
1:C:316:ILE:HD12	1:C:316:ILE:C	2.45	0.42
1:C:316:ILE:HD11	1:C:349:LYS:CG	2.50	0.42
1:C:344:ILE:HG12	1:C:345:ASP:N	2.34	0.42
1:D:282:VAL:HA	1:D:283:PRO:HD3	1.82	0.42
1:D:334:ASN:C	1:D:334:ASN:HD22	2.28	0.42
1:F:29:ASP:O	1:F:32:ILE:HG12	2.18	0.42
1:F:269:ASP:OD1	1:F:270:PRO:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:497:ARG:CG	1:A:497:ARG:NH1	2.80	0.42
1:B:197:TYR:HB3	1:B:198:TYR:H	1.67	0.42
1:B:204:PRO:HB3	1:B:215:VAL:CG1	2.48	0.42
1:B:385:ILE:HG22	1:E:184:ALA:HB2	2.01	0.42
1:D:198:TYR:CE2	1:D:218:GLN:OE1	2.72	0.42
1:E:72:LEU:HD21	1:E:142:GLN:HB3	2.01	0.42
1:E:495:THR:O	1:E:499:ILE:HG22	2.19	0.42
1:F:332:ALA:HB2	1:F:367:LEU:HB2	2.01	0.42
1:C:84:THR:HG22	1:C:97:TYR:CB	2.49	0.42
1:C:267:THR:HA	2:C:560:HOH:O	2.19	0.42
1:D:25:LYS:HA	1:D:25:LYS:HD3	1.92	0.42
1:D:455:GLN:CA	1:D:455:GLN:NE2	2.80	0.42
1:E:155:PHE:CZ	1:E:181:TYR:HB2	2.55	0.42
1:F:6:LYS:NZ	1:F:8:PRO:N	2.68	0.42
1:F:273:ARG:C	1:F:274:ASP:OD2	2.63	0.42
1:B:112:HIS:CD2	1:B:112:HIS:C	2.97	0.42
1:B:180:VAL:HG22	1:E:385:ILE:CG2	2.50	0.42
1:B:227:ALA:O	1:B:312:TRP:HB2	2.20	0.42
1:B:237:VAL:HG21	1:B:242:GLU:CB	2.49	0.42
1:D:50:LEU:HD13	1:D:244:ILE:CD1	2.49	0.42
1:D:227:ALA:O	1:D:312:TRP:HB2	2.20	0.42
1:F:6:LYS:NZ	1:F:8:PRO:O	2.50	0.42
1:A:418:MET:O	1:A:419:SER:CB	2.68	0.41
1:A:494:ASP:O	1:A:497:ARG:NH1	2.52	0.41
1:B:208:LYS:HD3	1:B:214:GLU:N	2.35	0.41
1:B:291:ASN:HD22	1:B:294:GLU:HG3	1.85	0.41
1:B:443:GLY:O	1:B:447:ILE:HG23	2.20	0.41
1:C:112:HIS:C	1:C:112:HIS:CD2	2.98	0.41
1:D:351:ALA:O	1:D:355:ARG:HG3	2.19	0.41
1:E:228:THR:HG22	1:E:311:HIS:CB	2.47	0.41
1:E:323:ILE:HG21	1:E:499:ILE:HD12	2.01	0.41
1:F:203:GLY:O	1:F:207:THR:HG23	2.20	0.41
1:F:316:ILE:HG12	1:F:346:ALA:HB1	2.02	0.41
1:B:226:HIS:HA	1:B:230:SER:OG	2.20	0.41
1:B:451:LYS:HA	1:B:451:LYS:HZ2	1.77	0.41
1:B:464:LYS:CG	1:B:464:LYS:O	2.67	0.41
1:F:447:ILE:HD12	1:F:447:ILE:N	2.36	0.41
1:A:54:GLY:O	1:A:55:LYS:HD3	2.19	0.41
1:A:278:VAL:HG13	1:A:279:GLU:N	2.35	0.41
1:C:55:LYS:HB3	1:C:55:LYS:HZ2	1.85	0.41
1:C:257:ASN:HD21	1:C:259:MET:HB2	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:206:ILE:HD13	1:D:206:ILE:C	2.45	0.41
1:E:283:PRO:C	1:E:285:ASP:N	2.78	0.41
1:F:128:ALA:N	1:F:165:ILE:HD13	2.35	0.41
1:F:257:ASN:ND2	1:F:260:GLU:HG3	2.35	0.41
1:F:296:ILE:HD12	1:F:296:ILE:O	2.20	0.41
1:A:342:ILE:HG23	1:A:373:TYR:CD2	2.56	0.41
1:A:365:ILE:HD11	1:A:499:ILE:HD11	2.02	0.41
1:A:369:ASP:CG	1:A:408:ARG:HB3	2.45	0.41
1:B:193:LYS:O	1:B:193:LYS:HG2	2.19	0.41
1:C:6:LYS:HE3	1:C:8:PRO:HD2	2.03	0.41
1:C:435:GLU:CD	1:C:475:ALA:HB1	2.46	0.41
1:D:323:ILE:O	1:D:324:ALA:HB3	2.21	0.41
1:E:168:ILE:CD1	1:E:250:LEU:HD23	2.50	0.41
1:E:228:THR:C	1:E:229:LYS:HD2	2.45	0.41
1:E:312:TRP:O	1:E:313:ALA:C	2.64	0.41
1:F:507:LYS:HD2	2:F:743:HOH:O	2.19	0.41
1:A:179:ALA:HB1	2:A:667:HOH:O	2.21	0.41
1:A:256:SER:HB2	1:A:260:GLU:OE1	2.20	0.41
1:B:208:LYS:HD2	1:B:212:GLY:HA2	2.03	0.41
1:C:46:ARG:HD3	1:C:133:ILE:HG21	2.01	0.41
1:C:247:THR:O	1:C:251:LEU:HD23	2.20	0.41
1:C:376:GLY:HA3	2:C:655:HOH:O	2.19	0.41
1:C:451:LYS:CD	1:C:452:GLU:N	2.83	0.41
1:E:9:VAL:HG13	1:E:10:GLU:N	2.36	0.41
1:F:177:GLY:O	1:F:180:VAL:HG22	2.21	0.41
1:F:191:MET:HE3	1:F:233:VAL:HG22	2.02	0.41
1:F:490:ILE:HG12	1:F:491:GLU:H	1.85	0.41
1:A:358:ASP:CG	1:A:398:ALA:HA	2.46	0.41
1:B:495:THR:HA	1:B:498:VAL:CG1	2.50	0.41
1:C:171:MET:HE1	2:C:689:HOH:O	2.19	0.41
1:C:497:ARG:HD2	1:C:497:ARG:C	2.45	0.41
1:D:255:PRO:HB2	1:D:260:GLU:HB3	2.03	0.41
1:F:89:VAL:O	1:F:89:VAL:HG22	2.20	0.41
1:F:273:ARG:CB	1:F:497:ARG:HH12	2.09	0.41
1:F:312:TRP:O	1:F:313:ALA:C	2.63	0.41
1:F:393:TYR:C	1:F:393:TYR:CD2	2.99	0.41
1:F:512:TYR:CD1	1:F:512:TYR:N	2.88	0.41
1:A:190:ILE:CD1	1:A:246:LEU:HD13	2.50	0.41
1:A:392:LEU:HD23	1:A:417:ALA:HA	2.01	0.41
1:A:450:ARG:CZ	1:A:450:ARG:N	2.84	0.41
1:C:160:MET:HE2	2:F:544:HOH:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:358:ASP:HA	1:C:400:VAL:HG11	2.03	0.41
1:D:17:ARG:HG2	2:E:614:HOH:O	2.21	0.41
1:D:198:TYR:HB2	1:D:199:MET:H	1.72	0.41
1:D:399:THR:HG22	1:D:513:ARG:NH1	2.36	0.41
1:D:418:MET:O	1:D:419:SER:CB	2.67	0.41
1:D:453:ILE:O	1:D:454:GLN:HG3	2.21	0.41
1:D:464:LYS:O	1:D:467:ILE:HG12	2.21	0.41
1:E:344:ILE:CD1	1:E:382:LYS:HB2	2.50	0.41
1:F:15:GLU:HA	1:F:18:GLN:HE21	1.86	0.41
1:F:129:PRO:HA	1:F:165:ILE:HG23	2.01	0.41
1:F:157:MET:HE3	2:F:573:HOH:O	2.19	0.41
1:F:273:ARG:CD	1:F:275:ALA:HB2	2.50	0.41
1:F:318:VAL:HG13	1:F:353:PHE:CD1	2.56	0.41
1:A:109:GLY:O	1:A:112:HIS:HB3	2.21	0.41
1:A:146:LEU:HD23	1:D:479:TRP:CZ3	2.56	0.41
1:A:467:ILE:O	1:A:471:ARG:HG3	2.21	0.41
1:B:225:VAL:CG2	1:B:226:HIS:N	2.84	0.41
1:B:392:LEU:HD23	1:B:417:ALA:HA	2.02	0.41
1:B:458:ASN:HA	1:B:459:PRO:HD3	1.84	0.41
1:E:200:PHE:CE1	1:E:203:GLY:HA2	2.55	0.41
1:F:71:GLY:O	1:F:74:LYS:HB3	2.21	0.41
1:A:177:GLY:O	1:A:180:VAL:HB	2.21	0.41
1:A:274:ASP:HB2	1:A:275:ALA:H	1.46	0.41
1:A:490:ILE:CG1	1:A:494:ASP:HB2	2.51	0.41
1:B:146:LEU:HD22	1:E:479:TRP:CH2	2.56	0.41
1:B:429:TYR:OH	1:C:57:ASN:ND2	2.54	0.41
1:B:449:TYR:O	1:B:453:ILE:HG22	2.21	0.41
1:B:495:THR:O	1:B:498:VAL:HG13	2.21	0.41
1:C:220:LEU:C	1:C:222:GLY:H	2.29	0.41
1:C:276:THR:O	1:C:276:THR:HG23	2.20	0.41
1:C:344:ILE:HG12	1:C:345:ASP:OD1	2.21	0.41
1:C:494:ASP:O	1:C:498:VAL:HG23	2.21	0.41
1:D:344:ILE:H	1:D:379:GLN:HE22	1.68	0.41
1:D:372:GLY:HA2	1:D:414:ALA:HB2	2.03	0.41
1:D:466:ARG:HB3	1:D:469:GLU:OE2	2.20	0.41
1:E:22:LYS:HG3	2:E:715:HOH:O	2.19	0.41
1:E:49:LEU:HD13	2:E:612:HOH:O	2.21	0.41
1:E:190:ILE:HD13	1:E:246:LEU:HD13	2.02	0.41
1:F:171:MET:CE	1:F:173:GLY:H	2.30	0.41
1:F:212:GLY:O	1:F:213:GLU:HG3	2.21	0.41
1:F:369:ASP:OD1	1:F:408:ARG:HB3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:490:ILE:CD1	1:F:494:ASP:HB2	2.48	0.41
1:A:108:LEU:HD22	1:A:151:TYR:CG	2.56	0.41
1:A:191:MET:SD	1:A:199:MET:HE2	2.61	0.41
1:C:7:PRO:HG2	1:C:8:PRO:CD	2.46	0.41
1:C:171:MET:HE2	1:C:173:GLY:H	1.85	0.41
1:D:68:THR:HA	1:D:73:ASP:HB3	2.03	0.41
1:A:57:ASN:O	1:A:85:GLY:HA3	2.21	0.40
1:B:20:LYS:HD2	1:B:62:PHE:CZ	2.56	0.40
1:B:300:VAL:HA	1:B:323:ILE:HD13	2.03	0.40
1:B:321:ALA:O	1:B:327:VAL:HA	2.21	0.40
1:B:451:LYS:HZ1	1:B:454:GLN:HE22	1.69	0.40
1:C:262:PRO:HB2	1:C:327:VAL:CG2	2.51	0.40
1:C:481:ALA:CA	1:C:486:VAL:HG22	2.47	0.40
1:D:281:ILE:CD1	1:D:294:GLU:HG2	2.51	0.40
1:D:461:ASP:OD2	1:D:465:GLN:NE2	2.53	0.40
1:E:198:TYR:CE2	1:E:218:GLN:NE2	2.89	0.40
1:F:214:GLU:O	1:F:215:VAL:C	2.64	0.40
1:F:441:PRO:O	1:F:445:VAL:HG23	2.21	0.40
1:F:442:GLU:HB2	1:F:467:ILE:HD11	2.03	0.40
1:A:446:ARG:O	1:A:450:ARG:CZ	2.69	0.40
1:B:310:LYS:HG2	1:B:311:HIS:CE1	2.56	0.40
1:C:285:ASP:OD1	1:C:288:LYS:NZ	2.51	0.40
1:C:439:THR:CG2	1:C:444:ALA:HB2	2.51	0.40
1:D:6:LYS:HB3	1:D:6:LYS:HZ3	1.85	0.40
1:D:266:ASP:O	1:D:266:ASP:OD1	2.39	0.40
1:D:432:PRO:HG3	1:F:16:LEU:HD22	2.02	0.40
1:E:178:GLY:C	1:E:180:VAL:H	2.29	0.40
1:E:204:PRO:HG2	1:E:217:PHE:CD2	2.56	0.40
1:A:273:ARG:NH1	1:A:497:ARG:CD	2.84	0.40
1:B:271:ALA:O	1:B:272:ASP:CG	2.65	0.40
1:C:451:LYS:HD2	1:C:451:LYS:C	2.46	0.40
1:D:445:VAL:HG21	1:D:467:ILE:CD1	2.46	0.40
1:E:448:LEU:HD12	1:E:449:TYR:N	2.36	0.40
1:E:471:ARG:O	1:E:475:ALA:HB3	2.21	0.40
1:F:464:LYS:NZ	1:F:464:LYS:HB3	2.36	0.40
1:F:491:GLU:O	1:F:492:PRO:C	2.64	0.40
1:B:280:GLN:NE2	2:B:671:HOH:O	2.54	0.40
1:B:374:VAL:HG13	1:B:374:VAL:O	2.21	0.40
1:B:464:LYS:O	1:B:464:LYS:HD2	2.21	0.40
1:C:270:PRO:HG2	1:C:496:ARG:HH21	1.86	0.40
1:C:385:ILE:HG22	1:F:184:ALA:HB2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:269:ASP:C	1:D:271:ALA:N	2.78	0.40
1:E:244:ILE:CD1	1:E:248:LYS:HE3	2.52	0.40
1:F:342:ILE:HG13	1:F:343:ASP:N	2.35	0.40
1:A:33:GLN:HB2	2:A:690:HOH:O	2.21	0.40
1:A:237:VAL:HG22	1:A:238:ASP:H	1.85	0.40
1:A:258:ASN:O	1:A:259:MET:HE2	2.22	0.40
1:A:449:TYR:H	1:A:450:ARG:NH1	2.14	0.40
1:A:451:LYS:N	1:A:451:LYS:CD	2.82	0.40
1:B:59:ILE:O	1:B:60:MET:C	2.62	0.40
1:B:445:VAL:C	1:B:447:ILE:N	2.79	0.40
1:C:32:ILE:C	1:C:34:PHE:N	2.77	0.40
1:C:70:PHE:CZ	1:F:448:LEU:HD13	2.56	0.40
1:F:382:LYS:HE2	1:F:382:LYS:HB3	1.87	0.40

There are no symmetry-related clashes.

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	516/522 (99%)	471 (91%)	31 (6%)	14 (3%)	4	2
1	B	516/522 (99%)	471 (91%)	30 (6%)	15 (3%)	3	2
1	C	516/522 (99%)	461 (89%)	37 (7%)	18 (4%)	3	1
1	D	516/522 (99%)	474 (92%)	25 (5%)	17 (3%)	3	1
1	E	516/522 (99%)	468 (91%)	37 (7%)	11 (2%)	5	3
1	F	516/522 (99%)	479 (93%)	25 (5%)	12 (2%)	5	3
All	All	3096/3132 (99%)	2824 (91%)	185 (6%)	87 (3%)	4	2

All (87) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	7	PRO
1	A	52	ASP
1	A	267	THR
1	A	270	PRO
1	A	273	ARG
1	A	459	PRO
1	B	194	GLY
1	B	265	ILE
1	B	464	LYS
1	C	195	ASP
1	C	216	SER
1	C	266	ASP
1	C	267	THR
1	C	453	ILE
1	D	197	TYR
1	D	266	ASP
1	D	267	THR
1	D	273	ARG
1	D	276	THR
1	E	52	ASP
1	E	196	ALA
1	E	197	TYR
1	E	273	ARG
1	E	274	ASP
1	E	276	THR
1	F	215	VAL
1	F	270	PRO
1	F	275	ALA
1	F	459	PRO
1	A	53	ASP
1	B	196	ALA
1	B	276	THR
1	C	27	GLY
1	C	277	GLY
1	C	464	LYS
1	D	265	ILE
1	D	268	GLY
1	D	442	GLU
1	D	454	GLN
1	D	457	SER
1	E	53	ASP
1	E	265	ILE
1	F	212	GLY

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Mol	Chain	Res	Type
1	F	276	THR
1	A	419	SER
1	B	267	THR
1	B	275	ALA
1	B	419	SER
1	C	37	SER
1	C	211	LEU
1	C	212	GLY
1	C	419	SER
1	C	452	GLU
1	D	419	SER
1	E	419	SER
1	F	269	ASP
1	F	419	SER
1	A	275	ALA
1	A	369	ASP
1	B	207	THR
1	B	459	PRO
1	C	7	PRO
1	C	56	PHE
1	C	219	ASP
1	D	286	ALA
1	D	450	ARG
1	A	174	PRO
1	A	210	VAL
1	A	266	ASP
1	B	266	ASP
1	B	457	SER
1	C	77	PHE
1	C	302	ASN
1	D	196	ALA
1	D	198	TYR
1	D	270	PRO
1	E	518	HIS
1	F	278	VAL
1	F	302	ASN
1	F	475	ALA
1	A	458	ASN
1	B	277	GLY
1	B	462	VAL
1	D	462	VAL
1	F	268	GLY

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Mol	Chain	Res	Type
1	B	7	PRO
1	E	174	PRO

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	413/416 (99%)	370 (90%)	43 (10%)	7	7
1	B	413/416 (99%)	373 (90%)	40 (10%)	8	8
1	C	413/416 (99%)	368 (89%)	45 (11%)	6	6
1	D	413/416 (99%)	373 (90%)	40 (10%)	8	8
1	E	413/416 (99%)	368 (89%)	45 (11%)	6	6
1	F	413/416 (99%)	373 (90%)	40 (10%)	8	8
All	All	2478/2496 (99%)	2225 (90%)	253 (10%)	7	7

All (253) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	LYS
1	A	11	LYS
1	A	21	GLU
1	A	32	ILE
1	A	49	LEU
1	A	61	THR
1	A	68	THR
1	A	94	VAL
1	A	108	LEU
1	A	131	VAL
1	A	141	ILE
1	A	154	VAL
1	A	180	VAL
1	A	215	VAL
1	A	244	ILE
1	A	246	LEU

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Mol	Chain	Res	Type
1	A	266	ASP
1	A	269	ASP
1	A	273	ARG
1	A	274	ASP
1	A	276	THR
1	A	304	GLU
1	A	316	ILE
1	A	342	ILE
1	A	352	ARG
1	A	354	ILE
1	A	423	LEU
1	A	435	GLU
1	A	450	ARG
1	A	451	LYS
1	A	452	GLU
1	A	455	GLN
1	A	458	ASN
1	A	459	PRO
1	A	463	LEU
1	A	464	LYS
1	A	467	ILE
1	A	472	LYS
1	A	486	VAL
1	A	497	ARG
1	A	498	VAL
1	A	499	ILE
1	A	513	ARG
1	B	13	ILE
1	B	14	GLU
1	B	32	ILE
1	B	61	THR
1	B	94	VAL
1	B	124	LEU
1	B	146	LEU
1	B	169	THR
1	B	210	VAL
1	B	211	LEU
1	B	214	GLU
1	B	225	VAL
1	B	241	GLN
1	B	244	ILE
1	B	250	LEU

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Mol	Chain	Res	Type
1	B	257	ASN
1	B	296	ILE
1	B	304	GLU
1	B	309	HIS
1	B	310	LYS
1	B	315	ASN
1	B	317	ILE
1	B	327	VAL
1	B	342	ILE
1	B	352	ARG
1	B	365	ILE
1	B	436	ILE
1	B	446	ARG
1	B	447	ILE
1	B	448	LEU
1	B	450	ARG
1	B	451	LYS
1	B	453	ILE
1	B	461	ASP
1	B	465	GLN
1	B	466	ARG
1	B	473	LEU
1	B	486	VAL
1	B	498	VAL
1	B	505	MET
1	C	6	LYS
1	C	11	LYS
1	C	31	ARG
1	C	32	ILE
1	C	33	GLN
1	C	38	LYS
1	C	55	LYS
1	C	75	GLN
1	C	76	ARG
1	C	108	LEU
1	C	160	MET
1	C	169	THR
1	C	205	GLU
1	C	206	ILE
1	C	207	THR
1	C	211	LEU
1	C	213	GLU

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Mol	Chain	Res	Type
1	C	214	GLU
1	C	215	VAL
1	C	217	PHE
1	C	218	GLN
1	C	220	LEU
1	C	264	TYR
1	C	288	LYS
1	C	296	ILE
1	C	298	LYS
1	C	304	GLU
1	C	315	ASN
1	C	318	VAL
1	C	327	VAL
1	C	342	ILE
1	C	344	ILE
1	C	377	THR
1	C	407	VAL
1	C	427	LEU
1	C	436	ILE
1	C	448	LEU
1	C	450	ARG
1	C	451	LYS
1	C	453	ILE
1	C	454	GLN
1	C	462	VAL
1	C	472	LYS
1	C	476	ASN
1	C	497	ARG
1	D	6	LYS
1	D	13	ILE
1	D	19	LEU
1	D	32	ILE
1	D	61	THR
1	D	68	THR
1	D	88	LYS
1	D	94	VAL
1	D	142	GLN
1	D	169	THR
1	D	197	TYR
1	D	206	ILE
1	D	208	LYS
1	D	241	GLN

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Mol	Chain	Res	Type
1	D	244	ILE
1	D	251	LEU
1	D	257	ASN
1	D	260	GLU
1	D	274	ASP
1	D	288	LYS
1	D	294	GLU
1	D	296	ILE
1	D	315	ASN
1	D	318	VAL
1	D	342	ILE
1	D	352	ARG
1	D	427	LEU
1	D	436	ILE
1	D	442	GLU
1	D	448	LEU
1	D	451	LYS
1	D	452	GLU
1	D	455	GLN
1	D	461	ASP
1	D	463	LEU
1	D	467	ILE
1	D	473	LEU
1	D	493	LYS
1	D	506	LEU
1	D	521	ILE
1	E	6	LYS
1	E	32	ILE
1	E	49	LEU
1	E	53	ASP
1	E	61	THR
1	E	68	THR
1	E	74	LYS
1	E	89	VAL
1	E	94	VAL
1	E	130	VAL
1	E	131	VAL
1	E	146	LEU
1	E	180	VAL
1	E	197	TYR
1	E	207	THR
1	E	208	LYS

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Mol	Chain	Res	Type
1	E	209	VAL
1	E	211	LEU
1	E	215	VAL
1	E	244	ILE
1	E	246	LEU
1	E	259	MET
1	E	273	ARG
1	E	276	THR
1	E	278	VAL
1	E	299	ILE
1	E	316	ILE
1	E	318	VAL
1	E	327	VAL
1	E	342	ILE
1	E	344	ILE
1	E	436	ILE
1	E	450	ARG
1	E	452	GLU
1	E	454	GLN
1	E	455	GLN
1	E	458	ASN
1	E	460	ASP
1	E	461	ASP
1	E	462	VAL
1	E	464	LYS
1	E	469	GLU
1	E	486	VAL
1	E	498	VAL
1	E	499	ILE
1	F	6	LYS
1	F	10	GLU
1	F	66	ARG
1	F	89	VAL
1	F	108	LEU
1	F	124	LEU
1	F	126	VAL
1	F	146	LEU
1	F	165	ILE
1	F	169	THR
1	F	185	LEU
1	F	205	GLU
1	F	206	ILE

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Mol	Chain	Res	Type
1	F	209	VAL
1	F	211	LEU
1	F	214	GLU
1	F	241	GLN
1	F	244	ILE
1	F	250	LEU
1	F	251	LEU
1	F	270	PRO
1	F	273	ARG
1	F	288	LYS
1	F	296	ILE
1	F	315	ASN
1	F	318	VAL
1	F	327	VAL
1	F	342	ILE
1	F	364	LEU
1	F	407	VAL
1	F	427	LEU
1	F	436	ILE
1	F	446	ARG
1	F	453	ILE
1	F	455	GLN
1	F	459	PRO
1	F	464	LYS
1	F	473	LEU
1	F	492	PRO
1	F	512	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (87) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	GLN
1	A	57	ASN
1	A	158	ASN
1	A	167	GLN
1	A	241	GLN
1	A	280	GLN
1	A	284	ASN
1	A	326	ASN
1	A	333	ASN
1	A	334	ASN
1	A	415	HIS

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Mol	Chain	Res	Type
1	A	454	GLN
1	A	455	GLN
1	A	458	ASN
1	A	465	GLN
1	A	518	HIS
1	B	18	GLN
1	B	57	ASN
1	B	99	GLN
1	B	112	HIS
1	B	158	ASN
1	B	241	GLN
1	B	245	ASN
1	B	257	ASN
1	B	291	ASN
1	B	302	ASN
1	B	326	ASN
1	B	334	ASN
1	B	379	GLN
1	B	387	HIS
1	B	415	HIS
1	B	454	GLN
1	B	455	GLN
1	B	458	ASN
1	B	465	GLN
1	B	518	HIS
1	C	36	HIS
1	C	57	ASN
1	C	75	GLN
1	C	158	ASN
1	C	218	GLN
1	C	226	HIS
1	C	245	ASN
1	C	257	ASN
1	C	291	ASN
1	C	326	ASN
1	C	379	GLN
1	C	415	HIS
1	C	476	ASN
1	D	18	GLN
1	D	36	HIS
1	D	75	GLN
1	D	99	GLN

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Mol	Chain	Res	Type
1	D	142	GLN
1	D	158	ASN
1	D	167	GLN
1	D	218	GLN
1	D	226	HIS
1	D	241	GLN
1	D	245	ASN
1	D	257	ASN
1	D	315	ASN
1	D	334	ASN
1	D	379	GLN
1	D	415	HIS
1	D	454	GLN
1	D	455	GLN
1	D	465	GLN
1	E	18	GLN
1	E	226	HIS
1	E	241	GLN
1	E	280	GLN
1	E	302	ASN
1	E	415	HIS
1	E	520	ASN
1	F	18	GLN
1	F	33	GLN
1	F	75	GLN
1	F	241	GLN
1	F	245	ASN
1	F	257	ASN
1	F	291	ASN
1	F	302	ASN
1	F	311	HIS
1	F	326	ASN
1	F	454	GLN
1	F	455	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [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	518/522 (99%)	-1.41	0 100 100	8, 17, 57, 83	0
1	B	518/522 (99%)	-1.37	0 100 100	7, 19, 61, 82	0
1	C	518/522 (99%)	-1.30	1 (0%) 91 90	9, 19, 68, 81	0
1	D	518/522 (99%)	-1.38	0 100 100	10, 19, 60, 83	0
1	E	518/522 (99%)	-1.38	0 100 100	9, 17, 57, 81	0
1	F	518/522 (99%)	-1.36	0 100 100	9, 19, 61, 82	0
All	All	3108/3132 (99%)	-1.37	1 (0%) 100 100	7, 19, 61, 83	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	54	GLY	2.8

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.