



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 02:47 PM UTC

PDB ID : 1HMV / pdb_00001hmv
Title : THE STRUCTURE OF UNLIGANDED REVERSE TRANSCRIPTASE
FROM THE HUMAN IMMUNODEFICIENCY VIRUS TYPE 1
Authors : Rodgers, D.W.; Gamblin, S.J.; Harris, B.A.; Ray, S.; Culp, J.S.; Hellmig, B.;
Woolf, D.J.; Debouck, C.; Harrison, S.C.
Deposited on : 1994-12-15
Resolution : 3.20 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

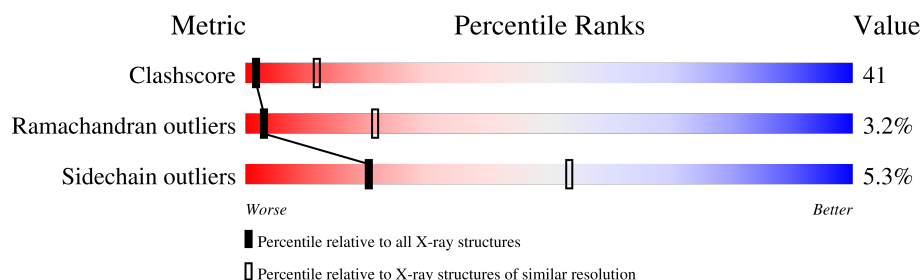
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	560	36% 50% 9% . .
1	C	560	36% 51% 9% . .
1	E	560	36% 51% 9% . .
1	G	560	36% 51% 8% . .
2	B	440	35% 45% 9% . 10%
2	D	440	35% 44% 9% . 10%
2	F	440	36% 44% 9% . 10%
2	H	440	35% 45% 8% . 10%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 29596 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 HIV-1 REVERSE TRANSCRIPTASE (SUBUNIT P66).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	536	Total	C	N	O	S	0	0	0
			4200	2711	698	784	7			
1	C	536	Total	C	N	O	S	0	0	0
			4200	2711	698	784	7			
1	E	536	Total	C	N	O	S	0	0	0
			4200	2711	698	784	7			
1	G	536	Total	C	N	O	S	0	0	0
			4200	2711	698	784	7			

- Molecule 2 is a protein called HIV-1 REVERSE TRANSCRIPTASE (SUBUNIT P51).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	395	Total	C	N	O	S	0	0	0
			3198	2079	531	582	6			
2	D	395	Total	C	N	O	S	0	0	0
			3198	2079	531	582	6			
2	F	395	Total	C	N	O	S	0	0	0
			3198	2079	531	582	6			
2	H	395	Total	C	N	O	S	0	0	0
			3198	2079	531	582	6			

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

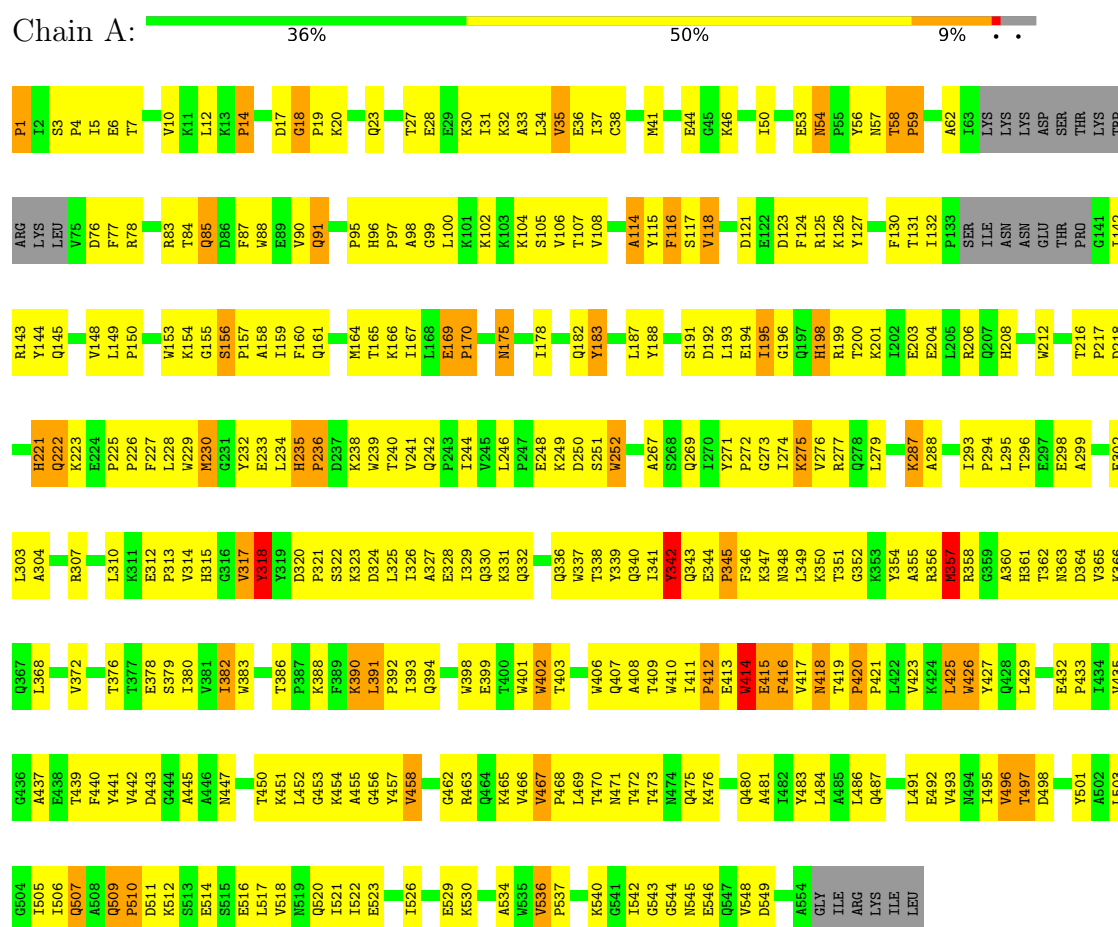
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Mg	0	0
			1	1		
3	D	1	Total	Mg	0	0
			1	1		
3	F	1	Total	Mg	0	0
			1	1		
3	H	1	Total	Mg	0	0
			1	1		

3 Residue-property plots

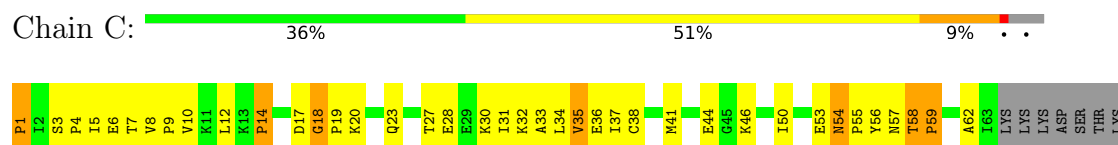
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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.

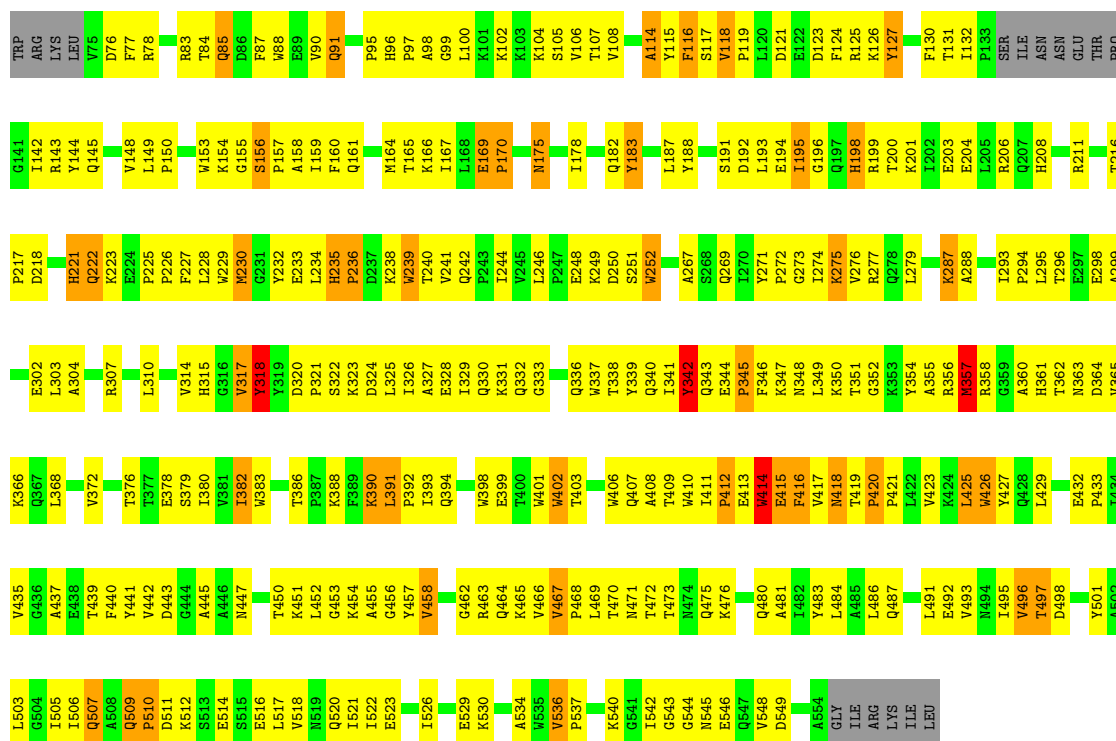
Note EDS was not executed.

• Molecule 1: HIV-1 REVERSE TRANSCRIPTASE (SUBUNIT P66)



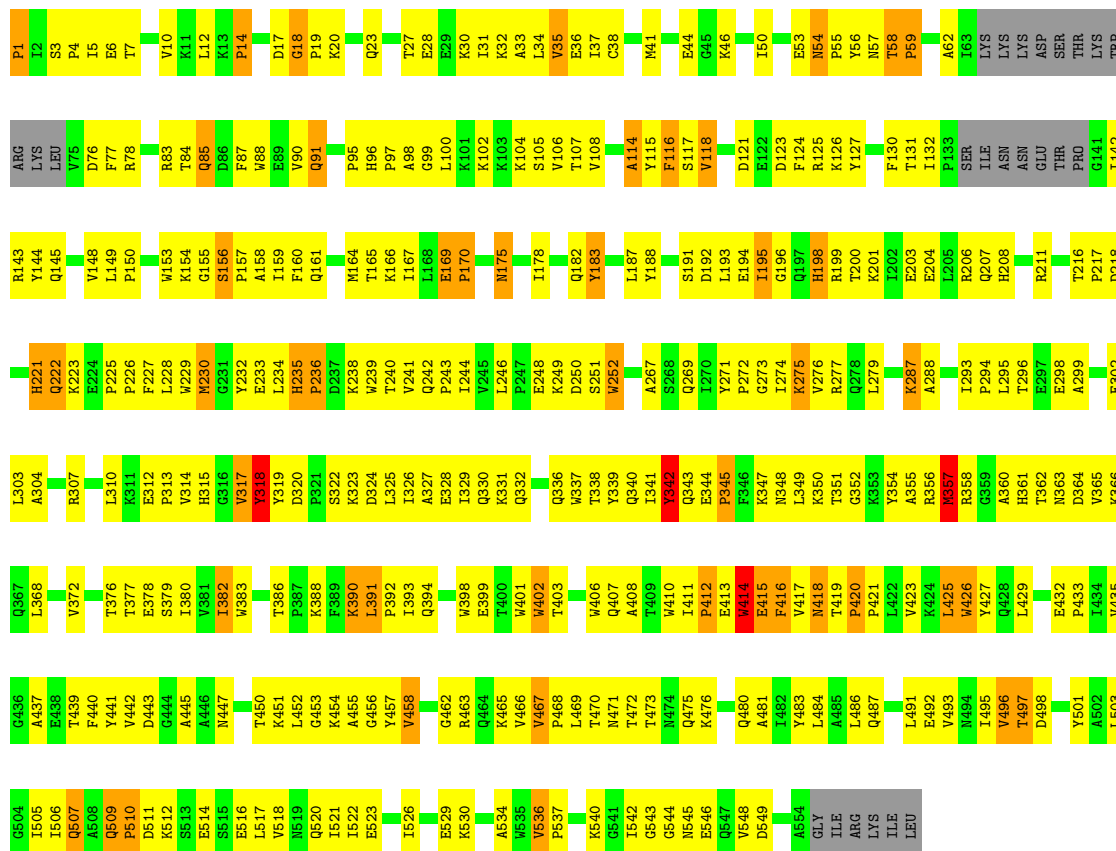
• Molecule 1: HIV-1 REVERSE TRANSCRIPTASE (SUBUNIT P66)



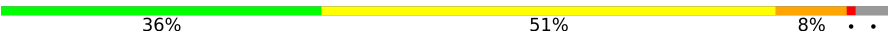


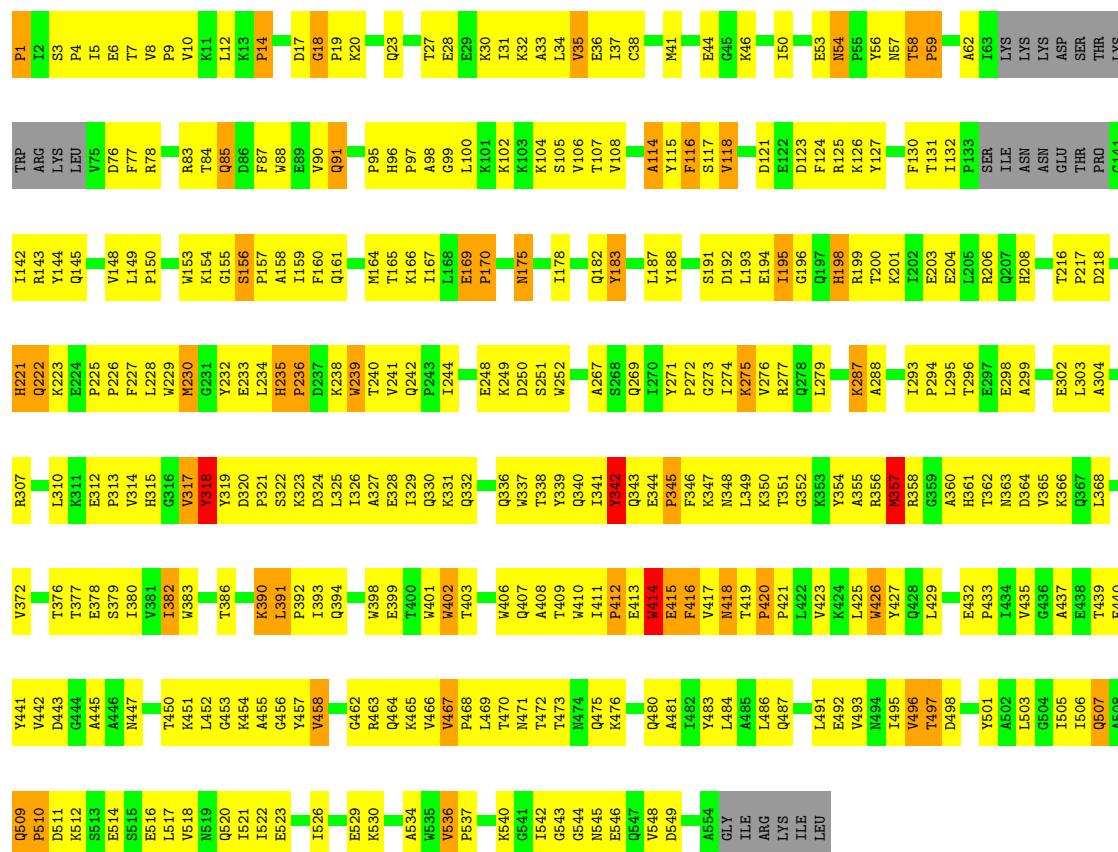
• Molecule 1: HIV-1 REVERSE TRANSCRIPTASE (SUBUNIT P66)

Chain E: 36% 51% 9% . .

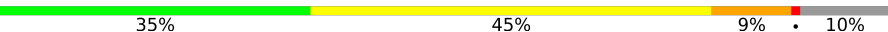


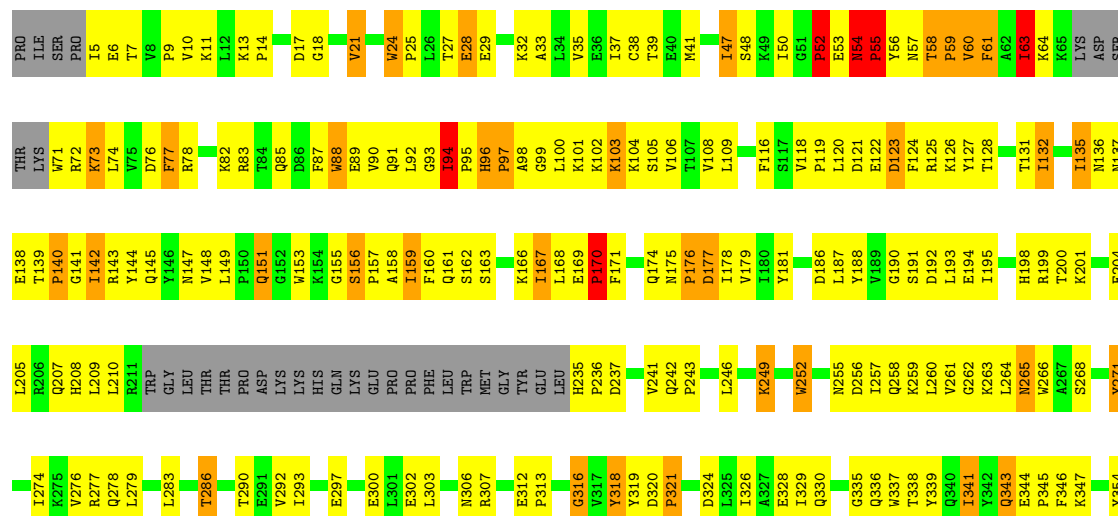
• Molecule 1: HIV-1 REVERSE TRANSCRIPTASE (SUBUNIT P66)

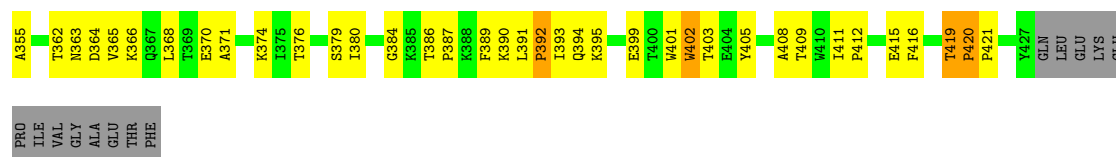
Chain G:  36% 51% 8% . .



• Molecule 2: HIV-1 REVERSE TRANSCRIPTASE (SUBUNIT P51)

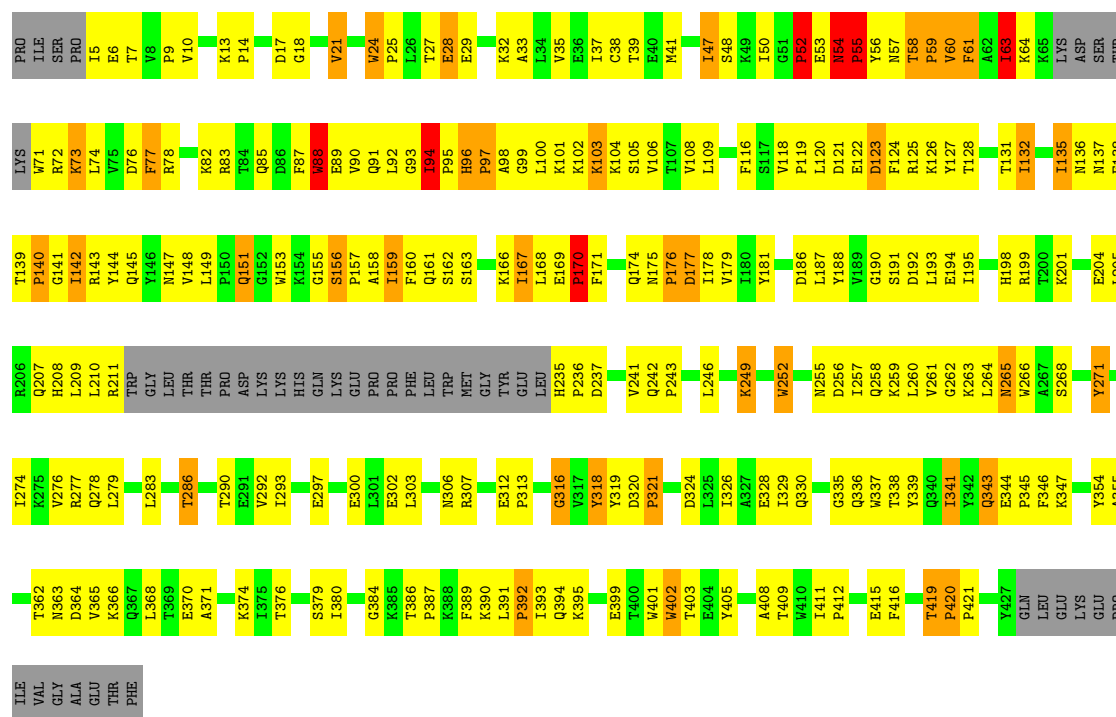
Chain B:  35% 45% 9% . 10%





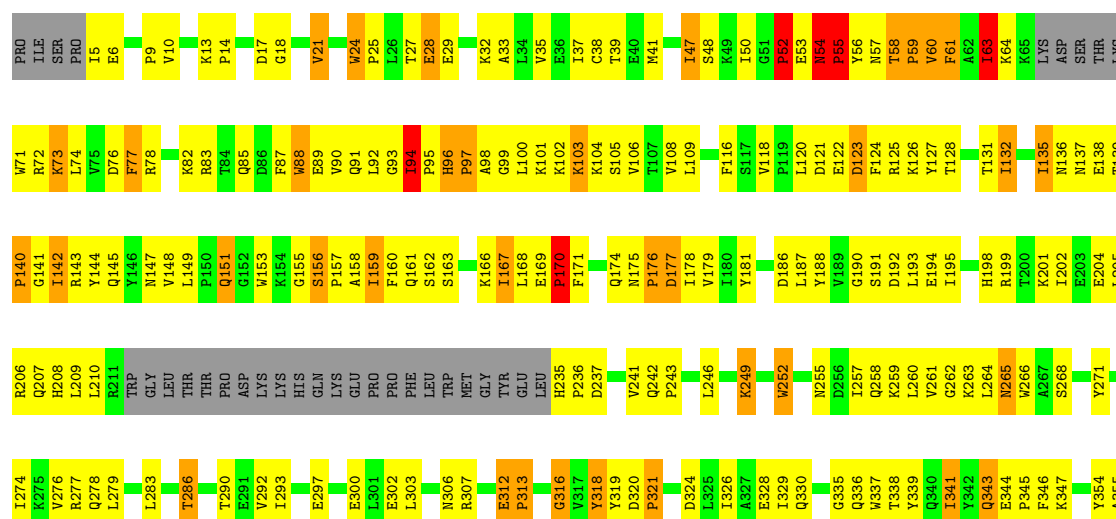
• Molecule 2: HIV-1 REVERSE TRANSCRIPTASE (SUBUNIT P51)

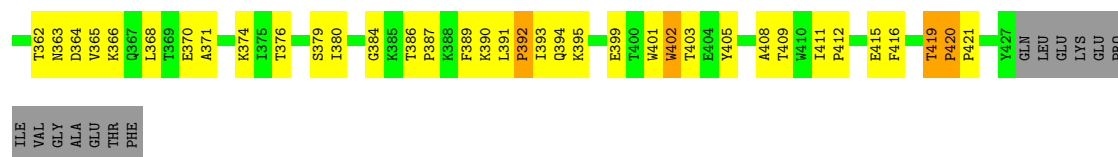
Chain D: 35% 44% 9% 10%



• Molecule 2: HIV-1 REVERSE TRANSCRIPTASE (SUBUNIT P51)

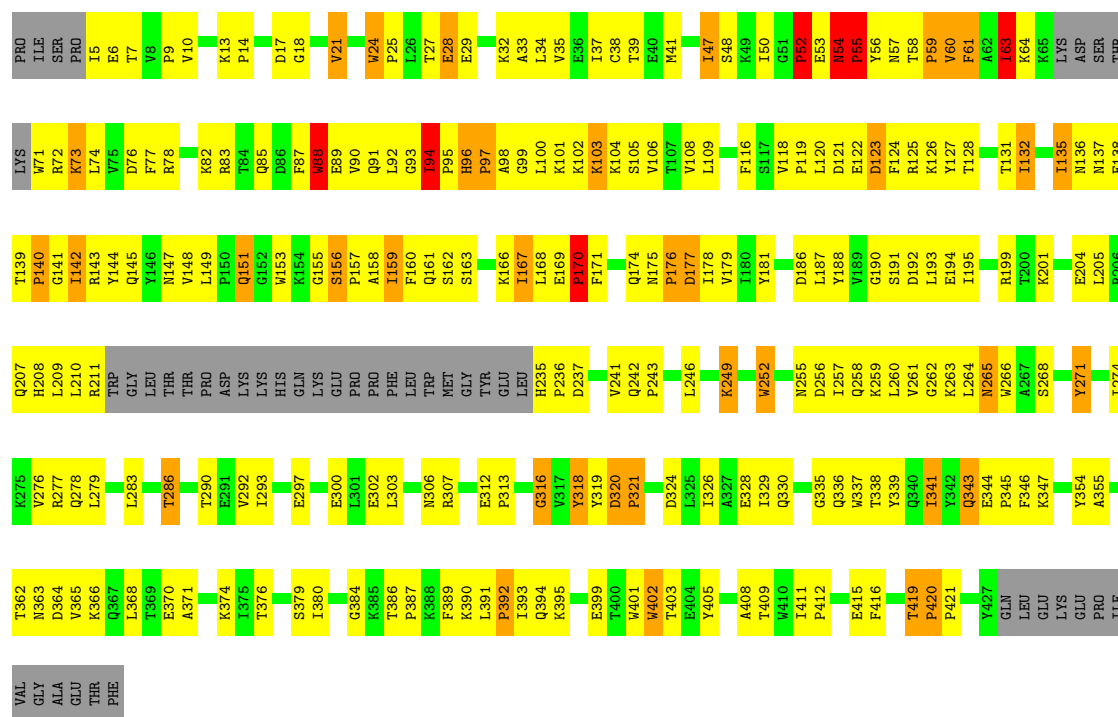
Chain F: 36% 44% 9% 10%





• Molecule 2: HIV-1 REVERSE TRANSCRIPTASE (SUBUNIT P51)

Chain H: 35% 45% 8% • 10%



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	168.70Å 162.80Å 331.80Å 90.00° 105.70° 90.00°	Depositor
Resolution (Å)	6.00 – 3.20	Depositor
% Data completeness (in resolution range)	(Not available) (6.00-3.20)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.254 , 0.297	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	29596	wwPDB-VP
Average B, all atoms (Å ²)	97.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG

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	0.93	6/4307 (0.1%)	1.44	57/5865 (1.0%)
1	C	0.93	6/4307 (0.1%)	1.44	58/5865 (1.0%)
1	E	0.93	6/4307 (0.1%)	1.44	58/5865 (1.0%)
1	G	0.93	6/4307 (0.1%)	1.44	57/5865 (1.0%)
2	B	0.92	4/3285 (0.1%)	1.47	54/4466 (1.2%)
2	D	0.92	4/3285 (0.1%)	1.47	54/4466 (1.2%)
2	F	0.92	4/3285 (0.1%)	1.47	52/4466 (1.2%)
2	H	0.92	4/3285 (0.1%)	1.47	53/4466 (1.2%)
All	All	0.92	40/30368 (0.1%)	1.45	443/41324 (1.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	C	0	2
1	E	0	2
1	G	0	2
2	B	0	1
2	D	0	1
2	F	0	1
2	H	0	1
All	All	0	12

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	230	MET	SD-CE	-9.25	1.56	1.79
1	E	230	MET	SD-CE	-9.24	1.56	1.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	230	MET	SD-CE	-9.23	1.56	1.79
1	A	230	MET	SD-CE	-9.22	1.56	1.79
1	C	222	GLN	C-O	7.57	1.33	1.24
1	A	222	GLN	C-O	7.54	1.33	1.24
1	G	222	GLN	C-O	7.53	1.33	1.24
1	E	222	GLN	C-O	7.52	1.33	1.24
1	G	118	VAL	CA-C	-6.31	1.48	1.53
1	A	118	VAL	CA-C	-6.20	1.48	1.53
1	C	118	VAL	CA-C	-6.14	1.48	1.53
1	E	118	VAL	CA-C	-6.14	1.48	1.53
2	B	21	VAL	CA-CB	-6.07	1.46	1.54
2	D	21	VAL	CA-CB	-6.05	1.46	1.54
2	H	21	VAL	CA-CB	-6.04	1.46	1.54
2	F	21	VAL	CA-CB	-6.03	1.46	1.54
1	E	269	GLN	C-N	-5.76	1.25	1.33
1	A	269	GLN	C-N	-5.72	1.25	1.33
1	C	269	GLN	C-N	-5.70	1.25	1.33
1	G	269	GLN	C-N	-5.70	1.25	1.33
2	D	362	THR	C-O	5.57	1.30	1.24
2	D	159	ILE	CA-CB	-5.55	1.48	1.54
2	H	159	ILE	CA-CB	-5.55	1.48	1.54
2	F	159	ILE	CA-CB	-5.54	1.48	1.54
2	B	159	ILE	CA-CB	-5.52	1.48	1.54
2	B	362	THR	C-O	5.51	1.30	1.24
2	H	362	THR	C-O	5.50	1.30	1.24
2	F	362	THR	C-O	5.48	1.30	1.24
2	B	341	ILE	CA-CB	-5.23	1.48	1.54
2	D	341	ILE	CA-CB	-5.22	1.48	1.54
1	G	183	TYR	CA-C	-5.22	1.48	1.53
2	F	341	ILE	CA-CB	-5.22	1.48	1.54
2	H	341	ILE	CA-CB	-5.21	1.48	1.54
1	C	279	LEU	C-O	-5.21	1.17	1.24
1	C	183	TYR	CA-C	-5.20	1.48	1.53
1	A	279	LEU	C-O	-5.17	1.17	1.24
1	A	183	TYR	CA-C	-5.17	1.48	1.53
1	E	183	TYR	CA-C	-5.16	1.48	1.53
1	G	279	LEU	C-O	-5.16	1.17	1.24
1	E	279	LEU	C-O	-5.14	1.17	1.24

All (443) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	94	ILE	CA-C-N	-13.14	106.58	119.85
2	H	94	ILE	C-N-CA	-13.14	106.58	119.85
2	F	94	ILE	CA-C-N	-13.13	106.58	119.85
2	F	94	ILE	C-N-CA	-13.13	106.58	119.85
2	B	94	ILE	CA-C-N	-13.13	106.59	119.85
2	B	94	ILE	C-N-CA	-13.13	106.59	119.85
2	D	94	ILE	CA-C-N	-13.12	106.60	119.85
2	D	94	ILE	C-N-CA	-13.12	106.60	119.85
2	F	54	ASN	CA-C-N	12.45	135.40	119.84
2	F	54	ASN	C-N-CA	12.45	135.40	119.84
2	B	54	ASN	CA-C-N	12.44	135.39	119.84
2	B	54	ASN	C-N-CA	12.44	135.39	119.84
2	H	54	ASN	CA-C-N	12.44	135.39	119.84
2	H	54	ASN	C-N-CA	12.44	135.39	119.84
2	D	54	ASN	CA-C-N	12.44	135.38	119.84
2	D	54	ASN	C-N-CA	12.44	135.38	119.84
1	G	118	VAL	CA-C-N	11.72	131.85	119.90
1	G	118	VAL	C-N-CA	11.72	131.85	119.90
1	C	118	VAL	CA-C-N	11.68	131.81	119.90
1	C	118	VAL	C-N-CA	11.68	131.81	119.90
1	A	118	VAL	CA-C-N	11.68	131.81	119.90
1	A	118	VAL	C-N-CA	11.68	131.81	119.90
1	E	118	VAL	CA-C-N	11.63	131.77	119.90
1	E	118	VAL	C-N-CA	11.63	131.77	119.90
1	A	271	TYR	CA-C-N	10.73	133.25	119.84
1	A	271	TYR	C-N-CA	10.73	133.25	119.84
1	E	271	TYR	CA-C-N	10.71	133.23	119.84
1	E	271	TYR	C-N-CA	10.71	133.23	119.84
1	G	271	TYR	CA-C-N	10.69	133.20	119.84
1	G	271	TYR	C-N-CA	10.69	133.20	119.84
1	C	271	TYR	CA-C-N	10.68	133.19	119.84
1	C	271	TYR	C-N-CA	10.68	133.19	119.84
1	C	382	ILE	N-CA-C	9.11	119.10	110.53
1	E	382	ILE	N-CA-C	9.11	119.10	110.53
1	A	382	ILE	N-CA-C	9.11	119.09	110.53
1	G	382	ILE	N-CA-C	9.06	119.05	110.53
2	H	102	LYS	N-CA-C	9.05	124.11	112.89
2	D	102	LYS	N-CA-C	9.05	124.11	112.89
2	F	102	LYS	N-CA-C	9.04	124.11	112.89
2	B	102	LYS	N-CA-C	9.04	124.10	112.89
2	H	312	GLU	CA-C-N	8.83	130.88	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	312	GLU	C-N-CA	8.83	130.88	119.84
2	F	312	GLU	CA-C-N	8.82	130.86	119.84
2	F	312	GLU	C-N-CA	8.82	130.86	119.84
2	B	312	GLU	CA-C-N	8.81	130.85	119.84
2	B	312	GLU	C-N-CA	8.81	130.85	119.84
2	D	312	GLU	CA-C-N	8.79	130.82	119.84
2	D	312	GLU	C-N-CA	8.79	130.82	119.84
2	H	60	VAL	CB-CA-C	-8.18	99.12	110.90
2	F	60	VAL	CB-CA-C	-8.16	99.14	110.90
2	B	60	VAL	CB-CA-C	-8.16	99.15	110.90
2	D	118	VAL	CA-C-N	8.16	127.92	119.76
2	D	118	VAL	C-N-CA	8.16	127.92	119.76
2	D	60	VAL	CB-CA-C	-8.14	99.17	110.90
2	B	118	VAL	CA-C-N	8.10	127.86	119.76
2	B	118	VAL	C-N-CA	8.10	127.86	119.76
1	E	118	VAL	N-CA-C	8.10	114.93	107.56
1	A	118	VAL	N-CA-C	8.10	114.93	107.56
1	G	118	VAL	N-CA-C	8.10	114.93	107.56
2	H	118	VAL	CA-C-N	8.09	127.85	119.76
2	H	118	VAL	C-N-CA	8.09	127.85	119.76
1	A	221	HIS	CA-C-N	8.08	136.97	121.54
1	A	221	HIS	C-N-CA	8.08	136.97	121.54
1	E	221	HIS	CA-C-N	8.08	136.96	121.54
1	E	221	HIS	C-N-CA	8.08	136.96	121.54
2	F	90	VAL	N-CA-C	-8.08	97.57	106.21
1	G	221	HIS	CA-C-N	8.07	136.95	121.54
1	G	221	HIS	C-N-CA	8.07	136.95	121.54
1	C	221	HIS	CA-C-N	8.07	136.95	121.54
1	C	221	HIS	C-N-CA	8.07	136.95	121.54
2	F	118	VAL	CA-C-N	8.06	127.82	119.76
2	F	118	VAL	C-N-CA	8.06	127.82	119.76
1	C	118	VAL	N-CA-C	8.05	114.89	107.56
2	B	90	VAL	N-CA-C	-8.05	97.59	106.21
2	H	90	VAL	N-CA-C	-8.03	97.62	106.21
2	D	90	VAL	N-CA-C	-8.03	97.62	106.21
1	E	351	THR	N-CA-C	-7.80	98.67	110.14
1	C	351	THR	N-CA-C	-7.80	98.67	110.14
1	A	351	THR	N-CA-C	-7.78	98.70	110.14
1	G	351	THR	N-CA-C	-7.78	98.70	110.14
2	F	103	LYS	N-CA-C	7.69	120.81	110.35
2	H	103	LYS	N-CA-C	7.68	120.80	110.35
2	D	103	LYS	N-CA-C	7.68	120.79	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	103	LYS	N-CA-C	7.68	120.79	110.35
1	C	498	ASP	N-CA-C	-7.66	101.83	112.25
1	G	498	ASP	N-CA-C	-7.66	101.83	112.25
1	A	498	ASP	N-CA-C	-7.65	101.85	112.25
1	E	498	ASP	N-CA-C	-7.61	101.89	112.25
1	E	3	SER	CA-C-N	7.41	129.60	121.00
1	E	3	SER	C-N-CA	7.41	129.60	121.00
1	A	3	SER	CA-C-N	7.40	129.59	121.00
1	A	3	SER	C-N-CA	7.40	129.59	121.00
1	C	3	SER	CA-C-N	7.40	129.59	121.00
1	C	3	SER	C-N-CA	7.40	129.59	121.00
1	G	3	SER	CA-C-N	7.39	129.57	121.00
1	G	3	SER	C-N-CA	7.39	129.57	121.00
1	E	18	GLY	CA-C-N	7.33	127.29	120.03
1	E	18	GLY	C-N-CA	7.33	127.29	120.03
1	C	18	GLY	CA-C-N	7.32	127.28	120.03
1	C	18	GLY	C-N-CA	7.32	127.28	120.03
1	A	18	GLY	CA-C-N	7.32	127.28	120.03
1	A	18	GLY	C-N-CA	7.32	127.28	120.03
1	G	18	GLY	CA-C-N	7.27	127.23	120.03
1	G	18	GLY	C-N-CA	7.27	127.23	120.03
1	C	536	VAL	CA-C-N	7.18	128.81	119.84
1	C	536	VAL	C-N-CA	7.18	128.81	119.84
1	E	536	VAL	CA-C-N	7.16	128.79	119.84
1	E	536	VAL	C-N-CA	7.16	128.79	119.84
1	A	536	VAL	CA-C-N	7.15	128.78	119.84
1	A	536	VAL	C-N-CA	7.15	128.78	119.84
1	G	536	VAL	CA-C-N	7.13	128.75	119.84
1	G	536	VAL	C-N-CA	7.13	128.75	119.84
1	E	496	VAL	N-CA-C	7.01	118.23	107.78
1	E	35	VAL	CB-CA-C	-6.92	103.16	111.81
1	G	35	VAL	CB-CA-C	-6.91	103.17	111.81
1	A	35	VAL	CB-CA-C	-6.91	103.18	111.81
1	C	35	VAL	CB-CA-C	-6.88	103.21	111.81
1	C	497	THR	N-CA-C	6.85	120.76	110.14
1	E	497	THR	N-CA-C	6.85	120.75	110.14
1	A	54	ASN	CA-C-N	6.85	127.41	119.47
1	A	54	ASN	C-N-CA	6.85	127.41	119.47
1	E	54	ASN	CA-C-N	6.85	127.41	119.47
1	E	54	ASN	C-N-CA	6.85	127.41	119.47
1	A	497	THR	N-CA-C	6.84	120.74	110.14
1	G	497	THR	N-CA-C	6.83	120.73	110.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	54	ASN	CA-C-N	6.82	127.38	119.47
1	G	54	ASN	C-N-CA	6.82	127.38	119.47
1	C	54	ASN	CA-C-N	6.80	127.36	119.47
1	C	54	ASN	C-N-CA	6.80	127.36	119.47
2	F	47	ILE	CB-CA-C	-6.65	100.39	111.29
1	C	391	LEU	CA-C-N	6.63	128.13	119.84
1	C	391	LEU	C-N-CA	6.63	128.13	119.84
2	H	47	ILE	CB-CA-C	-6.62	100.43	111.29
2	B	47	ILE	CB-CA-C	-6.62	100.43	111.29
2	D	47	ILE	CB-CA-C	-6.62	100.44	111.29
1	G	391	LEU	CA-C-N	6.60	128.09	119.84
1	G	391	LEU	C-N-CA	6.60	128.09	119.84
1	A	391	LEU	CA-C-N	6.59	128.08	119.84
1	A	391	LEU	C-N-CA	6.59	128.08	119.84
1	E	391	LEU	CA-C-N	6.57	128.06	119.84
1	E	391	LEU	C-N-CA	6.57	128.06	119.84
1	E	514	GLU	N-CA-C	-6.56	103.96	112.23
1	C	514	GLU	N-CA-C	-6.56	103.96	112.23
1	G	514	GLU	N-CA-C	-6.56	103.96	112.23
1	A	514	GLU	N-CA-C	-6.56	103.97	112.23
1	E	59	PRO	N-CA-C	6.54	121.11	111.03
2	B	89	GLU	N-CA-C	-6.54	103.77	111.03
2	F	89	GLU	N-CA-C	-6.54	103.77	111.03
1	G	59	PRO	N-CA-C	6.54	121.10	111.03
1	A	59	PRO	N-CA-C	6.54	121.09	111.03
1	C	59	PRO	N-CA-C	6.54	121.09	111.03
2	H	89	GLU	N-CA-C	-6.53	103.78	111.03
2	D	89	GLU	N-CA-C	-6.53	103.78	111.03
1	A	58	THR	CA-C-N	6.49	126.84	119.83
1	A	58	THR	C-N-CA	6.49	126.84	119.83
1	C	58	THR	CA-C-N	6.49	126.83	119.83
1	C	58	THR	C-N-CA	6.49	126.83	119.83
1	E	58	THR	CA-C-N	6.48	126.83	119.83
1	E	58	THR	C-N-CA	6.48	126.83	119.83
1	G	58	THR	CA-C-N	6.46	126.81	119.83
1	G	58	THR	C-N-CA	6.46	126.81	119.83
2	H	132	ILE	CA-C-N	6.45	127.33	120.11
2	H	132	ILE	C-N-CA	6.45	127.33	120.11
1	C	509	GLN	CA-C-N	6.45	127.90	119.84
1	C	509	GLN	C-N-CA	6.45	127.90	119.84
2	F	132	ILE	CA-C-N	6.45	127.33	120.11
2	F	132	ILE	C-N-CA	6.45	127.33	120.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	294	PRO	N-CA-CB	6.44	110.02	103.25
2	B	132	ILE	CA-C-N	6.43	127.32	120.11
2	B	132	ILE	C-N-CA	6.43	127.32	120.11
2	D	132	ILE	CA-C-N	6.43	127.31	120.11
2	D	132	ILE	C-N-CA	6.43	127.31	120.11
1	A	509	GLN	CA-C-N	6.42	127.87	119.84
1	A	509	GLN	C-N-CA	6.42	127.87	119.84
1	E	294	PRO	N-CA-CB	6.42	109.99	103.25
1	A	294	PRO	N-CA-CB	6.41	109.98	103.25
1	C	294	PRO	N-CA-CB	6.41	109.98	103.25
1	G	509	GLN	CA-C-N	6.40	127.84	119.84
1	G	509	GLN	C-N-CA	6.40	127.84	119.84
1	C	496	VAL	N-CA-C	6.40	118.25	107.18
1	E	509	GLN	CA-C-N	6.40	127.84	119.84
1	E	509	GLN	C-N-CA	6.40	127.84	119.84
1	G	496	VAL	N-CA-C	6.39	118.23	107.18
1	A	496	VAL	N-CA-C	6.38	118.22	107.18
1	A	272	PRO	N-CA-CB	6.37	109.94	103.25
1	E	272	PRO	N-CA-CB	6.37	109.94	103.25
1	C	272	PRO	N-CA-CB	6.36	109.93	103.25
1	G	287	LYS	CA-C-O	-6.36	114.59	121.14
2	F	249	LYS	N-CA-C	6.36	119.54	109.81
2	F	96	HIS	CA-C-N	6.36	127.79	119.84
2	F	96	HIS	C-N-CA	6.36	127.79	119.84
2	D	96	HIS	CA-C-N	6.35	127.78	119.84
2	D	96	HIS	C-N-CA	6.35	127.78	119.84
1	C	287	LYS	CA-C-O	-6.35	114.60	121.14
1	A	287	LYS	CA-C-O	-6.34	114.61	121.14
2	B	96	HIS	CA-C-N	6.34	127.77	119.84
2	B	96	HIS	C-N-CA	6.34	127.77	119.84
1	G	272	PRO	N-CA-CB	6.34	109.91	103.25
2	H	96	HIS	CA-C-N	6.34	127.76	119.84
2	H	96	HIS	C-N-CA	6.34	127.76	119.84
2	B	249	LYS	N-CA-C	6.34	119.50	109.81
2	D	249	LYS	N-CA-C	6.33	119.50	109.81
2	H	249	LYS	N-CA-C	6.32	119.48	109.81
1	E	287	LYS	CA-C-O	-6.31	114.64	121.14
2	D	156	SER	CA-C-N	6.24	125.73	119.24
2	D	156	SER	C-N-CA	6.24	125.73	119.24
2	F	156	SER	CA-C-N	6.23	125.72	119.24
2	F	156	SER	C-N-CA	6.23	125.72	119.24
2	H	156	SER	CA-C-N	6.21	125.69	119.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	156	SER	C-N-CA	6.21	125.69	119.24
2	B	156	SER	CA-C-N	6.19	125.68	119.24
2	B	156	SER	C-N-CA	6.19	125.68	119.24
1	E	357	MET	N-CA-C	-6.16	97.69	110.80
1	C	357	MET	N-CA-C	-6.14	97.71	110.80
1	G	357	MET	N-CA-C	-6.14	97.72	110.80
2	H	128	THR	N-CA-C	-6.13	104.29	112.94
2	B	128	THR	N-CA-C	-6.13	104.30	112.94
1	A	357	MET	N-CA-C	-6.13	97.74	110.80
2	F	128	THR	N-CA-C	-6.13	104.30	112.94
2	D	128	THR	N-CA-C	-6.11	104.32	112.94
1	E	416	PHE	N-CA-C	6.11	119.12	109.96
1	G	416	PHE	N-CA-C	6.10	119.11	109.96
1	A	416	PHE	N-CA-C	6.10	119.10	109.96
1	C	416	PHE	N-CA-C	6.09	119.10	109.96
1	C	293	ILE	CA-C-N	5.95	127.27	119.84
1	C	293	ILE	C-N-CA	5.95	127.27	119.84
1	G	293	ILE	CA-C-N	5.95	127.28	119.84
1	G	293	ILE	C-N-CA	5.95	127.28	119.84
1	E	293	ILE	CA-C-N	5.94	127.27	119.84
1	E	293	ILE	C-N-CA	5.94	127.27	119.84
1	A	293	ILE	CA-C-N	5.93	127.26	119.84
1	A	293	ILE	C-N-CA	5.93	127.26	119.84
1	G	41	MET	N-CA-C	-5.93	104.89	111.71
1	C	41	MET	N-CA-C	-5.91	104.92	111.71
1	E	41	MET	N-CA-C	-5.91	104.92	111.71
1	A	41	MET	N-CA-C	-5.90	104.92	111.71
2	D	63	ILE	N-CA-C	-5.89	97.09	109.34
2	F	140	PRO	N-CA-C	-5.88	102.03	111.38
2	F	63	ILE	N-CA-C	-5.87	97.12	109.34
2	B	63	ILE	N-CA-C	-5.87	97.14	109.34
2	H	63	ILE	N-CA-C	-5.86	97.15	109.34
2	B	140	PRO	N-CA-C	-5.85	102.08	111.38
2	H	58	THR	CA-C-N	-5.85	113.94	120.14
2	H	58	THR	C-N-CA	-5.85	113.94	120.14
2	H	140	PRO	N-CA-C	-5.84	102.09	111.38
2	D	58	THR	CA-C-N	-5.83	113.96	120.14
2	D	58	THR	C-N-CA	-5.83	113.96	120.14
2	D	140	PRO	N-CA-C	-5.83	102.11	111.38
2	B	58	THR	CA-C-N	-5.82	113.97	120.14
2	B	58	THR	C-N-CA	-5.82	113.97	120.14
1	C	198	HIS	N-CA-C	-5.81	104.58	111.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	317	VAL	CA-C-O	-5.80	117.10	121.68
1	G	382	ILE	CB-CA-C	-5.80	104.42	112.02
1	E	198	HIS	N-CA-C	-5.80	104.59	111.03
2	F	58	THR	CA-C-N	-5.80	113.99	120.14
2	F	58	THR	C-N-CA	-5.80	113.99	120.14
1	A	198	HIS	N-CA-C	-5.80	104.59	111.03
1	A	382	ILE	CB-CA-C	-5.79	104.44	112.02
1	E	317	VAL	CA-C-O	-5.79	117.11	121.68
1	E	382	ILE	CB-CA-C	-5.78	104.45	112.02
1	C	382	ILE	CB-CA-C	-5.78	104.45	112.02
1	C	317	VAL	CA-C-O	-5.78	117.12	121.68
1	G	317	VAL	CA-C-O	-5.78	117.12	121.68
1	G	239	TRP	N-CA-C	-5.77	101.14	110.32
1	E	239	TRP	N-CA-C	-5.76	101.15	110.32
2	B	52	PRO	N-CA-C	-5.76	106.49	114.27
2	H	52	PRO	N-CA-C	-5.76	106.49	114.27
1	G	198	HIS	N-CA-C	-5.76	104.64	111.03
1	A	239	TRP	N-CA-C	-5.76	101.16	110.32
1	C	360	ALA	N-CA-C	-5.75	106.10	113.23
1	C	239	TRP	N-CA-C	-5.75	101.19	110.32
2	F	408	ALA	N-CA-C	5.75	119.45	110.32
2	D	52	PRO	N-CA-C	-5.74	106.52	114.27
1	E	360	ALA	N-CA-C	-5.73	106.13	113.23
2	B	408	ALA	N-CA-C	5.73	119.43	110.32
2	F	52	PRO	N-CA-C	-5.73	106.54	114.27
1	A	360	ALA	N-CA-C	-5.72	106.14	113.23
1	G	360	ALA	N-CA-C	-5.71	106.15	113.23
2	D	408	ALA	N-CA-C	5.70	119.39	110.32
1	A	390	LYS	N-CA-C	-5.70	97.88	108.02
1	E	390	LYS	N-CA-C	-5.70	97.88	108.02
2	H	408	ALA	N-CA-C	5.70	119.38	110.32
1	G	390	LYS	N-CA-C	-5.69	97.89	108.02
1	C	390	LYS	N-CA-C	-5.69	97.89	108.02
2	D	344	GLU	CA-C-N	5.62	125.94	119.93
2	D	344	GLU	C-N-CA	5.62	125.94	119.93
2	H	344	GLU	CA-C-N	5.57	125.89	119.93
2	H	344	GLU	C-N-CA	5.57	125.89	119.93
2	B	344	GLU	CA-C-N	5.57	125.89	119.93
2	B	344	GLU	C-N-CA	5.57	125.89	119.93
1	A	458	VAL	N-CA-C	-5.55	100.29	108.23
2	D	131	THR	N-CA-C	5.55	117.44	108.34
2	F	344	GLU	CA-C-N	5.55	125.87	119.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	344	GLU	C-N-CA	5.55	125.87	119.93
1	G	458	VAL	N-CA-C	-5.55	100.29	108.23
1	C	458	VAL	N-CA-C	-5.55	100.30	108.23
1	E	458	VAL	N-CA-C	-5.55	100.30	108.23
2	H	131	THR	N-CA-C	5.55	117.44	108.34
2	B	131	THR	N-CA-C	5.54	117.43	108.34
2	H	21	VAL	N-CA-C	5.54	116.56	108.58
2	B	335	GLY	N-CA-C	-5.54	105.28	114.48
2	F	21	VAL	N-CA-C	5.54	116.56	108.58
2	F	335	GLY	N-CA-C	-5.54	105.28	114.48
2	D	21	VAL	N-CA-C	5.54	116.55	108.58
2	F	131	THR	N-CA-C	5.54	117.42	108.34
2	B	21	VAL	N-CA-C	5.54	116.55	108.58
2	H	335	GLY	N-CA-C	-5.53	105.31	114.48
2	D	335	GLY	N-CA-C	-5.52	105.32	114.48
1	A	7	THR	N-CA-C	5.51	118.90	110.20
1	C	7	THR	N-CA-C	5.50	118.89	110.20
1	E	7	THR	N-CA-C	5.50	118.89	110.20
1	G	7	THR	N-CA-C	5.50	118.88	110.20
1	A	175	ASN	CA-C-N	5.49	126.70	119.84
1	A	175	ASN	C-N-CA	5.49	126.70	119.84
2	F	419	THR	N-CA-C	5.48	117.38	109.48
1	C	234	LEU	N-CA-C	5.48	118.10	108.56
2	D	419	THR	N-CA-C	5.48	117.37	109.48
1	G	234	LEU	N-CA-C	5.48	118.09	108.56
1	A	234	LEU	N-CA-C	5.47	118.08	108.56
1	G	175	ASN	CA-C-N	5.47	126.67	119.84
1	G	175	ASN	C-N-CA	5.47	126.67	119.84
1	C	175	ASN	CA-C-N	5.47	126.67	119.84
1	C	175	ASN	C-N-CA	5.47	126.67	119.84
1	E	175	ASN	CA-C-N	5.46	126.67	119.84
1	E	175	ASN	C-N-CA	5.46	126.67	119.84
1	E	234	LEU	N-CA-C	5.46	118.06	108.56
2	B	419	THR	N-CA-C	5.46	117.34	109.48
2	H	419	THR	N-CA-C	5.46	117.34	109.48
2	H	265	ASN	N-CA-C	-5.46	104.97	111.03
1	C	318	TYR	CA-C-N	-5.44	115.04	122.93
1	C	318	TYR	C-N-CA	-5.44	115.04	122.93
1	C	495	ILE	CB-CA-C	5.43	119.38	110.69
2	H	343	GLN	N-CA-C	-5.43	105.46	112.68
1	G	495	ILE	CB-CA-C	5.43	119.37	110.69
2	D	265	ASN	N-CA-C	-5.42	105.01	111.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	265	ASN	N-CA-C	-5.42	105.01	111.03
1	A	495	ILE	CB-CA-C	5.42	119.36	110.69
1	A	318	TYR	CA-C-N	-5.41	115.08	122.93
1	A	318	TYR	C-N-CA	-5.41	115.08	122.93
1	E	318	TYR	CA-C-N	-5.41	115.08	122.93
1	E	318	TYR	C-N-CA	-5.41	115.08	122.93
2	F	252	TRP	N-CA-C	5.41	117.28	108.63
2	F	343	GLN	N-CA-C	-5.41	105.49	112.68
2	B	343	GLN	N-CA-C	-5.41	105.49	112.68
2	D	343	GLN	N-CA-C	-5.40	105.49	112.68
1	E	495	ILE	CB-CA-C	5.40	119.33	110.69
2	F	265	ASN	N-CA-C	-5.40	105.03	111.03
2	B	252	TRP	N-CA-C	5.39	117.25	108.63
2	H	252	TRP	N-CA-C	5.39	117.25	108.63
1	G	318	TYR	CA-C-N	-5.38	115.12	122.93
1	G	318	TYR	C-N-CA	-5.38	115.12	122.93
2	D	252	TRP	N-CA-C	5.38	117.23	108.63
1	G	317	VAL	CB-CA-C	-5.34	103.76	112.03
2	D	167	ILE	CB-CA-C	-5.32	104.96	112.14
1	A	317	VAL	CB-CA-C	-5.31	103.80	112.03
1	E	317	VAL	CB-CA-C	-5.31	103.80	112.03
2	B	167	ILE	CB-CA-C	-5.31	104.98	112.14
2	F	167	ILE	CB-CA-C	-5.30	104.98	112.14
2	H	167	ILE	CB-CA-C	-5.29	105.00	112.14
2	F	177	ASP	N-CA-C	5.28	119.46	108.53
1	C	317	VAL	CB-CA-C	-5.28	103.84	112.03
2	B	177	ASP	N-CA-C	5.28	119.45	108.53
2	H	177	ASP	N-CA-C	5.27	119.44	108.53
2	D	177	ASP	N-CA-C	5.26	119.43	108.53
2	H	419	THR	CA-C-N	5.22	125.76	120.38
2	H	419	THR	C-N-CA	5.22	125.76	120.38
1	G	414	TRP	N-CA-CB	-5.21	102.31	109.97
1	E	414	TRP	N-CA-CB	-5.21	102.31	109.97
1	A	414	TRP	N-CA-CB	-5.21	102.31	109.97
2	B	419	THR	CA-C-N	5.21	125.74	120.38
2	B	419	THR	C-N-CA	5.21	125.74	120.38
1	A	467	VAL	CB-CA-C	-5.20	101.89	111.36
1	C	414	TRP	N-CA-CB	-5.20	102.33	109.97
1	E	467	VAL	CB-CA-C	-5.20	101.90	111.36
1	C	467	VAL	CB-CA-C	-5.20	101.90	111.36
2	D	142	ILE	N-CA-C	-5.20	101.10	108.58
2	F	142	ILE	N-CA-C	-5.20	101.10	108.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	419	THR	CA-C-N	5.20	125.73	120.38
2	F	419	THR	C-N-CA	5.20	125.73	120.38
1	G	467	VAL	CB-CA-C	-5.19	101.91	111.36
2	H	142	ILE	N-CA-C	-5.19	101.10	108.58
2	B	142	ILE	N-CA-C	-5.18	101.11	108.58
2	H	302	GLU	N-CA-C	5.18	116.61	111.07
2	D	318	TYR	CA-C-N	-5.17	114.80	122.41
2	D	318	TYR	C-N-CA	-5.17	114.80	122.41
2	H	318	TYR	CA-C-N	-5.17	114.81	122.41
2	H	318	TYR	C-N-CA	-5.17	114.81	122.41
2	F	302	GLU	N-CA-C	5.16	116.59	111.07
2	B	318	TYR	CA-C-N	-5.16	114.82	122.41
2	B	318	TYR	C-N-CA	-5.16	114.82	122.41
2	F	318	TYR	CA-C-N	-5.16	114.83	122.41
2	F	318	TYR	C-N-CA	-5.16	114.83	122.41
2	D	419	THR	CA-C-N	5.15	125.69	120.38
2	D	419	THR	C-N-CA	5.15	125.69	120.38
2	B	302	GLU	N-CA-C	5.14	116.56	111.07
1	C	235	HIS	N-CA-C	-5.14	102.80	110.20
2	F	118	VAL	CB-CA-C	-5.13	104.78	110.68
2	D	151	GLN	N-CA-C	5.13	117.28	111.02
2	B	151	GLN	N-CA-C	5.12	117.26	111.02
2	H	151	GLN	N-CA-C	5.12	117.26	111.02
2	F	151	GLN	N-CA-C	5.12	117.26	111.02
2	D	302	GLU	N-CA-C	5.11	116.54	111.07
2	D	73	LYS	N-CA-C	-5.11	102.13	110.20
2	B	118	VAL	CB-CA-C	-5.11	104.81	110.68
2	H	118	VAL	CB-CA-C	-5.10	104.81	110.68
2	H	320	ASP	CA-C-N	5.10	126.21	119.84
2	H	320	ASP	C-N-CA	5.10	126.21	119.84
1	G	235	HIS	N-CA-C	-5.10	102.86	110.20
1	A	235	HIS	N-CA-C	-5.09	102.86	110.20
2	F	320	ASP	CA-C-N	5.09	126.21	119.84
2	F	320	ASP	C-N-CA	5.09	126.21	119.84
1	E	235	HIS	N-CA-C	-5.09	102.87	110.20
2	B	320	ASP	CA-C-N	5.09	126.20	119.84
2	B	320	ASP	C-N-CA	5.09	126.20	119.84
2	F	73	LYS	N-CA-C	-5.08	102.17	110.20
2	D	320	ASP	CA-C-N	5.08	126.19	119.84
2	D	320	ASP	C-N-CA	5.08	126.19	119.84
2	B	73	LYS	N-CA-C	-5.07	102.19	110.20
2	D	178	ILE	N-CA-C	-5.07	98.80	109.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	118	VAL	CB-CA-C	-5.06	104.86	110.68
1	G	193	LEU	N-CA-C	5.06	116.68	109.14
2	D	271	TYR	CA-C-N	5.06	126.16	119.84
2	D	271	TYR	C-N-CA	5.06	126.16	119.84
2	H	73	LYS	N-CA-C	-5.06	102.21	110.20
2	F	178	ILE	N-CA-C	-5.05	98.83	109.34
2	B	178	ILE	N-CA-C	-5.05	98.83	109.34
1	C	193	LEU	N-CA-C	5.05	116.67	109.14
1	A	193	LEU	N-CA-C	5.05	116.67	109.14
2	H	271	TYR	CA-C-N	5.04	126.14	119.84
2	H	271	TYR	C-N-CA	5.04	126.14	119.84
1	C	425	LEU	N-CA-C	-5.04	100.57	108.63
2	H	178	ILE	N-CA-C	-5.03	98.87	109.34
1	A	425	LEU	N-CA-C	-5.03	100.58	108.63
1	E	193	LEU	N-CA-C	5.03	116.63	109.14
2	F	198	HIS	N-CA-C	-5.03	104.76	111.24
2	D	198	HIS	N-CA-C	-5.03	104.76	111.24
2	B	271	TYR	CA-C-N	5.02	126.11	119.84
2	B	271	TYR	C-N-CA	5.02	126.11	119.84
1	G	319	TYR	N-CA-C	5.02	117.67	109.59
2	B	198	HIS	N-CA-C	-5.01	104.78	111.24
1	C	127	TYR	N-CA-C	5.01	117.47	111.71
1	E	319	TYR	N-CA-C	5.01	117.65	109.59
1	E	425	LEU	N-CA-C	-5.01	100.62	108.63

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	318	TYR	Sidechain
1	A	342	TYR	Sidechain
2	B	61	PHE	Sidechain
1	C	318	TYR	Sidechain
1	C	342	TYR	Sidechain
2	D	61	PHE	Sidechain
1	E	318	TYR	Sidechain
1	E	342	TYR	Sidechain
2	F	61	PHE	Sidechain
1	G	318	TYR	Sidechain
1	G	342	TYR	Sidechain
2	H	61	PHE	Sidechain

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	4200	0	4064	353	2
1	C	4200	0	4064	418	24
1	E	4200	0	4064	353	2
1	G	4200	0	4064	411	8
2	B	3198	0	3184	253	4
2	D	3198	0	3184	251	8
2	F	3198	0	3184	254	0
2	H	3198	0	3184	251	20
3	B	1	0	0	0	0
3	D	1	0	0	0	0
3	F	1	0	0	0	0
3	H	1	0	0	0	0
All	All	29596	0	28992	2389	34

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 41.

All (2389) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:345:PRO:HG3	1:G:326:ILE:CD1	1.22	1.68
1:C:346:PHE:CD1	1:G:390:LYS:CE	1.87	1.58
1:C:345:PRO:CG	1:G:326:ILE:CD1	1.79	1.54
1:C:346:PHE:CD1	1:G:390:LYS:HE3	0.98	1.51
1:C:346:PHE:CE1	1:G:390:LYS:HG3	1.60	1.36
1:C:346:PHE:HB2	1:G:390:LYS:NZ	1.46	1.28
1:C:417:VAL:HG11	1:G:346:PHE:CE2	1.67	1.27
1:C:417:VAL:CG1	1:G:346:PHE:CE2	2.19	1.25
1:C:345:PRO:CG	1:G:326:ILE:HD12	1.49	1.21
1:C:345:PRO:CG	1:G:326:ILE:HD13	1.56	1.12
1:C:345:PRO:HG2	1:G:326:ILE:CD1	1.70	1.11
1:C:346:PHE:CE1	1:G:390:LYS:HE3	1.89	1.07
1:C:345:PRO:HG2	1:G:326:ILE:HD13	1.23	1.07
1:E:393:ILE:HG23	1:E:414:TRP:CH2	1.93	1.04
1:C:393:ILE:HG23	1:C:414:TRP:CH2	1.93	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:393:ILE:HG23	1:G:414:TRP:CH2	1.93	1.03
1:A:393:ILE:HG23	1:A:414:TRP:CH2	1.93	1.02
2:B:264:LEU:HD22	2:B:274:ILE:HD11	1.42	1.02
2:D:264:LEU:HD22	2:D:274:ILE:HD11	1.42	1.02
2:H:264:LEU:HD22	2:H:274:ILE:HD11	1.42	1.02
2:F:264:LEU:HD22	2:F:274:ILE:HD11	1.42	1.02
1:C:346:PHE:CZ	1:G:390:LYS:HG3	1.95	1.00
1:C:346:PHE:CB	1:G:390:LYS:NZ	2.24	1.00
1:C:417:VAL:HG13	1:G:346:PHE:CE2	1.97	1.00
1:C:376:THR:HG23	1:C:386:THR:HG23	1.43	0.99
1:A:376:THR:HG23	1:A:386:THR:HG23	1.43	0.99
1:C:346:PHE:CE1	1:G:390:LYS:CG	2.46	0.98
1:C:346:PHE:CG	1:G:390:LYS:CE	2.47	0.98
1:G:376:THR:HG23	1:G:386:THR:HG23	1.43	0.97
1:C:346:PHE:HB2	1:G:390:LYS:HZ2	1.29	0.97
1:E:376:THR:HG23	1:E:386:THR:HG23	1.43	0.97
1:G:420:PRO:HG2	1:G:421:PRO:HD2	1.47	0.95
1:C:417:VAL:HG13	1:G:346:PHE:CD2	2.02	0.94
1:C:342:TYR:OH	1:G:345:PRO:HG3	1.68	0.94
2:D:103:LYS:HZ2	2:D:179:VAL:H	1.14	0.94
1:E:420:PRO:HG2	1:E:421:PRO:HD2	1.47	0.94
1:C:420:PRO:HG2	1:C:421:PRO:HD2	1.47	0.93
1:A:420:PRO:HG2	1:A:421:PRO:HD2	1.47	0.93
1:C:540:LYS:HZ1	2:D:265:ASN:HB2	1.34	0.93
1:C:417:VAL:HG11	1:G:346:PHE:CZ	2.03	0.92
2:F:103:LYS:HZ2	2:F:179:VAL:H	1.14	0.92
1:C:346:PHE:CE1	1:G:342:TYR:OH	2.22	0.92
2:B:103:LYS:HZ2	2:B:179:VAL:H	1.13	0.92
2:F:50:ILE:HG21	2:F:145:GLN:HB2	1.49	0.92
2:H:50:ILE:HG21	2:H:145:GLN:HB2	1.49	0.92
2:D:50:ILE:HG21	2:D:145:GLN:HB2	1.49	0.91
1:A:540:LYS:NZ	2:B:265:ASN:HB2	1.86	0.91
1:G:540:LYS:NZ	2:H:265:ASN:HB2	1.86	0.91
2:B:50:ILE:HG21	2:B:145:GLN:HB2	1.49	0.91
1:C:540:LYS:NZ	2:D:265:ASN:HB2	1.86	0.91
1:C:346:PHE:HB2	1:G:390:LYS:HZ1	1.10	0.90
1:C:346:PHE:HE1	1:G:342:TYR:OH	1.53	0.90
1:C:346:PHE:CB	1:G:390:LYS:HZ2	1.83	0.90
2:H:103:LYS:HZ2	2:H:179:VAL:H	1.14	0.90
2:H:260:LEU:HD21	2:H:303:LEU:HD21	1.53	0.90
1:E:540:LYS:NZ	2:F:265:ASN:HB2	1.86	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:107:THR:HG23	1:A:198:HIS:HE1	1.38	0.89
1:C:107:THR:HG23	1:C:198:HIS:HE1	1.38	0.89
1:G:107:THR:HG23	1:G:198:HIS:HE1	1.38	0.89
2:D:260:LEU:HD21	2:D:303:LEU:HD21	1.54	0.89
2:B:260:LEU:HD21	2:B:303:LEU:HD21	1.54	0.88
1:E:107:THR:HG23	1:E:198:HIS:HE1	1.38	0.88
2:F:104:LYS:HB3	2:F:192:ASP:HA	1.55	0.87
2:F:260:LEU:HD21	2:F:303:LEU:HD21	1.54	0.87
2:H:104:LYS:HB3	2:H:192:ASP:HA	1.55	0.86
1:C:346:PHE:CD1	1:G:390:LYS:CD	2.57	0.86
1:C:244:ILE:HD12	1:C:267:ALA:HB2	1.56	0.86
1:G:244:ILE:HD12	1:G:267:ALA:HB2	1.56	0.86
2:H:171:PHE:HE2	2:H:204:GLU:HB2	1.41	0.86
1:A:317:VAL:HG21	1:A:347:LYS:HB3	1.58	0.86
1:C:317:VAL:HG21	1:C:347:LYS:HB3	1.58	0.86
2:F:171:PHE:HE2	2:F:204:GLU:HB2	1.41	0.86
1:G:317:VAL:HG21	1:G:347:LYS:HB3	1.58	0.85
2:D:104:LYS:HB3	2:D:192:ASP:HA	1.55	0.85
2:B:104:LYS:HB3	2:B:192:ASP:HA	1.55	0.85
1:G:540:LYS:HZ1	2:H:265:ASN:HB2	1.39	0.85
1:E:317:VAL:HG21	1:E:347:LYS:HB3	1.58	0.85
1:A:244:ILE:HD12	1:A:267:ALA:HB2	1.56	0.84
1:E:244:ILE:HD12	1:E:267:ALA:HB2	1.56	0.84
2:F:365:VAL:HG11	2:F:401:TRP:HB2	1.59	0.84
2:B:365:VAL:HG11	2:B:401:TRP:HB2	1.59	0.84
1:C:417:VAL:CG1	1:G:346:PHE:CD2	2.59	0.84
1:E:391:LEU:HB2	1:E:414:TRP:CZ3	2.13	0.84
1:C:342:TYR:OH	1:G:345:PRO:CB	2.26	0.84
2:D:171:PHE:HE2	2:D:204:GLU:HB2	1.41	0.83
2:B:171:PHE:HE2	2:B:204:GLU:HB2	1.41	0.83
1:G:391:LEU:HB2	1:G:414:TRP:CZ3	2.13	0.83
1:A:391:LEU:HB2	1:A:414:TRP:CZ3	2.13	0.83
2:D:365:VAL:HG11	2:D:401:TRP:HB2	1.59	0.83
2:H:365:VAL:HG11	2:H:401:TRP:HB2	1.59	0.82
2:B:24:TRP:CH2	2:B:61:PHE:CD1	2.68	0.82
1:C:391:LEU:HB2	1:C:414:TRP:CZ3	2.13	0.82
2:D:24:TRP:CH2	2:D:61:PHE:CD1	2.68	0.82
1:C:342:TYR:OH	1:G:345:PRO:CG	2.26	0.82
2:H:61:PHE:CZ	2:H:74:LEU:HD23	2.14	0.82
2:D:61:PHE:CZ	2:D:74:LEU:HD23	2.14	0.82
2:F:61:PHE:CZ	2:F:74:LEU:HD23	2.14	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:326:ILE:HB	1:C:342:TYR:CE1	2.15	0.82
1:G:326:ILE:HB	1:G:342:TYR:CE1	2.15	0.82
1:A:326:ILE:HB	1:A:342:TYR:CE1	2.15	0.82
2:D:33:ALA:O	2:D:37:ILE:HG13	1.80	0.82
2:F:33:ALA:O	2:F:37:ILE:HG13	1.80	0.82
2:B:33:ALA:O	2:B:37:ILE:HG13	1.80	0.81
2:B:61:PHE:CZ	2:B:74:LEU:HD23	2.14	0.81
2:H:24:TRP:CH2	2:H:61:PHE:CD1	2.68	0.81
2:H:24:TRP:HH2	2:H:61:PHE:CE1	1.99	0.81
2:H:33:ALA:O	2:H:37:ILE:HG13	1.80	0.81
1:E:107:THR:HG23	1:E:198:HIS:CE1	2.16	0.81
1:E:326:ILE:HB	1:E:342:TYR:CE1	2.15	0.81
2:F:157:PRO:HG2	2:F:158:ALA:H	1.46	0.81
2:F:24:TRP:HH2	2:F:61:PHE:CE1	1.99	0.81
2:F:24:TRP:CH2	2:F:61:PHE:CD1	2.68	0.80
1:G:107:THR:HG23	1:G:198:HIS:CE1	2.16	0.80
2:H:157:PRO:HG2	2:H:158:ALA:H	1.46	0.80
1:A:107:THR:HG23	1:A:198:HIS:CE1	2.16	0.80
1:E:91:GLN:HE21	1:E:91:GLN:HA	1.47	0.80
1:G:91:GLN:HA	1:G:91:GLN:HE21	1.47	0.80
1:C:91:GLN:HA	1:C:91:GLN:HE21	1.47	0.80
2:D:24:TRP:HH2	2:D:61:PHE:CE1	1.99	0.80
1:C:107:THR:HG23	1:C:198:HIS:CE1	2.16	0.79
2:B:24:TRP:HH2	2:B:61:PHE:CE1	1.99	0.79
2:B:249:LYS:HB2	2:B:252:TRP:CE2	2.18	0.79
2:H:103:LYS:HZ1	2:H:179:VAL:HG23	1.46	0.79
1:G:393:ILE:HB	1:G:423:VAL:CG2	2.12	0.79
2:D:249:LYS:HB2	2:D:252:TRP:CE2	2.18	0.79
1:C:393:ILE:HB	1:C:423:VAL:CG2	2.12	0.79
2:F:103:LYS:HZ1	2:F:179:VAL:HG23	1.46	0.79
1:A:91:GLN:HA	1:A:91:GLN:HE21	1.47	0.79
1:A:391:LEU:HB2	1:A:414:TRP:HZ3	1.48	0.79
1:G:361:HIS:CD2	1:G:518:VAL:HG11	2.18	0.78
2:D:157:PRO:HG2	2:D:158:ALA:H	1.46	0.78
1:A:393:ILE:HB	1:A:423:VAL:CG2	2.12	0.78
1:C:95:PRO:HG2	1:C:230:MET:HE1	1.65	0.78
1:E:393:ILE:HB	1:E:423:VAL:CG2	2.12	0.78
1:G:95:PRO:HG2	1:G:230:MET:HE1	1.65	0.78
2:B:157:PRO:HG2	2:B:158:ALA:H	1.46	0.78
2:H:249:LYS:HB2	2:H:252:TRP:CE2	2.18	0.78
1:C:391:LEU:HB2	1:C:414:TRP:HZ3	1.48	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:420:PRO:HB2	2:F:421:PRO:HD2	1.66	0.78
2:F:249:LYS:HB2	2:F:252:TRP:CE2	2.18	0.78
1:E:540:LYS:HZ1	2:F:265:ASN:HB2	1.44	0.78
1:A:361:HIS:HD2	1:A:518:VAL:HG11	1.49	0.77
1:A:95:PRO:HG2	1:A:230:MET:HE1	1.65	0.77
1:C:346:PHE:CG	1:G:390:LYS:NZ	2.52	0.77
1:E:95:PRO:HG2	1:E:230:MET:HE1	1.65	0.77
1:E:361:HIS:CD2	1:E:518:VAL:HG11	2.18	0.77
1:A:361:HIS:CD2	1:A:518:VAL:HG11	2.18	0.77
1:G:361:HIS:HD2	1:G:518:VAL:HG11	1.49	0.77
1:C:361:HIS:HD2	1:C:518:VAL:HG11	1.49	0.77
1:C:361:HIS:CD2	1:C:518:VAL:HG11	2.18	0.77
2:B:420:PRO:HB2	2:B:421:PRO:HD2	1.66	0.76
1:G:391:LEU:HB2	1:G:414:TRP:HZ3	1.48	0.76
2:H:420:PRO:HB2	2:H:421:PRO:HD2	1.66	0.76
1:E:354:TYR:OH	1:E:356:ARG:HD3	1.85	0.76
2:D:420:PRO:HB2	2:D:421:PRO:HD2	1.66	0.76
2:D:103:LYS:HZ1	2:D:179:VAL:HG23	1.51	0.75
1:A:85:GLN:HG2	1:A:85:GLN:O	1.86	0.75
2:D:24:TRP:HH2	2:D:61:PHE:CD1	2.05	0.75
1:G:354:TYR:OH	1:G:356:ARG:HD3	1.85	0.75
1:E:85:GLN:O	1:E:85:GLN:HG2	1.86	0.75
1:C:354:TYR:OH	1:C:356:ARG:HD3	1.85	0.75
2:B:103:LYS:HZ1	2:B:179:VAL:HG23	1.52	0.74
1:C:131:THR:HG22	1:C:143:ARG:HG3	1.69	0.74
1:C:249:LYS:HE2	1:C:251:SER:HB3	1.69	0.74
1:E:391:LEU:HB2	1:E:414:TRP:HZ3	1.48	0.74
1:C:10:VAL:HG21	1:C:153:TRP:HH2	1.52	0.74
2:F:17:ASP:O	2:F:83:ARG:HD3	1.87	0.74
2:F:24:TRP:HH2	2:F:61:PHE:CD1	2.05	0.74
1:G:131:THR:HG22	1:G:143:ARG:HG3	1.69	0.74
1:A:10:VAL:HG21	1:A:153:TRP:HH2	1.52	0.74
1:A:354:TYR:OH	1:A:356:ARG:HD3	1.85	0.74
1:C:342:TYR:CZ	1:G:345:PRO:HG3	2.22	0.74
1:E:361:HIS:HD2	1:E:518:VAL:HG11	1.49	0.74
1:C:85:GLN:O	1:C:85:GLN:HG2	1.86	0.74
1:A:249:LYS:HE2	1:A:251:SER:HB3	1.69	0.74
1:A:131:THR:HG22	1:A:143:ARG:HG3	1.69	0.74
2:B:24:TRP:HH2	2:B:61:PHE:CD1	2.05	0.74
1:E:10:VAL:HG21	1:E:153:TRP:HH2	1.52	0.74
1:G:6:GLU:H	1:G:6:GLU:CD	1.95	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:6:GLU:CD	1:C:6:GLU:H	1.95	0.74
1:G:10:VAL:HG21	1:G:153:TRP:HH2	1.52	0.74
1:G:85:GLN:HG2	1:G:85:GLN:O	1.86	0.74
1:A:6:GLU:H	1:A:6:GLU:CD	1.95	0.74
1:G:249:LYS:HE2	1:G:251:SER:HB3	1.69	0.74
2:H:17:ASP:O	2:H:83:ARG:HD3	1.87	0.74
1:E:6:GLU:H	1:E:6:GLU:CD	1.95	0.73
1:E:249:LYS:HE2	1:E:251:SER:HB3	1.69	0.73
1:E:391:LEU:HD12	1:E:414:TRP:CE3	2.23	0.73
2:B:17:ASP:O	2:B:83:ARG:HD3	1.87	0.73
2:D:103:LYS:NZ	2:D:179:VAL:HG23	2.04	0.73
2:B:50:ILE:CG2	2:B:145:GLN:HB2	2.18	0.73
2:B:63:ILE:HG23	2:B:72:ARG:HB3	1.70	0.73
2:B:103:LYS:NZ	2:B:179:VAL:HG23	2.04	0.73
2:D:17:ASP:O	2:D:83:ARG:HD3	1.87	0.73
1:E:90:VAL:HG12	2:F:141:GLY:H	1.53	0.73
1:G:391:LEU:HD12	1:G:414:TRP:CE3	2.24	0.73
2:H:24:TRP:HH2	2:H:61:PHE:CD1	2.04	0.73
1:C:90:VAL:HG12	2:D:141:GLY:H	1.53	0.73
1:E:131:THR:HG22	1:E:143:ARG:HG3	1.69	0.73
2:H:103:LYS:NZ	2:H:179:VAL:HG23	2.04	0.73
2:D:63:ILE:HG23	2:D:72:ARG:HB3	1.70	0.73
1:G:90:VAL:HG12	2:H:141:GLY:H	1.53	0.73
1:E:442:VAL:CG1	1:E:481:ALA:HB1	2.19	0.72
2:H:171:PHE:HB2	2:H:208:HIS:CE1	2.24	0.72
1:A:391:LEU:HD12	1:A:414:TRP:CE3	2.24	0.72
1:C:157:PRO:HG2	1:C:158:ALA:H	1.54	0.72
1:G:157:PRO:HG2	1:G:158:ALA:H	1.54	0.72
2:B:171:PHE:HB2	2:B:208:HIS:CE1	2.24	0.72
2:D:171:PHE:HB2	2:D:208:HIS:CE1	2.25	0.72
2:D:246:LEU:HD11	2:D:264:LEU:HD21	1.72	0.72
2:F:50:ILE:CG2	2:F:145:GLN:HB2	2.18	0.72
2:H:246:LEU:HD11	2:H:264:LEU:HD21	1.72	0.72
1:A:90:VAL:HG12	2:B:141:GLY:H	1.53	0.72
2:B:246:LEU:HD11	2:B:264:LEU:HD21	1.72	0.72
1:A:393:ILE:O	1:A:414:TRP:HH2	1.73	0.72
1:C:391:LEU:HD12	1:C:414:TRP:CE3	2.23	0.72
1:E:157:PRO:HG2	1:E:158:ALA:H	1.54	0.72
1:C:393:ILE:O	1:C:414:TRP:HH2	1.73	0.72
2:F:103:LYS:NZ	2:F:179:VAL:HG23	2.04	0.72
2:F:171:PHE:HB2	2:F:208:HIS:CE1	2.25	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:442:VAL:CG1	1:G:481:ALA:HB1	2.19	0.72
1:C:442:VAL:CG1	1:C:481:ALA:HB1	2.19	0.72
2:D:50:ILE:CG2	2:D:145:GLN:HB2	2.18	0.72
2:F:63:ILE:HG23	2:F:72:ARG:HB3	1.70	0.71
2:F:92:LEU:HG	2:F:158:ALA:HB2	1.72	0.71
1:E:518:VAL:O	1:E:522:ILE:HG13	1.90	0.71
1:A:518:VAL:O	1:A:522:ILE:HG13	1.90	0.71
1:C:95:PRO:CG	1:C:230:MET:HE1	2.20	0.71
1:C:341:ILE:HD12	1:C:383:TRP:HE1	1.55	0.71
1:E:341:ILE:HD12	1:E:383:TRP:HE1	1.55	0.71
1:G:518:VAL:O	1:G:522:ILE:HG13	1.90	0.71
1:A:157:PRO:HG2	1:A:158:ALA:H	1.54	0.71
2:H:63:ILE:HG23	2:H:72:ARG:HB3	1.70	0.71
1:A:442:VAL:CG1	1:A:481:ALA:HB1	2.19	0.71
1:G:393:ILE:O	1:G:414:TRP:HH2	1.73	0.71
2:H:47:ILE:HG22	2:H:48:SER:H	1.56	0.71
1:E:393:ILE:O	1:E:414:TRP:HH2	1.73	0.71
2:F:246:LEU:HD11	2:F:264:LEU:HD21	1.72	0.71
1:A:95:PRO:CG	1:A:230:MET:HE1	2.20	0.71
2:B:47:ILE:HG22	2:B:48:SER:H	1.56	0.71
1:C:518:VAL:O	1:C:522:ILE:HG13	1.90	0.71
2:D:47:ILE:HG22	2:D:48:SER:H	1.56	0.71
2:H:50:ILE:CG2	2:H:145:GLN:HB2	2.18	0.71
1:A:225:PRO:HG2	1:A:226:PRO:HD3	1.73	0.70
1:A:341:ILE:HD12	1:A:383:TRP:HE1	1.55	0.70
1:C:225:PRO:HG2	1:C:226:PRO:HD3	1.73	0.70
1:G:95:PRO:CG	1:G:230:MET:HE1	2.20	0.70
1:G:341:ILE:HD12	1:G:383:TRP:HE1	1.55	0.70
2:H:92:LEU:HG	2:H:158:ALA:HB2	1.72	0.70
2:D:92:LEU:HG	2:D:158:ALA:HB2	1.72	0.70
1:A:540:LYS:HZ3	2:B:261:VAL:CG1	2.05	0.70
2:B:103:LYS:HZ2	2:B:179:VAL:N	1.89	0.70
2:F:47:ILE:HG22	2:F:48:SER:H	1.56	0.70
1:A:114:ALA:HB1	1:A:160:PHE:CZ	2.27	0.70
1:E:114:ALA:HB1	1:E:160:PHE:CZ	2.27	0.70
1:C:345:PRO:HG3	1:G:326:ILE:HD12	0.70	0.70
1:E:95:PRO:CG	1:E:230:MET:HE1	2.20	0.70
1:G:114:ALA:HB1	1:G:160:PHE:CZ	2.27	0.70
2:D:168:LEU:HD21	2:D:209:LEU:HD21	1.74	0.70
2:F:59:PRO:HG2	2:F:76:ASP:HB3	1.74	0.70
2:H:136:ASN:HB3	2:H:138:GLU:HG3	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:103:LYS:HZ2	2:D:179:VAL:N	1.89	0.69
1:E:225:PRO:HG2	1:E:226:PRO:HD3	1.73	0.69
2:B:92:LEU:HG	2:B:158:ALA:HB2	1.72	0.69
1:G:416:PHE:CD1	1:G:417:VAL:N	2.60	0.69
2:H:168:LEU:HD21	2:H:209:LEU:HD21	1.74	0.69
2:B:59:PRO:HG2	2:B:76:ASP:HB3	1.74	0.69
1:E:416:PHE:CD1	1:E:417:VAL:N	2.60	0.69
1:G:31:ILE:O	1:G:35:VAL:HG23	1.92	0.69
1:C:31:ILE:O	1:C:35:VAL:HG23	1.92	0.69
1:E:233:GLU:OE2	1:E:242:GLN:HG3	1.93	0.69
1:A:416:PHE:CD1	1:A:417:VAL:N	2.60	0.69
1:A:419:THR:HG23	1:A:420:PRO:HD2	1.74	0.69
1:A:540:LYS:HZ1	2:B:265:ASN:HB2	1.57	0.69
1:C:426:TRP:HA	1:C:426:TRP:CE3	2.28	0.69
1:G:225:PRO:HG2	1:G:226:PRO:HD3	1.73	0.69
1:G:233:GLU:OE2	1:G:242:GLN:HG3	1.93	0.69
1:A:31:ILE:O	1:A:35:VAL:HG23	1.92	0.69
1:A:442:VAL:HG12	1:A:481:ALA:HB1	1.75	0.69
1:C:114:ALA:HB1	1:C:160:PHE:CZ	2.27	0.69
1:C:233:GLU:OE2	1:C:242:GLN:HG3	1.93	0.69
1:C:416:PHE:CD1	1:C:417:VAL:N	2.60	0.69
1:C:419:THR:HG23	1:C:420:PRO:HD2	1.74	0.69
2:D:59:PRO:HG2	2:D:76:ASP:HB3	1.74	0.69
2:D:136:ASN:HB3	2:D:138:GLU:HG3	1.74	0.69
1:E:442:VAL:HG12	1:E:481:ALA:HB1	1.75	0.69
1:G:130:PHE:CZ	1:G:144:TYR:HB2	2.28	0.69
1:G:426:TRP:CE3	1:G:426:TRP:HA	2.28	0.69
2:H:316:GLY:O	2:H:318:TYR:HD1	1.76	0.69
1:E:426:TRP:HA	1:E:426:TRP:CE3	2.28	0.69
2:F:316:GLY:O	2:F:318:TYR:HD1	1.76	0.69
1:C:99:GLY:HA2	1:C:383:TRP:CZ3	2.28	0.69
1:C:221:HIS:O	1:C:223:LYS:N	2.26	0.69
1:A:99:GLY:HA2	1:A:383:TRP:CZ3	2.28	0.68
2:B:136:ASN:HB3	2:B:138:GLU:HG3	1.74	0.68
2:B:168:LEU:HD21	2:B:209:LEU:HD21	1.74	0.68
2:B:316:GLY:O	2:B:318:TYR:HD1	1.76	0.68
1:E:221:HIS:O	1:E:223:LYS:N	2.26	0.68
2:F:72:ARG:HH12	2:F:409:THR:HG22	1.58	0.68
1:G:221:HIS:O	1:G:223:LYS:N	2.26	0.68
2:H:59:PRO:HG2	2:H:76:ASP:HB3	1.74	0.68
1:A:221:HIS:O	1:A:223:LYS:N	2.27	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:426:TRP:HA	1:A:426:TRP:CE3	2.28	0.68
1:C:130:PHE:CZ	1:C:144:TYR:HB2	2.28	0.68
1:G:442:VAL:HG12	1:G:481:ALA:HB1	1.75	0.68
2:D:316:GLY:O	2:D:318:TYR:HD1	1.76	0.68
2:H:163:SER:O	2:H:167:ILE:HG13	1.94	0.68
1:A:130:PHE:CZ	1:A:144:TYR:HB2	2.28	0.68
1:A:233:GLU:OE2	1:A:242:GLN:HG3	1.93	0.68
2:F:104:LYS:HA	2:F:237:ASP:OD2	1.94	0.68
2:F:163:SER:O	2:F:167:ILE:HG13	1.93	0.68
2:B:72:ARG:HH12	2:B:409:THR:HG22	1.58	0.68
1:C:442:VAL:HG12	1:C:481:ALA:HB1	1.75	0.68
1:E:31:ILE:O	1:E:35:VAL:HG23	1.92	0.68
1:E:130:PHE:CZ	1:E:144:TYR:HB2	2.28	0.68
1:G:99:GLY:HA2	1:G:383:TRP:CZ3	2.28	0.68
2:H:104:LYS:HA	2:H:237:ASP:OD2	1.94	0.68
1:E:100:LEU:O	1:E:318:TYR:HB3	1.94	0.68
2:H:72:ARG:HH12	2:H:409:THR:HG22	1.58	0.68
2:B:163:SER:O	2:B:167:ILE:HG13	1.94	0.68
1:E:99:GLY:HA2	1:E:383:TRP:CZ3	2.28	0.68
2:F:136:ASN:HB3	2:F:138:GLU:HG3	1.74	0.68
2:F:168:LEU:HD21	2:F:209:LEU:HD21	1.74	0.68
1:G:420:PRO:HG2	1:G:421:PRO:CD	2.22	0.68
2:D:72:ARG:HH12	2:D:409:THR:HG22	1.58	0.68
2:D:97:PRO:HG2	2:D:181:TYR:HB2	1.76	0.68
2:D:163:SER:O	2:D:167:ILE:HG13	1.94	0.68
1:E:419:THR:HG23	1:E:420:PRO:HD2	1.74	0.68
2:B:104:LYS:HA	2:B:237:ASP:OD2	1.94	0.68
1:E:98:ALA:CB	1:E:383:TRP:HH2	2.07	0.68
2:F:123:ASP:HA	2:F:126:LYS:NZ	2.09	0.68
2:H:97:PRO:HG2	2:H:181:TYR:HB2	1.76	0.68
1:C:100:LEU:O	1:C:318:TYR:HB3	1.94	0.67
1:C:345:PRO:CD	1:G:326:ILE:HD12	2.24	0.67
2:D:104:LYS:HA	2:D:237:ASP:OD2	1.94	0.67
1:C:346:PHE:CD1	1:G:390:LYS:NZ	2.62	0.67
1:E:378:GLU:O	1:E:382:ILE:HG13	1.95	0.67
1:G:100:LEU:O	1:G:318:TYR:HB3	1.94	0.67
1:G:419:THR:HG23	1:G:420:PRO:HD2	1.74	0.67
1:A:426:TRP:HA	1:A:426:TRP:HE3	1.59	0.67
1:A:100:LEU:O	1:A:318:TYR:HB3	1.94	0.67
2:B:97:PRO:HG2	2:B:181:TYR:HB2	1.76	0.67
2:B:123:ASP:HA	2:B:126:LYS:NZ	2.10	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:244:ILE:CD1	1:E:267:ALA:HB2	2.25	0.67
2:F:41:MET:HE1	2:F:73:LYS:HD2	1.76	0.67
2:F:94:ILE:HG22	2:F:95:PRO:CD	2.24	0.67
2:F:97:PRO:HG2	2:F:181:TYR:HB2	1.76	0.67
1:G:378:GLU:O	1:G:382:ILE:HG13	1.95	0.67
1:G:393:ILE:O	1:G:414:TRP:CH2	2.48	0.67
1:A:378:GLU:O	1:A:382:ILE:HG13	1.95	0.67
2:D:41:MET:HE1	2:D:73:LYS:HD2	1.76	0.67
2:D:123:ASP:HA	2:D:126:LYS:NZ	2.10	0.67
1:A:244:ILE:CD1	1:A:267:ALA:HB2	2.25	0.67
1:G:98:ALA:CB	1:G:383:TRP:HH2	2.07	0.67
2:H:123:ASP:HA	2:H:126:LYS:NZ	2.10	0.67
2:F:153:TRP:CZ3	2:F:155:GLY:HA3	2.30	0.67
1:C:426:TRP:HA	1:C:426:TRP:HE3	1.59	0.67
1:C:457:TYR:CE1	1:C:465:LYS:HB3	2.30	0.67
2:D:94:ILE:HG22	2:D:95:PRO:CD	2.25	0.67
1:G:244:ILE:CD1	1:G:267:ALA:HB2	2.25	0.67
1:A:98:ALA:CB	1:A:383:TRP:HH2	2.07	0.66
2:B:153:TRP:CZ3	2:B:155:GLY:HA3	2.30	0.66
1:G:457:TYR:CE1	1:G:465:LYS:HB3	2.31	0.66
2:H:94:ILE:HG22	2:H:95:PRO:CD	2.25	0.66
2:H:103:LYS:HZ2	2:H:179:VAL:N	1.91	0.66
1:C:378:GLU:O	1:C:382:ILE:HG13	1.95	0.66
1:E:426:TRP:HA	1:E:426:TRP:HE3	1.59	0.66
1:A:457:TYR:CE1	1:A:465:LYS:HB3	2.31	0.66
1:E:393:ILE:O	1:E:414:TRP:CH2	2.48	0.66
1:E:420:PRO:HG2	1:E:421:PRO:CD	2.22	0.66
2:F:109:LEU:HD12	2:F:187:LEU:HD23	1.77	0.66
1:G:33:ALA:O	1:G:37:ILE:HG13	1.95	0.66
1:G:167:ILE:O	1:G:208:HIS:HE1	1.78	0.66
2:B:157:PRO:HG2	2:B:158:ALA:N	2.08	0.66
1:E:167:ILE:O	1:E:208:HIS:HE1	1.78	0.66
2:F:21:VAL:CG1	2:F:59:PRO:HD3	2.26	0.66
2:H:21:VAL:CG1	2:H:59:PRO:HD3	2.26	0.66
2:H:41:MET:HE1	2:H:73:LYS:HD2	1.76	0.66
2:B:41:MET:HE1	2:B:73:LYS:HD2	1.76	0.66
2:B:94:ILE:HG22	2:B:95:PRO:CD	2.25	0.66
2:D:153:TRP:CZ3	2:D:155:GLY:HA3	2.30	0.66
1:E:457:TYR:CE1	1:E:465:LYS:HB3	2.31	0.66
1:E:149:LEU:HD22	1:E:156:SER:HA	1.78	0.66
1:C:98:ALA:CB	1:C:383:TRP:HH2	2.07	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:393:ILE:O	1:C:414:TRP:CH2	2.48	0.66
2:H:109:LEU:HD12	2:H:187:LEU:HD23	1.77	0.66
2:H:153:TRP:CZ3	2:H:155:GLY:HA3	2.30	0.66
2:H:157:PRO:HG2	2:H:158:ALA:N	2.08	0.66
1:A:165:THR:HG21	2:B:140:PRO:HG2	1.77	0.66
2:B:21:VAL:CG1	2:B:59:PRO:HD3	2.26	0.66
1:C:537:PRO:HG2	2:D:262:GLY:HA2	1.78	0.66
1:G:165:THR:HG21	2:H:140:PRO:HG2	1.77	0.66
2:B:151:GLN:HE21	2:B:151:GLN:HA	1.61	0.66
2:F:151:GLN:HA	2:F:151:GLN:HE21	1.61	0.66
1:G:149:LEU:HD22	1:G:156:SER:HA	1.78	0.66
1:A:33:ALA:O	1:A:37:ILE:HG13	1.95	0.65
1:A:393:ILE:O	1:A:414:TRP:CH2	2.48	0.65
1:C:165:THR:HG21	2:D:140:PRO:HG2	1.77	0.65
1:C:167:ILE:O	1:C:208:HIS:HE1	1.78	0.65
2:D:21:VAL:CG1	2:D:59:PRO:HD3	2.26	0.65
1:E:33:ALA:O	1:E:37:ILE:HG13	1.95	0.65
1:A:27:THR:OG1	1:A:30:LYS:HG3	1.97	0.65
1:A:167:ILE:O	1:A:208:HIS:HE1	1.78	0.65
1:A:537:PRO:HG2	2:B:262:GLY:HA2	1.78	0.65
2:B:61:PHE:CE2	2:B:74:LEU:HD23	2.31	0.65
2:B:103:LYS:NZ	2:B:179:VAL:H	1.93	0.65
2:B:169:GLU:HB3	2:B:170:PRO:HD3	1.78	0.65
2:D:157:PRO:HG2	2:D:158:ALA:N	2.08	0.65
2:D:169:GLU:HB3	2:D:170:PRO:HD3	1.78	0.65
2:D:151:GLN:HA	2:D:151:GLN:HE21	1.61	0.65
1:G:27:THR:OG1	1:G:30:LYS:HG3	1.97	0.65
2:D:109:LEU:HD12	2:D:187:LEU:HD23	1.77	0.65
2:F:61:PHE:CE2	2:F:74:LEU:HD23	2.31	0.65
1:C:27:THR:OG1	1:C:30:LYS:HG3	1.97	0.65
1:C:33:ALA:O	1:C:37:ILE:HG13	1.95	0.65
1:C:420:PRO:HG2	1:C:421:PRO:CD	2.22	0.65
2:D:303:LEU:O	2:D:307:ARG:HG3	1.97	0.65
1:E:27:THR:OG1	1:E:30:LYS:HG3	1.97	0.65
1:G:406:TRP:CE3	1:G:407:GLN:HG3	2.32	0.65
2:H:151:GLN:HA	2:H:151:GLN:HE21	1.61	0.65
2:H:303:LEU:O	2:H:307:ARG:HG3	1.97	0.65
1:E:248:GLU:HG3	1:E:307:ARG:HH21	1.62	0.65
1:E:537:PRO:HG2	2:F:262:GLY:HA2	1.78	0.65
1:G:328:GLU:O	1:G:339:TYR:HA	1.97	0.65
1:G:426:TRP:HA	1:G:426:TRP:HE3	1.59	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:537:PRO:HG2	2:H:262:GLY:HA2	1.78	0.65
2:H:61:PHE:CE2	2:H:74:LEU:HD23	2.31	0.65
2:H:104:LYS:NZ	2:H:194:GLU:HA	2.12	0.65
1:A:406:TRP:CE3	1:A:407:GLN:HG3	2.32	0.65
2:B:303:LEU:O	2:B:307:ARG:HG3	1.97	0.65
2:D:61:PHE:CE2	2:D:74:LEU:HD23	2.31	0.65
2:F:103:LYS:HZ2	2:F:179:VAL:N	1.91	0.65
2:F:103:LYS:NZ	2:F:179:VAL:H	1.93	0.65
1:G:248:GLU:HG3	1:G:307:ARG:HH21	1.62	0.65
1:A:149:LEU:HD22	1:A:156:SER:HA	1.78	0.65
1:A:328:GLU:O	1:A:339:TYR:HA	1.97	0.65
2:B:109:LEU:HD12	2:B:187:LEU:HD23	1.77	0.65
1:C:406:TRP:CE3	1:C:407:GLN:HG3	2.32	0.65
2:F:28:GLU:HG3	2:F:135:ILE:CD1	2.27	0.65
1:A:248:GLU:HG3	1:A:307:ARG:HH21	1.62	0.65
2:B:28:GLU:HG3	2:B:135:ILE:CD1	2.27	0.65
1:C:328:GLU:O	1:C:339:TYR:HA	1.97	0.65
1:E:406:TRP:CE3	1:E:407:GLN:HG3	2.32	0.65
1:E:540:LYS:HZ3	2:F:261:VAL:CG1	2.10	0.65
2:F:303:LEU:O	2:F:307:ARG:HG3	1.97	0.65
2:H:28:GLU:HG3	2:H:135:ILE:CD1	2.27	0.65
1:C:248:GLU:HG3	1:C:307:ARG:HH21	1.62	0.64
2:D:28:GLU:HG3	2:D:135:ILE:CD1	2.27	0.64
1:E:328:GLU:O	1:E:339:TYR:HA	1.97	0.64
1:G:537:PRO:HD2	1:G:542:ILE:CD1	2.27	0.64
1:C:149:LEU:HD22	1:C:156:SER:HA	1.78	0.64
1:C:244:ILE:CD1	1:C:267:ALA:HB2	2.25	0.64
1:C:376:THR:HG23	1:C:386:THR:CG2	2.25	0.64
1:E:165:THR:HG21	2:F:140:PRO:HG2	1.77	0.64
2:B:24:TRP:CZ3	2:B:61:PHE:HB3	2.32	0.64
2:B:264:LEU:CD2	2:B:274:ILE:HD11	2.24	0.64
1:C:393:ILE:HG23	1:C:414:TRP:HH2	1.58	0.64
2:D:24:TRP:CZ3	2:D:61:PHE:HB3	2.32	0.64
2:D:149:LEU:HD22	2:D:156:SER:HA	1.79	0.64
1:E:537:PRO:HD2	1:E:542:ILE:CD1	2.27	0.64
2:B:104:LYS:NZ	2:B:194:GLU:HA	2.12	0.64
1:C:537:PRO:HD2	1:C:542:ILE:CD1	2.27	0.64
2:D:104:LYS:NZ	2:D:194:GLU:HA	2.12	0.64
2:F:24:TRP:CZ3	2:F:61:PHE:HB3	2.32	0.64
2:F:104:LYS:NZ	2:F:194:GLU:HA	2.12	0.64
2:F:246:LEU:HB2	2:F:307:ARG:NH1	2.13	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:246:LEU:CD1	2:B:264:LEU:HD21	2.27	0.64
2:D:103:LYS:NZ	2:D:179:VAL:H	1.93	0.64
2:F:157:PRO:HG2	2:F:158:ALA:N	2.08	0.64
2:H:126:LYS:HA	2:H:145:GLN:NE2	2.13	0.64
2:H:246:LEU:CD1	2:H:264:LEU:HD21	2.27	0.64
2:H:246:LEU:HB2	2:H:307:ARG:NH1	2.13	0.64
2:B:149:LEU:HD22	2:B:156:SER:HA	1.79	0.64
2:D:264:LEU:CD2	2:D:274:ILE:HD11	2.24	0.64
1:A:393:ILE:HG23	1:A:414:TRP:HH2	1.58	0.64
2:B:246:LEU:HB2	2:B:307:ARG:NH1	2.13	0.64
2:H:264:LEU:CD2	2:H:274:ILE:HD11	2.24	0.64
2:F:246:LEU:CD1	2:F:264:LEU:HD21	2.27	0.64
1:A:420:PRO:HG2	1:A:421:PRO:CD	2.22	0.64
1:A:540:LYS:HZ3	2:B:261:VAL:HG12	1.61	0.64
1:G:376:THR:HG23	1:G:386:THR:CG2	2.25	0.64
2:H:169:GLU:HB3	2:H:170:PRO:HD3	1.78	0.64
1:A:376:THR:HG23	1:A:386:THR:CG2	2.25	0.63
2:B:94:ILE:HG22	2:B:95:PRO:HD3	1.81	0.63
2:D:246:LEU:HB2	2:D:307:ARG:NH1	2.13	0.63
2:F:169:GLU:HB3	2:F:170:PRO:HD3	1.78	0.63
2:D:94:ILE:HG22	2:D:95:PRO:HD3	1.81	0.63
1:E:28:GLU:O	1:E:32:LYS:HG3	1.98	0.63
1:G:28:GLU:O	1:G:32:LYS:HG3	1.98	0.63
2:B:126:LYS:HA	2:B:145:GLN:NE2	2.13	0.63
2:D:246:LEU:CD1	2:D:264:LEU:HD21	2.27	0.63
2:H:63:ILE:HG12	2:H:64:LYS:N	2.14	0.63
1:C:342:TYR:CE1	1:G:345:PRO:HG3	2.33	0.63
1:E:376:THR:HG23	1:E:386:THR:CG2	2.25	0.63
2:F:126:LYS:HA	2:F:145:GLN:NE2	2.13	0.63
1:A:537:PRO:HD2	1:A:542:ILE:CD1	2.27	0.63
1:C:393:ILE:HB	1:C:423:VAL:HG21	1.79	0.63
2:H:94:ILE:HG22	2:H:95:PRO:HD3	1.81	0.63
2:F:264:LEU:CD2	2:F:274:ILE:HD11	2.24	0.63
2:H:24:TRP:CZ3	2:H:61:PHE:HB3	2.32	0.63
1:A:393:ILE:HB	1:A:423:VAL:HG21	1.79	0.63
1:E:206:ARG:HH22	1:E:218:ASP:HA	1.64	0.63
1:A:206:ARG:HH22	1:A:218:ASP:HA	1.64	0.63
2:D:126:LYS:HA	2:D:145:GLN:NE2	2.13	0.63
2:F:63:ILE:HG12	2:F:64:LYS:N	2.14	0.63
2:H:103:LYS:NZ	2:H:179:VAL:H	1.93	0.63
1:A:28:GLU:O	1:A:32:LYS:HG3	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:94:ILE:HG22	2:F:95:PRO:HD3	1.81	0.63
1:A:238:LYS:HE2	1:A:240:THR:CG2	2.29	0.62
2:B:21:VAL:HG11	2:B:59:PRO:HD3	1.80	0.62
1:C:238:LYS:HE2	1:C:240:THR:CG2	2.29	0.62
2:F:21:VAL:HG11	2:F:59:PRO:HD3	1.80	0.62
2:H:149:LEU:HD22	2:H:156:SER:HA	1.79	0.62
2:H:21:VAL:HG11	2:H:59:PRO:HD3	1.80	0.62
1:C:28:GLU:O	1:C:32:LYS:HG3	1.98	0.62
2:D:21:VAL:HG11	2:D:59:PRO:HD3	1.80	0.62
2:D:63:ILE:HG12	2:D:64:LYS:N	2.14	0.62
1:E:393:ILE:HB	1:E:423:VAL:HG21	1.80	0.62
2:F:125:ARG:NH1	2:F:147:ASN:HA	2.15	0.62
1:G:206:ARG:HH22	1:G:218:ASP:HA	1.64	0.62
2:B:125:ARG:NH1	2:B:147:ASN:HA	2.15	0.62
1:C:346:PHE:HD1	1:G:390:LYS:HE3	0.80	0.62
2:D:125:ARG:NH1	2:D:147:ASN:HA	2.15	0.62
2:F:149:LEU:HD22	2:F:156:SER:HA	1.79	0.62
1:E:418:ASN:C	1:E:418:ASN:HD22	2.08	0.62
1:C:206:ARG:HG3	1:C:216:THR:OG1	2.00	0.62
1:C:206:ARG:HH22	1:C:218:ASP:HA	1.64	0.62
1:E:206:ARG:HG3	1:E:216:THR:OG1	2.00	0.62
1:A:491:LEU:HB3	1:A:529:GLU:CB	2.30	0.62
1:C:249:LYS:HG2	1:C:250:ASP:N	2.15	0.62
1:E:491:LEU:HB3	1:E:529:GLU:CB	2.30	0.62
1:G:339:TYR:CE1	1:G:352:GLY:HA3	2.35	0.62
1:A:206:ARG:HG3	1:A:216:THR:OG1	2.00	0.62
1:C:491:LEU:HB3	1:C:529:GLU:CB	2.30	0.62
2:D:376:THR:HG22	2:D:389:PHE:CE1	2.35	0.62
2:F:376:THR:HG22	2:F:389:PHE:CE1	2.35	0.62
1:G:418:ASN:C	1:G:418:ASN:HD22	2.08	0.62
1:G:540:LYS:HZ3	2:H:261:VAL:CG1	2.13	0.62
2:H:125:ARG:NH1	2:H:147:ASN:HA	2.15	0.62
1:G:238:LYS:HE2	1:G:240:THR:CG2	2.29	0.61
1:G:249:LYS:HG2	1:G:250:ASP:N	2.15	0.61
2:B:47:ILE:HG21	2:B:144:TYR:HB3	1.82	0.61
2:D:354:TYR:OH	2:D:374:LYS:HG2	2.00	0.61
2:F:47:ILE:HG21	2:F:144:TYR:HB3	1.82	0.61
2:F:257:ILE:HB	2:F:283:LEU:HD21	1.82	0.61
1:A:249:LYS:HG2	1:A:250:ASP:N	2.15	0.61
1:A:418:ASN:HD22	1:A:418:ASN:C	2.08	0.61
2:B:354:TYR:OH	2:B:374:LYS:HG2	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:104:LYS:HB2	1:C:192:ASP:HA	1.82	0.61
1:C:339:TYR:CE1	1:C:352:GLY:HA3	2.35	0.61
1:E:238:LYS:HE2	1:E:240:THR:CG2	2.29	0.61
1:E:393:ILE:HG23	1:E:414:TRP:HH2	1.58	0.61
1:G:393:ILE:HB	1:G:423:VAL:HG21	1.79	0.61
2:H:376:THR:HG22	2:H:389:PHE:CE1	2.35	0.61
2:B:54:ASN:C	2:B:54:ASN:HD22	2.08	0.61
2:B:63:ILE:HG12	2:B:64:LYS:N	2.14	0.61
1:G:104:LYS:HB2	1:G:192:ASP:HA	1.82	0.61
1:G:435:VAL:HG22	2:H:290:THR:HG21	1.83	0.61
2:B:376:THR:HG22	2:B:389:PHE:CE1	2.35	0.61
1:C:418:ASN:C	1:C:418:ASN:HD22	2.08	0.61
2:D:87:PHE:CE2	2:D:155:GLY:HA2	2.36	0.61
1:G:206:ARG:HG3	1:G:216:THR:OG1	2.00	0.61
1:E:104:LYS:HB2	1:E:192:ASP:HA	1.82	0.61
1:E:376:THR:O	1:E:380:ILE:HG13	2.01	0.61
2:F:54:ASN:HD22	2:F:54:ASN:C	2.08	0.61
2:F:87:PHE:CE2	2:F:155:GLY:HA2	2.36	0.61
2:H:87:PHE:CE2	2:H:155:GLY:HA2	2.36	0.61
2:H:354:TYR:OH	2:H:374:LYS:HG2	2.00	0.61
1:C:225:PRO:HG2	1:C:226:PRO:CD	2.31	0.61
2:D:54:ASN:C	2:D:54:ASN:HD22	2.08	0.61
2:H:54:ASN:C	2:H:54:ASN:HD22	2.08	0.61
1:C:435:VAL:HG22	2:D:290:THR:HG21	1.83	0.61
1:E:435:VAL:HG22	2:F:290:THR:HG21	1.83	0.61
1:A:225:PRO:HG2	1:A:226:PRO:CD	2.31	0.61
1:A:339:TYR:CE1	1:A:352:GLY:HA3	2.35	0.61
1:A:376:THR:O	1:A:380:ILE:HG13	2.01	0.61
2:B:87:PHE:CE2	2:B:155:GLY:HA2	2.36	0.61
1:E:88:TRP:CH2	2:F:57:ASN:HB3	2.36	0.61
1:E:249:LYS:HG2	1:E:250:ASP:N	2.15	0.61
1:E:339:TYR:CE1	1:E:352:GLY:HA3	2.35	0.61
2:H:47:ILE:HG21	2:H:144:TYR:HB3	1.82	0.61
1:E:225:PRO:HG2	1:E:226:PRO:CD	2.31	0.61
1:E:238:LYS:HE2	1:E:240:THR:HG22	1.83	0.61
1:G:491:LEU:HB3	1:G:529:GLU:CB	2.30	0.61
1:A:104:LYS:HB2	1:A:192:ASP:HA	1.82	0.60
1:A:435:VAL:HG22	2:B:290:THR:HG21	1.83	0.60
1:G:225:PRO:HG2	1:G:226:PRO:CD	2.31	0.60
1:G:238:LYS:HE2	1:G:240:THR:HG22	1.83	0.60
2:F:354:TYR:OH	2:F:374:LYS:HG2	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:376:THR:O	1:G:380:ILE:HG13	2.01	0.60
1:G:393:ILE:HG23	1:G:414:TRP:HH2	1.58	0.60
2:B:257:ILE:HB	2:B:283:LEU:HD21	1.82	0.60
2:D:47:ILE:HG21	2:D:144:TYR:HB3	1.82	0.60
2:D:257:ILE:HB	2:D:283:LEU:HD21	1.82	0.60
1:E:326:ILE:HB	1:E:342:TYR:HE1	1.65	0.60
1:E:509:GLN:N	1:E:510:PRO:HD3	2.17	0.60
1:C:376:THR:O	1:C:380:ILE:HG13	2.01	0.60
2:F:151:GLN:HA	2:F:151:GLN:NE2	2.17	0.60
1:G:88:TRP:CH2	2:H:57:ASN:HB3	2.36	0.60
2:H:151:GLN:HA	2:H:151:GLN:NE2	2.17	0.60
2:B:47:ILE:CG2	2:B:144:TYR:HB3	2.31	0.60
1:C:88:TRP:CH2	2:D:57:ASN:HB3	2.36	0.60
2:D:171:PHE:CE2	2:D:204:GLU:HB2	2.31	0.60
2:H:47:ILE:CG2	2:H:144:TYR:HB3	2.31	0.60
2:H:257:ILE:HB	2:H:283:LEU:HD21	1.82	0.60
1:A:88:TRP:CH2	2:B:57:ASN:HB3	2.36	0.60
2:D:47:ILE:CG2	2:D:144:TYR:HB3	2.31	0.60
2:B:328:GLU:O	2:B:339:TYR:HA	2.02	0.60
1:C:160:PHE:CE1	1:C:164:MET:HG2	2.37	0.60
1:C:326:ILE:HB	1:C:342:TYR:HE1	1.66	0.60
2:D:328:GLU:O	2:D:339:TYR:HA	2.02	0.60
2:F:47:ILE:CG2	2:F:144:TYR:HB3	2.31	0.60
1:C:323:LYS:HE2	1:G:322:SER:O	2.01	0.60
1:C:363:ASN:OD1	1:C:364:ASP:N	2.35	0.60
1:A:160:PHE:CE1	1:A:164:MET:HG2	2.37	0.60
1:A:238:LYS:HE3	1:A:315:HIS:CD2	2.36	0.60
1:C:238:LYS:HE2	1:C:240:THR:HG22	1.83	0.60
1:G:509:GLN:N	1:G:510:PRO:HD3	2.17	0.60
2:H:328:GLU:O	2:H:339:TYR:HA	2.02	0.60
1:A:492:GLU:HG2	1:A:530:LYS:HB2	1.84	0.59
1:A:509:GLN:N	1:A:510:PRO:HD3	2.17	0.59
1:C:238:LYS:HE3	1:C:315:HIS:CD2	2.37	0.59
1:A:238:LYS:HE2	1:A:240:THR:HG22	1.83	0.59
1:A:326:ILE:HB	1:A:342:TYR:HE1	1.66	0.59
1:C:509:GLN:N	1:C:510:PRO:HD3	2.16	0.59
1:C:235:HIS:HB3	1:C:236:PRO:HD2	1.84	0.59
1:E:160:PHE:CE1	1:E:164:MET:HG2	2.37	0.59
1:G:363:ASN:OD1	1:G:364:ASP:N	2.35	0.59
1:A:235:HIS:HB3	1:A:236:PRO:HD2	1.84	0.59
1:A:392:PRO:O	1:A:423:VAL:HG22	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:492:GLU:HG2	1:C:530:LYS:HB2	1.84	0.59
1:E:238:LYS:HE3	1:E:315:HIS:CD2	2.36	0.59
1:G:160:PHE:CE1	1:G:164:MET:HG2	2.37	0.59
1:A:363:ASN:OD1	1:A:364:ASP:N	2.35	0.59
1:E:363:ASN:OD1	1:E:364:ASP:N	2.35	0.59
1:G:238:LYS:HE3	1:G:315:HIS:CD2	2.36	0.59
2:B:106:VAL:HA	2:B:190:GLY:HA2	1.85	0.59
1:C:392:PRO:O	1:C:423:VAL:HG22	2.03	0.59
2:F:328:GLU:O	2:F:339:TYR:HA	2.02	0.59
1:G:326:ILE:HB	1:G:342:TYR:HE1	1.66	0.59
2:B:153:TRP:CH2	2:B:155:GLY:HA3	2.38	0.59
2:D:151:GLN:HA	2:D:151:GLN:NE2	2.17	0.59
1:E:161:GLN:O	1:E:165:THR:HG23	2.03	0.59
1:E:392:PRO:O	1:E:423:VAL:HG22	2.03	0.59
2:D:106:VAL:HA	2:D:190:GLY:HA2	1.85	0.59
2:F:153:TRP:CH2	2:F:155:GLY:HA3	2.38	0.59
1:G:161:GLN:O	1:G:165:THR:HG23	2.03	0.59
1:G:295:LEU:CB	1:G:299:ALA:HB2	2.33	0.59
1:A:161:GLN:O	1:A:165:THR:HG23	2.03	0.59
1:C:161:GLN:O	1:C:165:THR:HG23	2.03	0.59
1:E:235:HIS:HB3	1:E:236:PRO:HD2	1.84	0.59
1:E:295:LEU:CB	1:E:299:ALA:HB2	2.33	0.59
1:G:164:MET:HE2	1:G:187:LEU:HD21	1.85	0.59
1:E:492:GLU:HG2	1:E:530:LYS:HB2	1.84	0.58
2:F:97:PRO:C	2:F:99:GLY:H	2.11	0.58
1:G:492:GLU:HG2	1:G:530:LYS:HB2	1.84	0.58
2:B:151:GLN:HA	2:B:151:GLN:NE2	2.17	0.58
2:D:153:TRP:CH2	2:D:155:GLY:HA3	2.38	0.58
2:B:171:PHE:CE2	2:B:204:GLU:HB2	2.31	0.58
1:C:346:PHE:CZ	1:G:390:LYS:CG	2.80	0.58
1:E:17:ASP:O	1:E:83:ARG:HD3	2.03	0.58
1:E:164:MET:HE2	1:E:187:LEU:HD21	1.85	0.58
1:G:167:ILE:O	1:G:170:PRO:HD2	2.04	0.58
1:A:295:LEU:CB	1:A:299:ALA:HB2	2.33	0.58
1:C:164:MET:HE2	1:C:187:LEU:HD21	1.85	0.58
1:C:295:LEU:CB	1:C:299:ALA:HB2	2.33	0.58
1:C:523:GLU:O	1:C:526:ILE:HG12	2.04	0.58
1:C:540:LYS:HZ3	2:D:261:VAL:CG1	2.16	0.58
1:E:167:ILE:O	1:E:170:PRO:HD2	2.03	0.58
1:G:235:HIS:HB3	1:G:236:PRO:HD2	1.84	0.58
1:G:402:TRP:CE3	1:G:402:TRP:C	2.82	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:97:PRO:C	2:H:99:GLY:H	2.11	0.58
1:C:17:ASP:O	1:C:83:ARG:HD3	2.03	0.58
1:C:402:TRP:CE3	1:C:402:TRP:C	2.82	0.58
1:E:393:ILE:HB	1:E:423:VAL:HG22	1.86	0.58
2:H:106:VAL:HA	2:H:190:GLY:HA2	1.85	0.58
1:A:164:MET:HE2	1:A:187:LEU:HD21	1.85	0.58
1:G:523:GLU:O	1:G:526:ILE:HG12	2.04	0.58
2:H:171:PHE:CE2	2:H:204:GLU:HB2	2.31	0.58
1:A:17:ASP:O	1:A:83:ARG:HD3	2.03	0.58
1:A:402:TRP:CE3	1:A:402:TRP:C	2.82	0.58
1:C:411:ILE:HG22	1:C:412:PRO:HD2	1.86	0.58
1:A:303:LEU:O	1:A:307:ARG:HG3	2.04	0.58
1:A:523:GLU:O	1:A:526:ILE:HG12	2.04	0.58
2:F:106:VAL:HA	2:F:190:GLY:HA2	1.84	0.58
2:H:55:PRO:HG2	2:H:56:TYR:N	2.19	0.58
2:H:153:TRP:CH2	2:H:155:GLY:HA3	2.38	0.58
2:F:55:PRO:HG2	2:F:56:TYR:N	2.19	0.58
2:F:395:LYS:HG3	2:F:416:PHE:CE2	2.39	0.58
1:A:411:ILE:HG22	1:A:412:PRO:HD2	1.86	0.57
2:B:395:LYS:HG3	2:B:416:PHE:CE2	2.39	0.57
2:D:10:VAL:CG1	2:D:159:ILE:HD11	2.34	0.57
2:F:171:PHE:CE2	2:F:204:GLU:HB2	2.31	0.57
1:E:406:TRP:CZ3	1:E:407:GLN:HG3	2.39	0.57
1:G:392:PRO:O	1:G:423:VAL:HG22	2.03	0.57
2:H:395:LYS:HG3	2:H:416:PHE:CE2	2.39	0.57
1:A:167:ILE:O	1:A:170:PRO:HD2	2.03	0.57
2:B:97:PRO:C	2:B:99:GLY:H	2.11	0.57
1:G:303:LEU:O	1:G:307:ARG:HG3	2.04	0.57
1:A:406:TRP:CZ3	1:A:407:GLN:HG3	2.40	0.57
2:D:395:LYS:HG3	2:D:416:PHE:CE2	2.39	0.57
1:E:429:LEU:HD11	1:E:506:ILE:HG22	1.87	0.57
1:A:393:ILE:HB	1:A:423:VAL:HG22	1.86	0.57
2:B:5:ILE:HG22	2:B:6:GLU:N	2.20	0.57
2:B:10:VAL:CG1	2:B:159:ILE:HD11	2.35	0.57
1:C:167:ILE:O	1:C:170:PRO:HD2	2.03	0.57
1:E:87:PHE:CE2	1:E:159:ILE:HD11	2.40	0.57
1:E:441:TYR:HE2	1:E:543:GLY:O	1.88	0.57
2:H:10:VAL:CG1	2:H:159:ILE:HD11	2.35	0.57
2:D:28:GLU:HG2	2:D:32:LYS:NZ	2.19	0.57
1:E:402:TRP:C	1:E:402:TRP:CE3	2.82	0.57
2:F:28:GLU:HG2	2:F:32:LYS:NZ	2.19	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:303:LEU:O	1:C:307:ARG:HG3	2.04	0.57
1:C:320:ASP:OD2	1:C:323:LYS:HG3	2.05	0.57
1:C:406:TRP:CZ3	1:C:407:GLN:HG3	2.39	0.57
1:E:232:TYR:HD1	1:E:241:VAL:HG22	1.70	0.57
2:H:395:LYS:O	2:H:399:GLU:HG3	2.05	0.57
2:B:54:ASN:HD21	2:B:56:TYR:HB2	1.70	0.57
2:D:54:ASN:HD21	2:D:56:TYR:HB2	1.70	0.57
1:E:523:GLU:O	1:E:526:ILE:HG12	2.04	0.57
2:F:54:ASN:HD21	2:F:56:TYR:HB2	1.70	0.57
1:G:393:ILE:HB	1:G:423:VAL:HG22	1.86	0.57
1:G:406:TRP:CZ3	1:G:407:GLN:HG3	2.40	0.57
2:D:5:ILE:HG22	2:D:6:GLU:N	2.20	0.57
2:F:5:ILE:HG22	2:F:6:GLU:N	2.20	0.57
1:G:17:ASP:O	1:G:83:ARG:HD3	2.03	0.57
1:G:458:VAL:HG23	1:G:548:VAL:HG22	1.87	0.57
1:E:56:TYR:O	1:E:143:ARG:NH2	2.38	0.57
1:E:320:ASP:OD2	1:E:323:LYS:HG3	2.05	0.57
2:F:395:LYS:O	2:F:399:GLU:HG3	2.05	0.57
2:H:28:GLU:HG2	2:H:32:LYS:NZ	2.19	0.57
1:A:320:ASP:OD2	1:A:323:LYS:HG3	2.05	0.56
1:C:393:ILE:HB	1:C:423:VAL:HG22	1.86	0.56
2:D:97:PRO:C	2:D:99:GLY:H	2.11	0.56
1:E:98:ALA:HB1	1:E:383:TRP:HH2	1.70	0.56
1:E:411:ILE:HG22	1:E:412:PRO:HD2	1.86	0.56
2:H:379:SER:OG	2:H:387:PRO:HD3	2.05	0.56
2:B:28:GLU:HG2	2:B:32:LYS:NZ	2.19	0.56
1:C:346:PHE:CG	1:G:390:LYS:CD	2.87	0.56
1:G:429:LEU:HD11	1:G:506:ILE:HG22	1.87	0.56
1:G:441:TYR:HE2	1:G:543:GLY:O	1.88	0.56
1:A:87:PHE:CE2	1:A:159:ILE:HD11	2.40	0.56
1:A:98:ALA:HB1	1:A:383:TRP:HH2	1.70	0.56
1:A:458:VAL:HG23	1:A:548:VAL:HG22	1.87	0.56
2:B:61:PHE:CE2	2:B:403:THR:HG22	2.41	0.56
2:B:271:TYR:O	2:B:274:ILE:HG22	2.06	0.56
1:C:87:PHE:CE2	1:C:159:ILE:HD11	2.40	0.56
1:C:517:LEU:O	1:C:521:ILE:HG13	2.06	0.56
2:D:55:PRO:HG2	2:D:56:TYR:N	2.19	0.56
2:D:271:TYR:O	2:D:274:ILE:HG22	2.06	0.56
2:D:395:LYS:O	2:D:399:GLU:HG3	2.05	0.56
2:F:379:SER:OG	2:F:387:PRO:HD3	2.05	0.56
1:G:411:ILE:HG22	1:G:412:PRO:HD2	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:5:ILE:HG22	2:H:6:GLU:N	2.20	0.56
2:H:61:PHE:CE2	2:H:403:THR:HG22	2.41	0.56
2:H:139:THR:HG22	2:H:140:PRO:O	2.06	0.56
1:A:329:ILE:HD12	1:A:391:LEU:CD2	2.36	0.56
1:A:453:GLY:O	1:A:469:LEU:HB2	2.06	0.56
1:A:517:LEU:O	1:A:521:ILE:HG13	2.06	0.56
2:B:55:PRO:HG2	2:B:56:TYR:N	2.19	0.56
2:B:105:SER:HB3	2:B:235:HIS:CE1	2.41	0.56
1:C:329:ILE:HD12	1:C:391:LEU:CD2	2.36	0.56
1:G:56:TYR:O	1:G:143:ARG:NH2	2.38	0.56
1:G:87:PHE:CE2	1:G:159:ILE:HD11	2.40	0.56
1:G:320:ASP:OD2	1:G:323:LYS:HG3	2.05	0.56
2:B:395:LYS:O	2:B:399:GLU:HG3	2.05	0.56
2:D:61:PHE:CE2	2:D:403:THR:HG22	2.41	0.56
2:D:105:SER:HB3	2:D:235:HIS:CE1	2.41	0.56
1:E:303:LEU:O	1:E:307:ARG:HG3	2.04	0.56
2:F:105:SER:HB3	2:F:235:HIS:CE1	2.41	0.56
1:G:453:GLY:O	1:G:469:LEU:HB2	2.06	0.56
1:G:517:LEU:O	1:G:521:ILE:HG13	2.06	0.56
1:C:98:ALA:HB1	1:C:383:TRP:HH2	1.71	0.56
2:F:10:VAL:CG1	2:F:159:ILE:HD11	2.35	0.56
1:G:98:ALA:HB1	1:G:383:TRP:HH2	1.70	0.56
2:H:271:TYR:O	2:H:274:ILE:HG22	2.06	0.56
1:A:441:TYR:HE2	1:A:543:GLY:O	1.88	0.56
1:C:441:TYR:HE2	1:C:543:GLY:O	1.88	0.56
2:F:125:ARG:HG2	2:F:125:ARG:HH11	1.71	0.56
2:F:139:THR:HG22	2:F:140:PRO:O	2.06	0.56
2:H:54:ASN:HD21	2:H:56:TYR:HB2	1.70	0.56
1:A:56:TYR:O	1:A:143:ARG:NH2	2.38	0.56
1:A:248:GLU:HG3	1:A:307:ARG:NH2	2.20	0.56
1:A:429:LEU:HD11	1:A:506:ILE:HG22	1.87	0.56
1:C:453:GLY:O	1:C:469:LEU:HB2	2.06	0.56
1:C:458:VAL:HG23	1:C:548:VAL:HG22	1.86	0.56
1:G:491:LEU:HB3	1:G:529:GLU:HB3	1.88	0.56
2:B:379:SER:OG	2:B:387:PRO:HD3	2.05	0.56
1:C:56:TYR:O	1:C:143:ARG:NH2	2.38	0.56
1:C:429:LEU:HD11	1:C:506:ILE:HG22	1.87	0.56
1:E:458:VAL:HG23	1:E:548:VAL:HG22	1.87	0.56
2:F:271:TYR:O	2:F:274:ILE:HG22	2.06	0.56
1:A:232:TYR:HD1	1:A:241:VAL:HG22	1.70	0.55
1:C:248:GLU:HG3	1:C:307:ARG:NH2	2.20	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:139:THR:HG22	2:D:140:PRO:O	2.06	0.55
1:E:453:GLY:O	1:E:469:LEU:HB2	2.06	0.55
1:G:232:TYR:HD1	1:G:241:VAL:HG22	1.70	0.55
1:G:248:GLU:HG3	1:G:307:ARG:NH2	2.20	0.55
2:F:72:ARG:HH12	2:F:409:THR:HA	1.71	0.55
2:H:105:SER:HB3	2:H:235:HIS:CE1	2.41	0.55
1:E:248:GLU:HG3	1:E:307:ARG:NH2	2.20	0.55
1:E:298:GLU:O	1:E:302:GLU:HG3	2.06	0.55
1:G:298:GLU:O	1:G:302:GLU:HG3	2.06	0.55
2:H:72:ARG:HH12	2:H:409:THR:HA	1.71	0.55
2:H:125:ARG:HG2	2:H:125:ARG:HH11	1.71	0.55
1:A:337:TRP:HZ3	1:A:368:LEU:HD13	1.72	0.55
2:B:139:THR:HG22	2:B:140:PRO:O	2.06	0.55
2:D:72:ARG:HH12	2:D:409:THR:HA	1.71	0.55
1:E:337:TRP:HZ3	1:E:368:LEU:HD13	1.72	0.55
1:E:439:THR:HG22	1:E:441:TYR:CE1	2.42	0.55
2:F:376:THR:HB	2:F:386:THR:HG22	1.88	0.55
1:G:98:ALA:HB1	1:G:349:LEU:HB3	1.89	0.55
1:G:337:TRP:HZ3	1:G:368:LEU:HD13	1.72	0.55
1:A:98:ALA:HB1	1:A:349:LEU:HB3	1.89	0.55
2:B:125:ARG:HG2	2:B:125:ARG:HH11	1.71	0.55
1:C:439:THR:HG22	1:C:441:TYR:CE1	2.42	0.55
1:E:28:GLU:HB3	1:E:32:LYS:HE3	1.88	0.55
2:F:61:PHE:CE2	2:F:403:THR:HG22	2.41	0.55
2:F:97:PRO:O	2:F:98:ALA:HB3	2.07	0.55
1:G:329:ILE:HD12	1:G:391:LEU:CD2	2.36	0.55
2:H:368:LEU:O	2:H:371:ALA:HB3	2.07	0.55
1:A:439:THR:HG22	1:A:441:TYR:CE1	2.42	0.55
2:B:97:PRO:O	2:B:98:ALA:HB3	2.07	0.55
1:C:298:GLU:O	1:C:302:GLU:HG3	2.06	0.55
1:G:28:GLU:HB3	1:G:32:LYS:HE3	1.88	0.55
2:H:366:LYS:O	2:H:370:GLU:HG3	2.07	0.55
1:A:298:GLU:O	1:A:302:GLU:HG3	2.06	0.55
2:B:72:ARG:HH12	2:B:409:THR:HA	1.71	0.55
2:B:101:LYS:O	2:B:236:PRO:HB2	2.07	0.55
2:B:201:LYS:HD3	2:B:204:GLU:OE1	2.07	0.55
1:C:98:ALA:HB1	1:C:349:LEU:HB3	1.89	0.55
1:C:232:TYR:HD1	1:C:241:VAL:HG22	1.70	0.55
1:C:337:TRP:HZ3	1:C:368:LEU:HD13	1.72	0.55
2:D:101:LYS:O	2:D:236:PRO:HB2	2.07	0.55
2:D:379:SER:OG	2:D:387:PRO:HD3	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:323:LYS:HD3	1:E:344:GLU:OE2	2.07	0.55
1:E:517:LEU:O	1:E:521:ILE:HG13	2.06	0.55
1:G:323:LYS:HD3	1:G:344:GLU:OE2	2.07	0.55
1:G:537:PRO:HD2	1:G:542:ILE:HD11	1.88	0.55
2:H:61:PHE:CZ	2:H:402:TRP:CZ2	2.95	0.55
1:A:401:TRP:HB2	1:A:425:LEU:HD21	1.89	0.55
1:C:332:GLN:HG2	1:C:332:GLN:O	2.07	0.55
2:D:201:LYS:HD3	2:D:204:GLU:OE1	2.07	0.55
1:E:98:ALA:HB1	1:E:349:LEU:HB3	1.89	0.55
1:E:491:LEU:HB3	1:E:529:GLU:HB3	1.88	0.55
1:E:537:PRO:HD2	1:E:542:ILE:HD11	1.88	0.55
1:G:439:THR:HG22	1:G:441:TYR:CE1	2.42	0.55
2:H:201:LYS:HD3	2:H:204:GLU:OE1	2.07	0.55
1:A:332:GLN:O	1:A:332:GLN:HG2	2.07	0.55
1:A:496:VAL:HG22	1:A:534:ALA:HB3	1.89	0.55
1:C:346:PHE:CE1	1:G:390:LYS:CD	2.86	0.55
1:C:491:LEU:HB3	1:C:529:GLU:HB3	1.88	0.55
1:C:496:VAL:HG22	1:C:534:ALA:HB3	1.89	0.55
1:A:99:GLY:HA2	1:A:383:TRP:HZ3	1.72	0.54
1:A:463:ARG:HH11	1:A:463:ARG:HG3	1.72	0.54
2:B:366:LYS:O	2:B:370:GLU:HG3	2.07	0.54
1:C:323:LYS:HD3	1:C:344:GLU:OE2	2.07	0.54
2:D:125:ARG:HH11	2:D:125:ARG:HG2	1.71	0.54
1:E:329:ILE:HD12	1:E:391:LEU:CD2	2.36	0.54
1:G:5:ILE:HD11	1:G:166:LYS:HD2	1.89	0.54
1:A:201:LYS:HD3	1:A:204:GLU:OE2	2.07	0.54
2:B:376:THR:HB	2:B:386:THR:HG22	1.88	0.54
2:D:27:THR:O	2:D:29:GLU:N	2.41	0.54
2:D:104:LYS:HZ3	2:D:194:GLU:HA	1.72	0.54
1:E:332:GLN:O	1:E:332:GLN:HG2	2.07	0.54
1:G:201:LYS:HD3	1:G:204:GLU:OE2	2.07	0.54
2:H:27:THR:C	2:H:29:GLU:H	2.15	0.54
2:H:97:PRO:O	2:H:98:ALA:HB3	2.07	0.54
1:A:200:THR:O	1:A:203:GLU:HB3	2.07	0.54
1:A:491:LEU:HB3	1:A:529:GLU:HB3	1.88	0.54
1:C:5:ILE:HD11	1:C:166:LYS:HD2	1.89	0.54
1:E:342:TYR:HB3	1:E:348:ASN:HB3	1.89	0.54
2:F:318:TYR:HE1	2:F:347:LYS:HD3	1.73	0.54
1:A:126:LYS:HA	1:A:145:GLN:HE21	1.73	0.54
1:A:475:GLN:HB3	1:A:501:TYR:CE2	2.43	0.54
1:A:537:PRO:CG	2:B:262:GLY:HA2	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:318:TYR:HE1	2:B:347:LYS:HD3	1.73	0.54
1:C:99:GLY:HA2	1:C:383:TRP:HZ3	1.72	0.54
2:D:97:PRO:O	2:D:98:ALA:HB3	2.07	0.54
2:D:303:LEU:HD13	2:D:307:ARG:NH2	2.23	0.54
2:F:104:LYS:HZ3	2:F:194:GLU:HA	1.73	0.54
1:G:131:THR:HA	1:G:142:ILE:O	2.07	0.54
1:A:537:PRO:HD2	1:A:542:ILE:HD11	1.88	0.54
2:B:27:THR:O	2:B:29:GLU:N	2.41	0.54
1:C:463:ARG:HG3	1:C:463:ARG:HH11	1.72	0.54
1:C:537:PRO:CG	2:D:262:GLY:HA2	2.38	0.54
1:E:131:THR:HA	1:E:142:ILE:O	2.07	0.54
2:F:303:LEU:HD13	2:F:307:ARG:NH2	2.23	0.54
2:F:366:LYS:O	2:F:370:GLU:HG3	2.07	0.54
1:G:99:GLY:HA2	1:G:383:TRP:HZ3	1.72	0.54
1:G:200:THR:O	1:G:203:GLU:HB3	2.07	0.54
1:G:332:GLN:O	1:G:332:GLN:HG2	2.07	0.54
1:A:5:ILE:HD11	1:A:166:LYS:HD2	1.89	0.54
1:A:98:ALA:O	1:A:383:TRP:HZ3	1.91	0.54
1:A:323:LYS:HD3	1:A:344:GLU:OE2	2.07	0.54
2:B:93:GLY:O	2:B:94:ILE:O	2.26	0.54
2:B:303:LEU:HD13	2:B:307:ARG:NH2	2.23	0.54
1:C:98:ALA:O	1:C:383:TRP:HZ3	1.91	0.54
1:C:342:TYR:HB3	1:C:348:ASN:HB3	1.89	0.54
1:C:346:PHE:HD1	1:G:390:LYS:CE	1.66	0.54
2:D:27:THR:C	2:D:29:GLU:H	2.15	0.54
2:D:318:TYR:HE1	2:D:347:LYS:HD3	1.72	0.54
2:F:27:THR:O	2:F:29:GLU:N	2.41	0.54
2:F:93:GLY:O	2:F:94:ILE:O	2.26	0.54
1:G:97:PRO:HD3	1:G:232:TYR:CZ	2.43	0.54
1:G:406:TRP:CD1	1:G:406:TRP:H	2.25	0.54
2:H:303:LEU:HD13	2:H:307:ARG:NH2	2.23	0.54
2:B:27:THR:C	2:B:29:GLU:H	2.15	0.54
1:C:200:THR:O	1:C:203:GLU:HB3	2.07	0.54
1:C:401:TRP:HB2	1:C:425:LEU:HD21	1.89	0.54
1:C:475:GLN:HB3	1:C:501:TYR:CE2	2.43	0.54
2:D:366:LYS:O	2:D:370:GLU:HG3	2.07	0.54
1:E:200:THR:O	1:E:203:GLU:HB3	2.07	0.54
1:E:401:TRP:HB2	1:E:425:LEU:HD21	1.89	0.54
2:F:27:THR:C	2:F:29:GLU:H	2.15	0.54
2:F:61:PHE:CZ	2:F:402:TRP:CZ2	2.95	0.54
2:F:392:PRO:HG2	2:F:392:PRO:O	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:463:ARG:HH11	1:G:463:ARG:HG3	1.72	0.54
1:G:496:VAL:HG22	1:G:534:ALA:HB3	1.89	0.54
2:H:27:THR:C	2:H:29:GLU:N	2.66	0.54
1:A:341:ILE:HD11	1:A:350:LYS:HB3	1.90	0.54
1:C:201:LYS:HD3	1:C:204:GLU:OE2	2.07	0.54
2:D:61:PHE:CZ	2:D:402:TRP:CZ2	2.95	0.54
2:D:376:THR:HB	2:D:386:THR:HG22	1.88	0.54
2:F:368:LEU:O	2:F:371:ALA:HB3	2.07	0.54
1:G:341:ILE:HD11	1:G:350:LYS:HB3	1.90	0.54
2:H:376:THR:HB	2:H:386:THR:HG22	1.88	0.54
1:A:131:THR:HA	1:A:142:ILE:O	2.07	0.54
2:B:61:PHE:CZ	2:B:402:TRP:CZ2	2.95	0.54
1:E:126:LYS:HA	1:E:145:GLN:HE21	1.73	0.54
2:H:318:TYR:HE1	2:H:347:LYS:HD3	1.73	0.54
1:A:28:GLU:HB3	1:A:32:LYS:HE3	1.88	0.54
2:B:365:VAL:HG12	2:B:405:TYR:CE2	2.43	0.54
1:C:28:GLU:HB3	1:C:32:LYS:HE3	1.88	0.54
1:C:126:LYS:HA	1:C:145:GLN:HE21	1.72	0.54
1:C:182:GLN:HG2	1:C:183:TYR:N	2.23	0.54
1:C:341:ILE:HD11	1:C:350:LYS:HB3	1.90	0.54
1:E:540:LYS:HZ3	2:F:261:VAL:HG12	1.71	0.54
2:H:27:THR:O	2:H:29:GLU:N	2.41	0.54
2:B:104:LYS:HZ3	2:B:194:GLU:HA	1.73	0.53
2:D:368:LEU:O	2:D:371:ALA:HB3	2.07	0.53
1:G:98:ALA:O	1:G:383:TRP:HZ3	1.91	0.53
1:A:182:GLN:HG2	1:A:183:TYR:N	2.23	0.53
2:B:27:THR:C	2:B:29:GLU:N	2.66	0.53
2:B:368:LEU:O	2:B:371:ALA:HB3	2.07	0.53
1:C:97:PRO:HD3	1:C:232:TYR:CZ	2.43	0.53
2:D:93:GLY:O	2:D:94:ILE:O	2.26	0.53
1:E:97:PRO:HD3	1:E:232:TYR:CZ	2.43	0.53
1:E:463:ARG:HH11	1:E:463:ARG:HG3	1.72	0.53
1:E:537:PRO:CG	2:F:262:GLY:HA2	2.38	0.53
2:F:101:LYS:O	2:F:236:PRO:HB2	2.07	0.53
1:G:441:TYR:CD2	1:G:544:GLY:HA3	2.44	0.53
1:G:475:GLN:HB3	1:G:501:TYR:CE2	2.43	0.53
1:A:342:TYR:C	1:A:342:TYR:CD1	2.87	0.53
1:E:341:ILE:HD11	1:E:350:LYS:HB3	1.90	0.53
1:E:496:VAL:HG22	1:E:534:ALA:HB3	1.89	0.53
2:F:153:TRP:CE3	2:F:155:GLY:HA3	2.43	0.53
1:G:401:TRP:HB2	1:G:425:LEU:HD21	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:537:PRO:CG	2:H:262:GLY:HA2	2.38	0.53
2:H:101:LYS:O	2:H:236:PRO:HB2	2.07	0.53
2:H:365:VAL:HG12	2:H:405:TYR:CE2	2.43	0.53
1:A:341:ILE:HD12	1:A:383:TRP:NE1	2.23	0.53
1:C:131:THR:HA	1:C:142:ILE:O	2.07	0.53
1:C:537:PRO:HD2	1:C:542:ILE:HD11	1.88	0.53
2:D:27:THR:C	2:D:29:GLU:N	2.66	0.53
2:D:103:LYS:NZ	2:D:179:VAL:N	2.55	0.53
2:D:153:TRP:CE3	2:D:155:GLY:HA3	2.43	0.53
1:E:6:GLU:CD	1:E:6:GLU:N	2.66	0.53
1:A:97:PRO:HD3	1:A:232:TYR:CZ	2.43	0.53
2:B:103:LYS:NZ	2:B:179:VAL:N	2.55	0.53
2:D:268:SER:HA	2:D:274:ILE:HG22	1.90	0.53
2:F:201:LYS:HD3	2:F:204:GLU:OE1	2.07	0.53
1:G:342:TYR:HB3	1:G:348:ASN:HB3	1.89	0.53
1:C:341:ILE:HD12	1:C:383:TRP:NE1	2.23	0.53
1:E:201:LYS:HD3	1:E:204:GLU:OE2	2.07	0.53
2:F:27:THR:C	2:F:29:GLU:N	2.66	0.53
2:F:365:VAL:HG12	2:F:405:TYR:CE2	2.43	0.53
1:G:342:TYR:CD1	1:G:342:TYR:C	2.87	0.53
2:H:153:TRP:CE3	2:H:155:GLY:HA3	2.43	0.53
1:A:106:VAL:O	1:A:227:PHE:CZ	2.62	0.53
1:A:342:TYR:HB3	1:A:348:ASN:HB3	1.89	0.53
2:B:392:PRO:O	2:B:392:PRO:HG2	2.08	0.53
1:C:196:GLY:O	1:C:199:ARG:HB3	2.09	0.53
1:C:346:PHE:CG	1:G:390:LYS:HD2	2.44	0.53
1:E:196:GLY:O	1:E:199:ARG:HB3	2.09	0.53
1:E:475:GLN:HB3	1:E:501:TYR:CE2	2.43	0.53
2:F:268:SER:HA	2:F:274:ILE:HG22	1.90	0.53
1:G:126:LYS:HA	1:G:145:GLN:HE21	1.73	0.53
1:A:465:LYS:O	1:A:466:VAL:HG23	2.08	0.53
2:B:153:TRP:CE3	2:B:155:GLY:HA3	2.43	0.53
1:C:106:VAL:O	1:C:227:PHE:CZ	2.62	0.53
1:C:342:TYR:CD1	1:C:342:TYR:C	2.87	0.53
1:C:345:PRO:CG	1:G:326:ILE:HD11	2.19	0.53
2:D:365:VAL:HG12	2:D:405:TYR:CE2	2.43	0.53
1:E:5:ILE:HD11	1:E:166:LYS:HD2	1.89	0.53
1:E:408:ALA:HB1	2:F:364:ASP:HB3	1.91	0.53
2:F:264:LEU:HB2	2:F:276:VAL:CG1	2.39	0.53
2:H:93:GLY:O	2:H:94:ILE:O	2.26	0.53
1:C:441:TYR:CD2	1:C:544:GLY:HA3	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:441:TYR:CD2	1:E:544:GLY:HA3	2.44	0.53
1:E:99:GLY:HA2	1:E:383:TRP:HZ3	1.72	0.53
1:E:106:VAL:O	1:E:227:PHE:CZ	2.62	0.53
1:G:372:VAL:HG11	1:G:411:ILE:HG23	1.91	0.53
2:H:13:LYS:HB3	2:H:14:PRO:HD2	1.91	0.53
1:A:441:TYR:CD2	1:A:544:GLY:HA3	2.44	0.52
1:C:417:VAL:CG2	1:G:346:PHE:CG	2.92	0.52
2:D:264:LEU:HB2	2:D:276:VAL:CG1	2.39	0.52
1:G:196:GLY:O	1:G:199:ARG:HB3	2.09	0.52
1:G:408:ALA:HB1	2:H:364:ASP:HB3	1.91	0.52
1:G:491:LEU:HB3	1:G:529:GLU:HB2	1.91	0.52
1:A:105:SER:HB3	1:A:198:HIS:CG	2.44	0.52
1:A:157:PRO:HG2	1:A:158:ALA:N	2.24	0.52
2:B:264:LEU:HB2	2:B:276:VAL:CG1	2.39	0.52
1:C:105:SER:HB3	1:C:198:HIS:CG	2.45	0.52
1:C:408:ALA:HB1	2:D:364:ASP:HB3	1.91	0.52
1:E:98:ALA:O	1:E:383:TRP:HZ3	1.91	0.52
1:E:465:LYS:O	1:E:466:VAL:HG23	2.08	0.52
1:G:465:LYS:O	1:G:466:VAL:HG23	2.08	0.52
2:H:268:SER:HA	2:H:274:ILE:HG22	1.90	0.52
1:A:196:GLY:O	1:A:199:ARG:HB3	2.09	0.52
2:H:392:PRO:O	2:H:392:PRO:HG2	2.08	0.52
1:A:540:LYS:CE	2:B:265:ASN:HB2	2.40	0.52
2:B:72:ARG:NH1	2:B:409:THR:HG22	2.25	0.52
2:D:246:LEU:HB2	2:D:307:ARG:HH12	1.75	0.52
1:E:406:TRP:CD1	1:E:406:TRP:H	2.26	0.52
1:G:105:SER:HB3	1:G:198:HIS:CG	2.44	0.52
1:G:414:TRP:CE3	1:G:415:GLU:N	2.78	0.52
1:A:408:ALA:HB1	2:B:364:ASP:HB3	1.91	0.52
1:A:452:LEU:HD22	1:A:470:THR:HG22	1.92	0.52
2:B:246:LEU:HB2	2:B:307:ARG:HH12	1.75	0.52
2:B:268:SER:HA	2:B:274:ILE:HG22	1.90	0.52
1:C:126:LYS:HA	1:C:145:GLN:NE2	2.25	0.52
1:C:372:VAL:HG11	1:C:411:ILE:HG23	1.91	0.52
1:C:414:TRP:CE3	1:C:415:GLU:N	2.78	0.52
2:D:35:VAL:O	2:D:39:THR:HG23	2.10	0.52
1:E:157:PRO:HG2	1:E:158:ALA:N	2.24	0.52
1:E:540:LYS:CE	2:F:265:ASN:HB2	2.40	0.52
2:F:329:ILE:HA	2:F:338:THR:O	2.10	0.52
2:H:264:LEU:HB2	2:H:276:VAL:CG1	2.39	0.52
1:A:402:TRP:CE3	1:A:403:THR:HA	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:35:VAL:O	2:B:39:THR:HG23	2.10	0.52
1:C:326:ILE:HG21	1:G:345:PRO:HG3	1.91	0.52
1:C:406:TRP:CD1	1:C:406:TRP:H	2.26	0.52
1:C:465:LYS:O	1:C:466:VAL:HG23	2.08	0.52
1:E:342:TYR:CD1	1:E:342:TYR:C	2.87	0.52
1:E:452:LEU:HD22	1:E:470:THR:HG22	1.92	0.52
1:G:106:VAL:O	1:G:227:PHE:CZ	2.62	0.52
1:G:454:LYS:HA	1:G:467:VAL:O	2.10	0.52
1:A:126:LYS:HA	1:A:145:GLN:NE2	2.25	0.52
2:D:392:PRO:HG2	2:D:392:PRO:O	2.08	0.52
1:E:414:TRP:CE3	1:E:415:GLU:N	2.78	0.52
2:F:326:ILE:O	2:F:341:ILE:HA	2.10	0.52
1:G:126:LYS:HA	1:G:145:GLN:NE2	2.25	0.52
2:H:35:VAL:O	2:H:39:THR:HG23	2.10	0.52
1:A:372:VAL:HG11	1:A:411:ILE:HG23	1.91	0.52
1:A:406:TRP:H	1:A:406:TRP:CD1	2.26	0.52
1:A:441:TYR:CE2	1:A:543:GLY:O	2.63	0.52
1:A:540:LYS:HZ2	2:B:265:ASN:HB2	1.71	0.52
1:E:441:TYR:CE2	1:E:543:GLY:O	2.63	0.52
1:G:91:GLN:HE21	1:G:91:GLN:CA	2.22	0.52
2:H:329:ILE:HA	2:H:338:THR:O	2.10	0.52
1:A:324:ASP:O	1:A:343:GLN:HG2	2.09	0.52
1:A:402:TRP:O	1:A:402:TRP:HE3	1.93	0.52
1:A:491:LEU:HB3	1:A:529:GLU:HB2	1.91	0.52
1:C:249:LYS:HG2	1:C:250:ASP:H	1.75	0.52
1:C:441:TYR:CE2	1:C:543:GLY:O	2.63	0.52
1:E:454:LYS:HA	1:E:467:VAL:O	2.10	0.52
1:E:491:LEU:HB3	1:E:529:GLU:HB2	1.91	0.52
2:F:13:LYS:HB3	2:F:14:PRO:HD2	1.91	0.52
2:F:103:LYS:NZ	2:F:179:VAL:N	2.55	0.52
1:C:491:LEU:HB3	1:C:529:GLU:HB2	1.91	0.52
2:D:13:LYS:HB3	2:D:14:PRO:HD2	1.91	0.52
2:F:9:PRO:HA	2:F:121:ASP:OD2	2.10	0.52
2:F:35:VAL:O	2:F:39:THR:HG23	2.10	0.52
1:G:182:GLN:HG2	1:G:183:TYR:N	2.23	0.52
1:G:341:ILE:HD12	1:G:383:TRP:NE1	2.23	0.52
2:B:9:PRO:HA	2:B:121:ASP:OD2	2.10	0.51
2:B:13:LYS:HB3	2:B:14:PRO:HD2	1.91	0.51
1:C:157:PRO:HG2	1:C:158:ALA:N	2.24	0.51
1:C:326:ILE:CB	1:C:342:TYR:CE1	2.92	0.51
1:C:402:TRP:CE3	1:C:403:THR:HA	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:126:LYS:HA	1:E:145:GLN:NE2	2.25	0.51
1:E:182:GLN:HG2	1:E:183:TYR:N	2.23	0.51
1:E:324:ASP:O	1:E:343:GLN:HG2	2.09	0.51
1:E:361:HIS:CD2	1:E:505:ILE:CG2	2.93	0.51
2:H:376:THR:HG22	2:H:389:PHE:CZ	2.45	0.51
1:A:6:GLU:CD	1:A:6:GLU:N	2.66	0.51
1:A:118:VAL:O	1:A:118:VAL:HG12	2.10	0.51
1:A:249:LYS:HG2	1:A:250:ASP:H	1.75	0.51
1:C:402:TRP:HE3	1:C:402:TRP:O	1.93	0.51
1:C:452:LEU:HD22	1:C:470:THR:HG22	1.92	0.51
1:C:540:LYS:CE	2:D:265:ASN:HB2	2.40	0.51
2:D:376:THR:HG22	2:D:389:PHE:CZ	2.45	0.51
1:G:410:TRP:CH2	1:G:412:PRO:HA	2.46	0.51
2:H:103:LYS:NZ	2:H:179:VAL:N	2.55	0.51
2:H:104:LYS:HZ1	2:H:194:GLU:HA	1.74	0.51
2:H:326:ILE:O	2:H:341:ILE:HA	2.10	0.51
1:A:454:LYS:HA	1:A:467:VAL:O	2.10	0.51
2:B:376:THR:HG22	2:B:389:PHE:CZ	2.45	0.51
2:D:97:PRO:HB3	2:D:179:VAL:HG11	1.93	0.51
1:E:105:SER:HB3	1:E:198:HIS:CG	2.45	0.51
1:E:341:ILE:HD12	1:E:383:TRP:NE1	2.23	0.51
1:E:410:TRP:CH2	1:E:412:PRO:HA	2.46	0.51
1:G:157:PRO:HG2	1:G:158:ALA:N	2.24	0.51
1:G:206:ARG:NH2	1:G:218:ASP:HA	2.25	0.51
1:G:540:LYS:CE	2:H:265:ASN:HB2	2.40	0.51
1:G:542:ILE:O	1:G:545:ASN:HB3	2.11	0.51
2:H:24:TRP:CH2	2:H:61:PHE:CE1	2.88	0.51
2:B:329:ILE:HA	2:B:338:THR:O	2.10	0.51
1:C:118:VAL:O	1:C:118:VAL:HG12	2.10	0.51
1:C:324:ASP:O	1:C:343:GLN:HG2	2.09	0.51
1:E:249:LYS:HG2	1:E:250:ASP:H	1.75	0.51
1:E:326:ILE:CB	1:E:342:TYR:CE1	2.92	0.51
1:E:372:VAL:HG11	1:E:411:ILE:HG23	1.91	0.51
1:G:402:TRP:CE3	1:G:403:THR:HA	2.45	0.51
1:G:441:TYR:CE2	1:G:543:GLY:O	2.63	0.51
2:H:246:LEU:HB2	2:H:307:ARG:HH12	1.75	0.51
1:C:391:LEU:HD12	1:C:414:TRP:CZ3	2.46	0.51
2:D:54:ASN:ND2	2:D:56:TYR:HB2	2.25	0.51
1:G:118:VAL:HG12	1:G:118:VAL:O	2.10	0.51
2:H:54:ASN:ND2	2:H:56:TYR:HB2	2.25	0.51
1:A:361:HIS:CD2	1:A:505:ILE:CG2	2.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:391:LEU:HD12	1:A:414:TRP:CZ3	2.46	0.51
2:D:9:PRO:HA	2:D:121:ASP:OD2	2.10	0.51
2:D:10:VAL:HG21	2:D:153:TRP:CH2	2.46	0.51
1:E:91:GLN:HE21	1:E:91:GLN:CA	2.21	0.51
1:G:391:LEU:HD12	1:G:414:TRP:CZ3	2.46	0.51
2:B:10:VAL:HG21	2:B:153:TRP:CH2	2.46	0.51
1:C:6:GLU:CD	1:C:6:GLU:N	2.66	0.51
1:C:451:LYS:O	1:C:471:ASN:HA	2.11	0.51
2:D:326:ILE:O	2:D:341:ILE:HA	2.10	0.51
1:E:342:TYR:C	1:E:342:TYR:HD1	2.19	0.51
1:E:402:TRP:CE3	1:E:403:THR:HA	2.45	0.51
1:G:160:PHE:CZ	1:G:164:MET:HG2	2.46	0.51
1:A:326:ILE:CB	1:A:342:TYR:CE1	2.92	0.51
2:B:10:VAL:HG21	2:B:153:TRP:HH2	1.76	0.51
1:C:342:TYR:OH	1:G:345:PRO:HB3	2.08	0.51
1:C:454:LYS:HA	1:C:467:VAL:O	2.10	0.51
1:C:542:ILE:O	1:C:545:ASN:HB3	2.11	0.51
2:D:10:VAL:HG21	2:D:153:TRP:HH2	1.76	0.51
2:F:376:THR:HG22	2:F:389:PHE:CZ	2.45	0.51
2:H:10:VAL:HG21	2:H:153:TRP:CH2	2.46	0.51
1:A:118:VAL:C	1:A:148:VAL:HG13	2.36	0.51
2:B:97:PRO:HB3	2:B:179:VAL:HG11	1.93	0.51
1:C:12:LEU:HD11	1:C:127:TYR:CE1	2.46	0.51
1:E:118:VAL:O	1:E:118:VAL:HG12	2.10	0.51
2:F:54:ASN:ND2	2:F:56:TYR:HB2	2.25	0.51
2:F:194:GLU:HG2	2:F:195:ILE:N	2.26	0.51
1:G:452:LEU:HD22	1:G:470:THR:HG22	1.92	0.51
2:H:9:PRO:HA	2:H:121:ASP:OD2	2.10	0.51
2:H:10:VAL:HG21	2:H:153:TRP:HH2	1.76	0.51
1:A:451:LYS:O	1:A:471:ASN:HA	2.11	0.51
2:B:326:ILE:O	2:B:341:ILE:HA	2.10	0.51
1:C:160:PHE:CZ	1:C:164:MET:HG2	2.46	0.51
1:C:206:ARG:NH2	1:C:218:ASP:HA	2.25	0.51
1:C:410:TRP:CH2	1:C:412:PRO:HA	2.46	0.51
1:E:361:HIS:NE2	1:E:518:VAL:HG21	2.26	0.51
1:E:540:LYS:NZ	2:F:276:VAL:HG21	2.26	0.51
1:G:326:ILE:CG2	1:G:342:TYR:CE1	2.94	0.51
1:G:342:TYR:C	1:G:342:TYR:HD1	2.19	0.51
1:G:451:LYS:O	1:G:471:ASN:HA	2.11	0.51
2:H:135:ILE:C	2:H:137:ASN:H	2.20	0.51
1:A:363:ASN:ND2	1:A:365:VAL:HB	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:326:ILE:CG2	1:C:342:TYR:CE1	2.94	0.50
1:C:342:TYR:C	1:C:342:TYR:HD1	2.19	0.50
2:D:24:TRP:HZ3	2:D:61:PHE:HB3	1.77	0.50
2:D:329:ILE:HA	2:D:338:THR:O	2.10	0.50
1:E:391:LEU:HD12	1:E:414:TRP:CZ3	2.46	0.50
1:E:402:TRP:O	1:E:402:TRP:HE3	1.93	0.50
1:E:542:ILE:O	1:E:545:ASN:HB3	2.11	0.50
1:G:361:HIS:NE2	1:G:518:VAL:HG21	2.26	0.50
1:A:342:TYR:C	1:A:342:TYR:HD1	2.19	0.50
1:A:414:TRP:CE3	1:A:415:GLU:N	2.78	0.50
2:B:54:ASN:ND2	2:B:56:TYR:HB2	2.25	0.50
1:C:118:VAL:C	1:C:148:VAL:HG13	2.36	0.50
1:C:361:HIS:CD2	1:C:505:ILE:CG2	2.93	0.50
1:C:363:ASN:ND2	1:C:365:VAL:HB	2.26	0.50
1:G:361:HIS:CD2	1:G:505:ILE:CG2	2.93	0.50
1:G:402:TRP:O	1:G:402:TRP:HE3	1.93	0.50
1:G:540:LYS:HZ3	2:H:261:VAL:HG13	1.76	0.50
2:H:72:ARG:NH1	2:H:409:THR:HA	2.26	0.50
1:A:12:LEU:HD11	1:A:127:TYR:CE1	2.46	0.50
1:A:116:PHE:C	1:A:148:VAL:HG11	2.37	0.50
1:A:240:THR:HG22	1:A:315:HIS:CB	2.42	0.50
1:A:410:TRP:CH2	1:A:412:PRO:HA	2.46	0.50
1:C:417:VAL:CG1	1:G:346:PHE:HE2	2.12	0.50
1:E:125:ARG:O	1:E:126:LYS:C	2.55	0.50
1:E:160:PHE:CZ	1:E:164:MET:HG2	2.46	0.50
2:F:135:ILE:C	2:F:137:ASN:H	2.19	0.50
1:G:90:VAL:HG12	2:H:141:GLY:N	2.24	0.50
1:G:125:ARG:O	1:G:126:LYS:C	2.55	0.50
1:G:132:ILE:HD11	1:G:144:TYR:HE2	1.77	0.50
1:G:244:ILE:HB	1:G:310:LEU:HD22	1.94	0.50
1:G:249:LYS:HG2	1:G:250:ASP:H	1.75	0.50
2:H:97:PRO:HB3	2:H:179:VAL:HG11	1.93	0.50
1:A:160:PHE:CZ	1:A:164:MET:HG2	2.46	0.50
1:A:194:GLU:O	1:A:196:GLY:N	2.45	0.50
1:A:419:THR:CG2	1:A:420:PRO:HD2	2.41	0.50
1:A:542:ILE:O	1:A:545:ASN:HB3	2.11	0.50
2:B:135:ILE:C	2:B:137:ASN:H	2.19	0.50
1:C:417:VAL:HG22	1:G:346:PHE:CG	2.47	0.50
1:C:419:THR:CG2	1:C:420:PRO:HD2	2.41	0.50
1:C:468:PRO:HG2	1:C:468:PRO:O	2.12	0.50
1:E:540:LYS:NZ	2:F:261:VAL:O	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:324:ASP:O	1:G:343:GLN:HG2	2.09	0.50
1:A:345:PRO:HG3	1:E:326:ILE:HD13	1.94	0.50
1:A:361:HIS:NE2	1:A:518:VAL:HG21	2.26	0.50
1:C:116:PHE:C	1:C:148:VAL:HG11	2.37	0.50
1:C:361:HIS:NE2	1:C:518:VAL:HG21	2.26	0.50
1:E:244:ILE:HB	1:E:310:LEU:HD22	1.94	0.50
1:E:451:LYS:O	1:E:471:ASN:HA	2.11	0.50
2:F:10:VAL:HG21	2:F:153:TRP:HH2	1.76	0.50
1:G:318:TYR:N	1:G:318:TYR:HD1	2.10	0.50
1:A:244:ILE:HB	1:A:310:LEU:HD22	1.94	0.50
1:A:326:ILE:CG2	1:A:342:TYR:CE1	2.94	0.50
1:A:328:GLU:HG2	1:A:330:GLN:HE21	1.77	0.50
1:A:540:LYS:NZ	2:B:276:VAL:HG21	2.26	0.50
1:C:240:THR:HG22	1:C:315:HIS:CB	2.42	0.50
1:E:194:GLU:O	1:E:196:GLY:N	2.45	0.50
2:F:72:ARG:NH1	2:F:409:THR:HG22	2.25	0.50
1:G:540:LYS:HZ3	2:H:261:VAL:HG12	1.76	0.50
1:A:206:ARG:NH2	1:A:218:ASP:HA	2.25	0.50
2:D:61:PHE:CZ	2:D:402:TRP:HZ2	2.30	0.50
1:G:118:VAL:C	1:G:148:VAL:HG13	2.36	0.50
1:G:540:LYS:NZ	2:H:276:VAL:HG21	2.26	0.50
2:H:194:GLU:HG2	2:H:195:ILE:N	2.26	0.50
2:B:156:SER:N	2:B:157:PRO:HD2	2.27	0.50
1:C:53:GLU:H	1:C:53:GLU:CD	2.20	0.50
1:C:194:GLU:O	1:C:196:GLY:N	2.45	0.50
1:C:342:TYR:CZ	1:G:345:PRO:CG	2.92	0.50
1:C:540:LYS:NZ	2:D:261:VAL:O	2.45	0.50
1:E:90:VAL:HG12	1:E:90:VAL:O	2.12	0.50
1:E:363:ASN:ND2	1:E:365:VAL:HB	2.27	0.50
1:E:399:GLU:O	1:E:399:GLU:HG2	2.12	0.50
2:F:246:LEU:HB2	2:F:307:ARG:HH12	1.75	0.50
1:G:53:GLU:CD	1:G:53:GLU:H	2.20	0.50
1:G:468:PRO:O	1:G:468:PRO:HG2	2.12	0.50
2:H:61:PHE:CZ	2:H:402:TRP:HZ2	2.30	0.50
1:A:540:LYS:NZ	2:B:261:VAL:O	2.45	0.50
1:C:328:GLU:HG2	1:C:330:GLN:HE21	1.76	0.50
2:D:194:GLU:HG2	2:D:195:ILE:N	2.26	0.50
1:E:12:LEU:HD11	1:E:127:TYR:CE1	2.46	0.50
1:E:344:GLU:HB2	1:E:347:LYS:HB2	1.94	0.50
2:F:72:ARG:NH1	2:F:409:THR:HA	2.26	0.50
1:G:12:LEU:HD11	1:G:127:TYR:CE1	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:399:GLU:O	1:G:399:GLU:HG2	2.12	0.50
1:G:540:LYS:NZ	2:H:261:VAL:O	2.45	0.50
2:B:61:PHE:CZ	2:B:402:TRP:HZ2	2.30	0.49
2:B:72:ARG:NH1	2:B:409:THR:HA	2.26	0.49
1:C:244:ILE:HB	1:C:310:LEU:HD22	1.94	0.49
2:D:135:ILE:C	2:D:137:ASN:H	2.20	0.49
1:E:118:VAL:C	1:E:148:VAL:HG13	2.36	0.49
2:F:24:TRP:CH2	2:F:61:PHE:CE1	2.88	0.49
1:G:90:VAL:HG12	1:G:90:VAL:O	2.12	0.49
1:G:116:PHE:C	1:G:148:VAL:HG11	2.37	0.49
1:G:194:GLU:O	1:G:196:GLY:N	2.45	0.49
1:G:328:GLU:HG2	1:G:330:GLN:HE21	1.76	0.49
1:G:394:GLN:HG2	1:G:416:PHE:CE2	2.47	0.49
2:B:207:GLN:O	2:B:208:HIS:C	2.56	0.49
1:C:90:VAL:HG12	1:C:90:VAL:O	2.12	0.49
1:E:206:ARG:NH2	1:E:218:ASP:HA	2.25	0.49
1:E:240:THR:HG22	1:E:315:HIS:CB	2.42	0.49
2:F:10:VAL:HG21	2:F:153:TRP:CH2	2.46	0.49
2:F:156:SER:N	2:F:157:PRO:HD2	2.27	0.49
1:G:447:ASN:HB3	1:G:450:THR:OG1	2.12	0.49
1:A:53:GLU:CD	1:A:53:GLU:H	2.20	0.49
1:A:90:VAL:O	1:A:91:GLN:NE2	2.45	0.49
1:A:468:PRO:HG2	1:A:468:PRO:O	2.12	0.49
2:B:54:ASN:HD22	2:B:56:TYR:H	1.60	0.49
2:B:194:GLU:HG2	2:B:195:ILE:N	2.26	0.49
1:C:125:ARG:O	1:C:126:LYS:C	2.55	0.49
1:C:132:ILE:HD11	1:C:144:TYR:HE2	1.77	0.49
1:C:169:GLU:HB3	1:C:170:PRO:HD3	1.95	0.49
1:C:345:PRO:HG3	1:G:326:ILE:HD13	1.34	0.49
1:G:183:TYR:CD2	1:G:230:MET:HG2	2.47	0.49
1:G:240:THR:HG22	1:G:315:HIS:CB	2.42	0.49
1:C:229:TRP:O	1:C:230:MET:HB2	2.12	0.49
1:C:394:GLN:HG2	1:C:416:PHE:CE2	2.47	0.49
1:C:540:LYS:NZ	2:D:276:VAL:HG21	2.26	0.49
1:E:326:ILE:CG2	1:E:342:TYR:CE1	2.94	0.49
2:F:97:PRO:HB3	2:F:179:VAL:HG11	1.93	0.49
1:G:363:ASN:ND2	1:G:365:VAL:HB	2.27	0.49
2:B:24:TRP:CZ3	2:B:61:PHE:CG	3.00	0.49
1:C:90:VAL:O	1:C:91:GLN:NE2	2.45	0.49
2:D:156:SER:N	2:D:157:PRO:HD2	2.27	0.49
1:E:90:VAL:HG12	2:F:141:GLY:N	2.25	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:318:TYR:N	1:E:318:TYR:HD1	2.10	0.49
1:E:468:PRO:O	1:E:468:PRO:HG2	2.12	0.49
1:E:540:LYS:C	1:E:542:ILE:H	2.20	0.49
2:F:61:PHE:CZ	2:F:402:TRP:HZ2	2.30	0.49
2:B:142:ILE:HG22	2:B:144:TYR:CE1	2.48	0.49
1:C:90:VAL:HG12	2:D:141:GLY:N	2.24	0.49
1:C:318:TYR:N	1:C:318:TYR:HD1	2.10	0.49
2:D:72:ARG:NH1	2:D:409:THR:HA	2.26	0.49
1:E:132:ILE:HD11	1:E:144:TYR:HE2	1.77	0.49
1:E:191:SER:OG	1:E:198:HIS:CD2	2.66	0.49
2:F:24:TRP:CZ3	2:F:61:PHE:CG	3.00	0.49
2:F:54:ASN:HD22	2:F:56:TYR:H	1.60	0.49
1:G:229:TRP:CZ3	1:G:230:MET:HE3	2.48	0.49
2:H:72:ARG:NH1	2:H:409:THR:HG22	2.25	0.49
1:A:540:LYS:HZ3	2:B:261:VAL:HG13	1.76	0.49
1:E:229:TRP:CZ3	1:E:230:MET:HE3	2.48	0.49
1:E:540:LYS:HZ3	2:F:261:VAL:HG13	1.75	0.49
1:G:473:THR:OG1	1:G:476:LYS:HG2	2.13	0.49
2:H:156:SER:N	2:H:157:PRO:HD2	2.27	0.49
1:A:132:ILE:HD11	1:A:144:TYR:HE2	1.77	0.49
1:A:394:GLN:HG2	1:A:416:PHE:CE2	2.47	0.49
1:C:346:PHE:HZ	1:G:328:GLU:OE1	1.96	0.49
2:D:24:TRP:CZ3	2:D:61:PHE:CG	3.00	0.49
2:D:108:VAL:HG12	2:D:188:TYR:CD2	2.48	0.49
1:E:183:TYR:CD2	1:E:230:MET:HG2	2.47	0.49
1:E:328:GLU:HG2	1:E:330:GLN:HE21	1.77	0.49
1:G:169:GLU:HB3	1:G:170:PRO:HD3	1.95	0.49
1:A:46:LYS:HD2	1:A:116:PHE:HB3	1.94	0.49
1:A:169:GLU:HB3	1:A:170:PRO:HD3	1.95	0.49
1:A:191:SER:OG	1:A:198:HIS:CD2	2.66	0.49
1:A:318:TYR:N	1:A:318:TYR:HD1	2.10	0.49
2:D:41:MET:HE1	2:D:73:LYS:CD	2.43	0.49
2:D:72:ARG:NH1	2:D:409:THR:HG22	2.25	0.49
1:E:116:PHE:C	1:E:148:VAL:HG11	2.37	0.49
1:E:394:GLN:HG2	1:E:416:PHE:CE2	2.47	0.49
1:E:447:ASN:HB3	1:E:450:THR:OG1	2.12	0.49
2:F:207:GLN:O	2:F:210:LEU:N	2.46	0.49
1:G:344:GLU:HB2	1:G:347:LYS:HB2	1.94	0.49
2:H:108:VAL:HG12	2:H:188:TYR:CD2	2.48	0.49
1:A:125:ARG:O	1:A:126:LYS:C	2.55	0.49
1:A:229:TRP:CZ3	1:A:230:MET:HE3	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:229:TRP:O	1:A:230:MET:HB2	2.12	0.49
1:C:46:LYS:HD2	1:C:116:PHE:HB3	1.94	0.49
1:C:229:TRP:CZ3	1:C:230:MET:HE3	2.48	0.49
1:E:229:TRP:O	1:E:230:MET:HB2	2.12	0.49
1:G:6:GLU:CD	1:G:6:GLU:N	2.66	0.49
1:G:356:ARG:HH21	1:G:358:ARG:NH1	2.11	0.49
2:H:142:ILE:HG22	2:H:144:TYR:CE1	2.48	0.49
2:H:207:GLN:O	2:H:210:LEU:N	2.46	0.49
2:B:108:VAL:HG12	2:B:188:TYR:CD2	2.48	0.48
1:C:183:TYR:CD2	1:C:230:MET:HG2	2.47	0.48
1:C:540:LYS:HZ3	2:D:261:VAL:HG13	1.77	0.48
2:D:142:ILE:HG22	2:D:144:TYR:CE1	2.48	0.48
1:E:53:GLU:H	1:E:53:GLU:CD	2.20	0.48
1:E:473:THR:OG1	1:E:476:LYS:HG2	2.13	0.48
2:H:395:LYS:HG3	2:H:416:PHE:HE2	1.78	0.48
1:A:90:VAL:HG12	1:A:90:VAL:O	2.12	0.48
1:A:337:TRP:N	1:A:337:TRP:CD1	2.81	0.48
1:A:344:GLU:HB2	1:A:347:LYS:HB2	1.94	0.48
2:B:41:MET:HE1	2:B:73:LYS:CD	2.43	0.48
1:C:416:PHE:HD1	1:C:417:VAL:H	1.61	0.48
1:G:90:VAL:O	1:G:91:GLN:NE2	2.45	0.48
1:G:191:SER:OG	1:G:198:HIS:CD2	2.66	0.48
1:G:326:ILE:CB	1:G:342:TYR:CE1	2.92	0.48
1:G:540:LYS:C	1:G:542:ILE:H	2.20	0.48
1:A:88:TRP:CZ2	2:B:57:ASN:CB	2.96	0.48
1:A:447:ASN:HB3	1:A:450:THR:OG1	2.12	0.48
2:B:97:PRO:HD3	2:B:181:TYR:CD1	2.49	0.48
1:C:10:VAL:HA	1:C:85:GLN:OE1	2.13	0.48
1:C:344:GLU:HB2	1:C:347:LYS:HB2	1.94	0.48
2:D:54:ASN:HD22	2:D:56:TYR:H	1.60	0.48
1:E:452:LEU:HD23	1:E:471:ASN:H	1.78	0.48
2:F:108:VAL:HG12	2:F:188:TYR:CD2	2.48	0.48
2:F:142:ILE:HG22	2:F:144:TYR:CE1	2.48	0.48
1:G:229:TRP:O	1:G:230:MET:HB2	2.12	0.48
1:G:452:LEU:HD23	1:G:471:ASN:H	1.78	0.48
1:G:543:GLY:C	1:G:545:ASN:H	2.22	0.48
1:A:98:ALA:O	1:A:383:TRP:CZ3	2.66	0.48
1:A:356:ARG:HH21	1:A:358:ARG:NH1	2.11	0.48
1:A:452:LEU:HD23	1:A:471:ASN:H	1.78	0.48
2:B:153:TRP:CE3	2:B:156:SER:N	2.82	0.48
2:B:241:VAL:HG12	2:B:242:GLN:N	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:191:SER:OG	1:C:198:HIS:CD2	2.66	0.48
1:C:336:GLN:C	1:C:337:TRP:CD1	2.92	0.48
1:C:447:ASN:HB3	1:C:450:THR:OG1	2.12	0.48
2:D:97:PRO:HD3	2:D:181:TYR:CD1	2.49	0.48
2:D:153:TRP:CE3	2:D:156:SER:N	2.82	0.48
2:D:241:VAL:HG12	2:D:242:GLN:N	2.28	0.48
1:E:96:HIS:CG	1:E:97:PRO:HD2	2.49	0.48
1:E:356:ARG:HH21	1:E:358:ARG:NH1	2.11	0.48
1:E:543:GLY:C	1:E:545:ASN:H	2.22	0.48
1:G:98:ALA:O	1:G:383:TRP:CZ3	2.66	0.48
1:G:336:GLN:C	1:G:337:TRP:CD1	2.92	0.48
1:G:416:PHE:HD1	1:G:417:VAL:H	1.61	0.48
1:G:511:ASP:O	1:G:512:LYS:HD3	2.14	0.48
1:A:10:VAL:HA	1:A:85:GLN:OE1	2.13	0.48
1:A:183:TYR:CD2	1:A:230:MET:HG2	2.47	0.48
2:D:24:TRP:CH2	2:D:61:PHE:CE1	2.88	0.48
2:D:249:LYS:HZ3	2:D:256:ASP:CG	2.22	0.48
1:E:98:ALA:O	1:E:383:TRP:CZ3	2.66	0.48
1:E:336:GLN:C	1:E:337:TRP:CD1	2.92	0.48
1:G:419:THR:CG2	1:G:420:PRO:HD2	2.42	0.48
2:H:24:TRP:CZ3	2:H:61:PHE:CG	3.00	0.48
2:H:153:TRP:CE3	2:H:156:SER:N	2.82	0.48
2:H:207:GLN:O	2:H:208:HIS:C	2.56	0.48
1:A:76:ASP:OD1	1:A:78:ARG:HG3	2.14	0.48
1:A:543:GLY:C	1:A:545:ASN:H	2.22	0.48
1:C:399:GLU:HG2	1:C:399:GLU:O	2.12	0.48
1:C:452:LEU:HD23	1:C:471:ASN:H	1.78	0.48
1:E:46:LYS:HD2	1:E:116:PHE:HB3	1.94	0.48
1:E:510:PRO:O	1:E:522:ILE:HD13	2.14	0.48
2:F:268:SER:HA	2:F:274:ILE:CG2	2.43	0.48
1:G:510:PRO:O	1:G:522:ILE:HD13	2.14	0.48
1:A:90:VAL:HG12	2:B:141:GLY:N	2.24	0.48
2:D:268:SER:HA	2:D:274:ILE:CG2	2.43	0.48
1:E:88:TRP:CZ2	2:F:57:ASN:CB	2.96	0.48
1:E:108:VAL:HG22	1:E:188:TYR:HA	1.96	0.48
2:F:153:TRP:CE3	2:F:156:SER:N	2.82	0.48
1:G:10:VAL:HA	1:G:85:GLN:OE1	2.13	0.48
1:A:164:MET:HG3	1:A:182:GLN:NE2	2.29	0.48
1:A:336:GLN:C	1:A:337:TRP:CD1	2.92	0.48
1:A:416:PHE:HD1	1:A:417:VAL:H	1.61	0.48
1:A:473:THR:OG1	1:A:476:LYS:HG2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:207:GLN:O	2:D:210:LEU:N	2.46	0.48
2:D:274:ILE:HG13	2:D:306:ASN:CG	2.39	0.48
2:D:395:LYS:HG3	2:D:416:PHE:HE2	1.78	0.48
1:E:10:VAL:HA	1:E:85:GLN:OE1	2.13	0.48
1:E:90:VAL:O	1:E:91:GLN:NE2	2.45	0.48
1:E:455:ALA:HB2	1:E:469:LEU:HD11	1.96	0.48
2:F:207:GLN:O	2:F:208:HIS:C	2.55	0.48
2:F:336:GLN:HG2	2:F:355:ALA:CB	2.44	0.48
1:G:46:LYS:HD2	1:G:116:PHE:HB3	1.94	0.48
1:A:455:ALA:HB2	1:A:469:LEU:HD11	1.96	0.48
2:B:207:GLN:O	2:B:210:LEU:N	2.46	0.48
2:B:249:LYS:HZ3	2:B:256:ASP:CG	2.22	0.48
1:C:88:TRP:CZ2	2:D:57:ASN:CB	2.96	0.48
1:C:98:ALA:O	1:C:383:TRP:CZ3	2.66	0.48
1:C:473:THR:OG1	1:C:476:LYS:HG2	2.13	0.48
1:C:511:ASP:O	1:C:512:LYS:HD3	2.14	0.48
1:E:76:ASP:OD1	1:E:78:ARG:HG3	2.14	0.48
1:E:511:ASP:O	1:E:512:LYS:HD3	2.14	0.48
1:G:76:ASP:OD1	1:G:78:ARG:HG3	2.14	0.48
1:G:455:ALA:HB2	1:G:469:LEU:HD11	1.96	0.48
2:H:54:ASN:HD22	2:H:56:TYR:H	1.60	0.48
2:H:91:GLN:CD	2:H:94:ILE:HG23	2.39	0.48
1:A:108:VAL:HG22	1:A:188:TYR:HA	1.96	0.48
2:B:52:PRO:HD2	2:B:53:GLU:OE1	2.14	0.48
2:B:123:ASP:HA	2:B:126:LYS:HZ2	1.78	0.48
2:B:274:ILE:HG13	2:B:306:ASN:CG	2.39	0.48
2:D:52:PRO:HD2	2:D:53:GLU:OE1	2.14	0.48
1:G:132:ILE:HB	1:G:142:ILE:HG12	1.96	0.48
1:G:164:MET:HG3	1:G:182:GLN:NE2	2.29	0.48
2:H:41:MET:HE1	2:H:73:LYS:CD	2.43	0.48
2:H:241:VAL:HG12	2:H:242:GLN:N	2.28	0.48
1:A:96:HIS:CG	1:A:97:PRO:HD2	2.49	0.47
1:A:540:LYS:C	1:A:542:ILE:H	2.20	0.47
1:C:76:ASP:OD1	1:C:78:ARG:HG3	2.14	0.47
1:C:108:VAL:HG22	1:C:188:TYR:HA	1.96	0.47
1:C:356:ARG:HH21	1:C:358:ARG:NH1	2.11	0.47
1:C:540:LYS:C	1:C:542:ILE:H	2.20	0.47
1:E:169:GLU:HB3	1:E:170:PRO:HD3	1.95	0.47
2:F:41:MET:HE1	2:F:73:LYS:CD	2.43	0.47
2:F:158:ALA:O	2:F:161:GLN:HB2	2.15	0.47
1:G:108:VAL:HG22	1:G:188:TYR:HA	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:337:TRP:CD1	1:G:337:TRP:N	2.81	0.47
1:A:132:ILE:HB	1:A:142:ILE:HG12	1.96	0.47
1:A:399:GLU:HG2	1:A:399:GLU:O	2.12	0.47
1:C:164:MET:HG3	1:C:182:GLN:NE2	2.29	0.47
1:G:336:GLN:HG2	1:G:355:ALA:HB2	1.97	0.47
1:A:46:LYS:HG3	1:A:116:PHE:CD2	2.50	0.47
2:B:268:SER:HA	2:B:274:ILE:CG2	2.43	0.47
2:B:395:LYS:HG3	2:B:416:PHE:HE2	1.78	0.47
2:D:123:ASP:HA	2:D:126:LYS:HZ2	1.79	0.47
2:D:336:GLN:HG2	2:D:355:ALA:CB	2.44	0.47
2:F:24:TRP:HZ3	2:F:61:PHE:HB3	1.76	0.47
2:F:91:GLN:CD	2:F:94:ILE:HG23	2.39	0.47
2:F:97:PRO:HD3	2:F:181:TYR:CD1	2.49	0.47
2:F:241:VAL:HG12	2:F:242:GLN:N	2.28	0.47
1:A:354:TYR:CZ	1:A:356:ARG:HD3	2.49	0.47
1:A:511:ASP:O	1:A:512:LYS:HD3	2.14	0.47
2:B:91:GLN:CD	2:B:94:ILE:HG23	2.39	0.47
1:C:46:LYS:HG3	1:C:116:PHE:CD2	2.50	0.47
1:C:132:ILE:HB	1:C:142:ILE:HG12	1.96	0.47
1:C:390:LYS:HB3	1:C:417:VAL:HG21	1.96	0.47
1:E:102:LYS:CG	1:E:318:TYR:HB2	2.45	0.47
1:E:304:ALA:HA	1:E:307:ARG:HD2	1.96	0.47
1:E:336:GLN:HG2	1:E:355:ALA:HB2	1.97	0.47
1:E:419:THR:CG2	1:E:420:PRO:HD2	2.42	0.47
1:G:88:TRP:CZ2	2:H:57:ASN:CB	2.96	0.47
1:G:354:TYR:CZ	1:G:356:ARG:HD3	2.49	0.47
2:H:158:ALA:O	2:H:161:GLN:HB2	2.14	0.47
2:H:274:ILE:HG13	2:H:306:ASN:CG	2.39	0.47
2:H:336:GLN:HG2	2:H:355:ALA:CB	2.44	0.47
1:A:20:LYS:HG2	1:A:56:TYR:HA	1.96	0.47
1:A:23:GLN:HG2	1:A:59:PRO:HA	1.96	0.47
1:A:304:ALA:HA	1:A:307:ARG:HD2	1.96	0.47
1:A:510:PRO:O	1:A:522:ILE:HD13	2.14	0.47
2:B:24:TRP:CH2	2:B:61:PHE:CE1	2.88	0.47
2:B:64:LYS:HB2	2:B:71:TRP:CE3	2.50	0.47
1:C:96:HIS:CG	1:C:97:PRO:HD2	2.49	0.47
1:C:455:ALA:HB2	1:C:469:LEU:HD11	1.96	0.47
1:C:543:GLY:C	1:C:545:ASN:H	2.22	0.47
1:E:164:MET:HG3	1:E:182:GLN:NE2	2.29	0.47
1:E:318:TYR:N	1:E:318:TYR:CD1	2.82	0.47
2:H:97:PRO:HD3	2:H:181:TYR:CD1	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:228:LEU:HD21	1:A:233:GLU:HG2	1.96	0.47
1:A:318:TYR:N	1:A:318:TYR:CD1	2.82	0.47
1:A:342:TYR:HB3	1:A:348:ASN:CB	2.44	0.47
1:A:390:LYS:HB3	1:A:417:VAL:HG21	1.96	0.47
1:C:23:GLN:HG2	1:C:59:PRO:HA	1.97	0.47
1:C:228:LEU:HD21	1:C:233:GLU:HG2	1.96	0.47
1:C:354:TYR:CZ	1:C:356:ARG:HD3	2.49	0.47
2:D:207:GLN:O	2:D:208:HIS:C	2.55	0.47
2:F:56:TYR:O	2:F:143:ARG:NH2	2.48	0.47
2:F:64:LYS:HB2	2:F:71:TRP:CZ3	2.50	0.47
1:G:23:GLN:HG2	1:G:59:PRO:HA	1.97	0.47
1:G:46:LYS:HG3	1:G:116:PHE:CD2	2.50	0.47
2:H:24:TRP:HZ3	2:H:61:PHE:HB3	1.76	0.47
2:H:56:TYR:O	2:H:143:ARG:NH2	2.48	0.47
2:H:64:LYS:HB2	2:H:71:TRP:CZ3	2.50	0.47
2:H:268:SER:HA	2:H:274:ILE:CG2	2.43	0.47
1:A:336:GLN:HG2	1:A:355:ALA:HB2	1.97	0.47
1:A:345:PRO:HG3	1:E:326:ILE:CD1	2.44	0.47
2:B:336:GLN:HG2	2:B:355:ALA:CB	2.44	0.47
1:C:326:ILE:HB	1:C:342:TYR:CD1	2.50	0.47
1:C:417:VAL:CG2	1:G:346:PHE:CD2	2.98	0.47
1:C:442:VAL:HG12	1:C:443:ASP:N	2.30	0.47
2:D:56:TYR:O	2:D:143:ARG:NH2	2.48	0.47
1:E:23:GLN:HG2	1:E:59:PRO:HA	1.97	0.47
1:E:132:ILE:HB	1:E:142:ILE:HG12	1.96	0.47
1:E:228:LEU:HD21	1:E:233:GLU:HG2	1.96	0.47
1:E:337:TRP:CD1	1:E:337:TRP:N	2.81	0.47
1:E:442:VAL:HG12	1:E:443:ASP:N	2.30	0.47
1:G:102:LYS:CG	1:G:318:TYR:HB2	2.45	0.47
1:G:318:TYR:N	1:G:318:TYR:CD1	2.82	0.47
1:G:326:ILE:HB	1:G:342:TYR:CD1	2.50	0.47
1:G:390:LYS:HB3	1:G:417:VAL:HG21	1.96	0.47
2:H:52:PRO:HD2	2:H:53:GLU:OE1	2.14	0.47
1:A:442:VAL:HG12	1:A:443:ASP:N	2.30	0.47
2:B:158:ALA:O	2:B:161:GLN:HB2	2.15	0.47
2:D:64:LYS:HB2	2:D:71:TRP:CZ3	2.50	0.47
1:E:20:LYS:HG2	1:E:56:TYR:HA	1.96	0.47
1:E:354:TYR:CZ	1:E:356:ARG:HD3	2.49	0.47
2:F:274:ILE:HG13	2:F:306:ASN:CG	2.39	0.47
1:G:78:ARG:NH1	1:G:287:LYS:O	2.39	0.47
1:G:228:LEU:HD21	1:G:233:GLU:HG2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:20:LYS:HG2	1:C:56:TYR:HA	1.96	0.47
1:C:121:ASP:O	1:C:125:ARG:HG3	2.15	0.47
1:C:191:SER:OG	1:C:198:HIS:HD2	1.98	0.47
1:C:318:TYR:N	1:C:318:TYR:CD1	2.82	0.47
1:C:342:TYR:HB3	1:C:348:ASN:CB	2.44	0.47
1:C:391:LEU:HA	1:C:392:PRO:HD3	1.72	0.47
2:D:64:LYS:HB2	2:D:71:TRP:CE3	2.50	0.47
1:E:390:LYS:HB3	1:E:417:VAL:HG21	1.96	0.47
1:E:416:PHE:HD1	1:E:417:VAL:H	1.61	0.47
2:F:24:TRP:HZ3	2:F:61:PHE:CB	2.28	0.47
2:H:276:VAL:HG12	2:H:279:LEU:HD12	1.97	0.47
1:A:33:ALA:O	1:A:36:GLU:HB3	2.15	0.47
1:A:102:LYS:CG	1:A:318:TYR:HB2	2.45	0.47
1:A:326:ILE:HB	1:A:342:TYR:CD1	2.50	0.47
2:B:64:LYS:HB2	2:B:71:TRP:CZ3	2.50	0.47
1:C:336:GLN:HG2	1:C:355:ALA:HB2	1.97	0.47
2:D:158:ALA:O	2:D:161:GLN:HB2	2.15	0.47
2:D:330:GLN:HG3	2:D:419:THR:HG21	1.96	0.47
1:E:537:PRO:HB2	1:E:540:LYS:HD2	1.97	0.47
2:F:52:PRO:HD2	2:F:53:GLU:OE1	2.14	0.47
2:F:108:VAL:HA	2:F:187:LEU:O	2.15	0.47
1:G:96:HIS:CG	1:G:97:PRO:HD2	2.49	0.47
1:A:191:SER:OG	1:A:198:HIS:HD2	1.98	0.46
2:B:55:PRO:HG2	2:B:56:TYR:CD2	2.51	0.46
2:B:56:TYR:O	2:B:143:ARG:NH2	2.48	0.46
1:C:510:PRO:O	1:C:522:ILE:HD13	2.14	0.46
2:D:91:GLN:CD	2:D:94:ILE:HG23	2.39	0.46
2:D:108:VAL:HA	2:D:187:LEU:O	2.15	0.46
1:E:437:ALA:HB1	1:E:493:VAL:HA	1.97	0.46
2:F:135:ILE:H	2:F:135:ILE:HG12	1.38	0.46
2:F:345:PRO:O	2:F:346:PHE:HB2	2.15	0.46
1:G:33:ALA:O	1:G:36:GLU:HB3	2.15	0.46
1:G:53:GLU:CD	1:G:53:GLU:N	2.73	0.46
1:G:442:VAL:HG12	1:G:443:ASP:N	2.30	0.46
2:H:55:PRO:HG2	2:H:56:TYR:CD2	2.51	0.46
1:A:121:ASP:O	1:A:125:ARG:HG3	2.15	0.46
2:B:108:VAL:HA	2:B:187:LEU:O	2.15	0.46
1:C:304:ALA:HA	1:C:307:ARG:HD2	1.96	0.46
1:C:346:PHE:CB	1:G:390:LYS:HZ1	1.98	0.46
2:D:55:PRO:HG2	2:D:56:TYR:CD2	2.51	0.46
2:F:64:LYS:HB2	2:F:71:TRP:CE3	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:121:ASP:O	1:G:125:ARG:HG3	2.15	0.46
1:G:240:THR:HG22	1:G:315:HIS:HB3	1.97	0.46
1:G:248:GLU:CG	1:G:307:ARG:HH21	2.28	0.46
1:A:503:LEU:O	1:A:507:GLN:HG2	2.16	0.46
1:C:33:ALA:O	1:C:36:GLU:HB3	2.15	0.46
1:C:337:TRP:CD1	1:C:337:TRP:N	2.81	0.46
1:C:503:LEU:O	1:C:507:GLN:HG2	2.16	0.46
1:E:33:ALA:O	1:E:36:GLU:HB3	2.15	0.46
1:E:229:TRP:CE3	1:E:230:MET:HE3	2.50	0.46
1:E:248:GLU:CG	1:E:307:ARG:HH21	2.28	0.46
1:E:326:ILE:HB	1:E:342:TYR:CD1	2.50	0.46
1:G:342:TYR:HB3	1:G:348:ASN:CB	2.44	0.46
2:H:108:VAL:HA	2:H:187:LEU:O	2.15	0.46
1:A:102:LYS:HG3	1:A:318:TYR:HB2	1.97	0.46
1:A:398:TRP:CZ3	1:A:411:ILE:HD11	2.51	0.46
2:B:276:VAL:HG12	2:B:279:LEU:HD12	1.98	0.46
2:F:259:LYS:HE3	2:F:263:LYS:NZ	2.30	0.46
2:F:330:GLN:HG3	2:F:419:THR:HG21	1.96	0.46
1:G:191:SER:OG	1:G:198:HIS:HD2	1.99	0.46
2:H:64:LYS:HB2	2:H:71:TRP:CE3	2.50	0.46
1:A:537:PRO:HB2	1:A:540:LYS:HD2	1.97	0.46
2:D:24:TRP:HZ3	2:D:61:PHE:CB	2.28	0.46
1:E:115:TYR:CE2	1:E:156:SER:HB3	2.51	0.46
1:E:516:GLU:O	1:E:520:GLN:HG2	2.15	0.46
1:G:304:ALA:HA	1:G:307:ARG:HD2	1.96	0.46
1:G:451:LYS:O	1:G:452:LEU:HD23	2.15	0.46
2:H:330:GLN:HG3	2:H:419:THR:HG21	1.96	0.46
1:E:59:PRO:HG2	1:E:76:ASP:HB3	1.98	0.46
1:E:240:THR:HG22	1:E:315:HIS:HB3	1.97	0.46
1:E:451:LYS:O	1:E:452:LEU:HD23	2.15	0.46
1:E:540:LYS:NZ	2:F:261:VAL:HG12	2.31	0.46
2:F:55:PRO:HG2	2:F:56:TYR:CD2	2.51	0.46
2:B:28:GLU:HG2	2:B:32:LYS:HZ2	1.81	0.46
2:B:259:LYS:HE3	2:B:263:LYS:NZ	2.30	0.46
2:B:345:PRO:O	2:B:346:PHE:HB2	2.15	0.46
1:C:53:GLU:CD	1:C:53:GLU:N	2.73	0.46
1:C:91:GLN:HE21	1:C:91:GLN:CA	2.21	0.46
1:C:102:LYS:CG	1:C:318:TYR:HB2	2.45	0.46
1:C:451:LYS:O	1:C:452:LEU:HD23	2.15	0.46
1:C:540:LYS:NZ	2:D:261:VAL:HG12	2.31	0.46
2:D:276:VAL:HG12	2:D:279:LEU:HD12	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:121:ASP:O	1:E:125:ARG:HG3	2.15	0.46
2:F:123:ASP:HA	2:F:126:LYS:HZ2	1.81	0.46
2:F:276:VAL:HG12	2:F:279:LEU:HD12	1.98	0.46
1:G:59:PRO:HG2	1:G:76:ASP:HB3	1.98	0.46
2:H:259:LYS:HE3	2:H:263:LYS:NZ	2.30	0.46
1:A:451:LYS:O	1:A:452:LEU:HD23	2.15	0.46
1:A:516:GLU:O	1:A:520:GLN:HG2	2.15	0.46
2:B:72:ARG:HH22	2:B:409:THR:HB	1.81	0.46
1:C:241:VAL:HB	1:C:314:VAL:HG22	1.98	0.46
2:D:259:LYS:HE3	2:D:263:LYS:NZ	2.30	0.46
1:G:46:LYS:HG3	1:G:116:PHE:HD2	1.81	0.46
1:G:229:TRP:CE3	1:G:230:MET:HE3	2.50	0.46
1:G:398:TRP:CZ3	1:G:411:ILE:HD11	2.51	0.46
2:H:10:VAL:HG11	2:H:153:TRP:HH2	1.81	0.46
1:A:59:PRO:HG2	1:A:76:ASP:HB3	1.98	0.46
1:A:91:GLN:HE21	1:A:91:GLN:CA	2.22	0.46
1:A:115:TYR:CE2	1:A:156:SER:HB3	2.51	0.46
1:A:175:ASN:ND2	1:A:201:LYS:NZ	2.64	0.46
1:A:241:VAL:HB	1:A:314:VAL:HG22	1.98	0.46
2:B:104:LYS:HZ1	2:B:194:GLU:HA	1.81	0.46
2:B:297:GLU:HA	2:B:300:GLU:HB3	1.98	0.46
2:B:365:VAL:HG12	2:B:405:TYR:HE2	1.80	0.46
1:C:175:ASN:ND2	1:C:201:LYS:NZ	2.64	0.46
1:C:417:VAL:HG22	1:G:346:PHE:CD2	2.51	0.46
2:D:72:ARG:HH22	2:D:409:THR:HB	1.81	0.46
2:D:297:GLU:HA	2:D:300:GLU:HB3	1.98	0.46
1:E:46:LYS:HG3	1:E:116:PHE:CD2	2.50	0.46
1:E:53:GLU:CD	1:E:53:GLU:N	2.73	0.46
1:E:102:LYS:HG3	1:E:318:TYR:HB2	1.97	0.46
1:E:398:TRP:CZ3	1:E:411:ILE:HD11	2.51	0.46
1:G:102:LYS:HG3	1:G:318:TYR:HB2	1.97	0.46
1:G:540:LYS:NZ	2:H:261:VAL:HG12	2.31	0.46
1:C:102:LYS:HG3	1:C:318:TYR:HB2	1.97	0.46
1:C:398:TRP:CZ3	1:C:411:ILE:HD11	2.51	0.46
1:C:537:PRO:HB2	1:C:540:LYS:HD2	1.97	0.46
1:E:95:PRO:HG3	1:E:230:MET:HE1	1.96	0.46
1:E:175:ASN:ND2	1:E:201:LYS:NZ	2.64	0.46
2:F:390:LYS:HA	2:F:415:GLU:O	2.17	0.46
1:G:20:LYS:HG2	1:G:56:TYR:HA	1.96	0.46
1:A:53:GLU:CD	1:A:53:GLU:N	2.73	0.45
1:A:229:TRP:CE3	1:A:230:MET:HE3	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:24:TRP:HZ3	2:B:61:PHE:CB	2.28	0.45
2:B:330:GLN:HG3	2:B:419:THR:HG21	1.96	0.45
2:B:390:LYS:HA	2:B:415:GLU:O	2.17	0.45
1:C:229:TRP:CE3	1:C:230:MET:HE3	2.50	0.45
2:D:171:PHE:HA	2:D:174:GLN:HB3	1.98	0.45
2:D:345:PRO:O	2:D:346:PHE:HB2	2.15	0.45
1:E:342:TYR:HB3	1:E:348:ASN:CB	2.44	0.45
2:F:96:HIS:CD2	2:F:384:GLY:HA3	2.51	0.45
1:G:115:TYR:CE2	1:G:156:SER:HB3	2.51	0.45
1:G:418:ASN:C	1:G:418:ASN:ND2	2.74	0.45
2:H:171:PHE:HA	2:H:174:GLN:HB3	1.98	0.45
1:A:95:PRO:HG3	1:A:230:MET:HE1	1.96	0.45
1:A:418:ASN:C	1:A:418:ASN:ND2	2.74	0.45
1:A:437:ALA:HB1	1:A:493:VAL:HA	1.97	0.45
2:B:24:TRP:HZ3	2:B:61:PHE:HB3	1.76	0.45
2:B:116:PHE:CZ	2:B:151:GLN:HG2	2.52	0.45
1:C:34:LEU:HD21	1:C:62:ALA:HB2	1.98	0.45
1:C:115:TYR:CE2	1:C:156:SER:HB3	2.51	0.45
1:C:437:ALA:HB1	1:C:493:VAL:HA	1.97	0.45
1:C:540:LYS:HZ3	2:D:261:VAL:HG12	1.81	0.45
2:D:28:GLU:HG2	2:D:32:LYS:HZ2	1.81	0.45
1:E:46:LYS:HG3	1:E:116:PHE:HD2	1.81	0.45
1:G:437:ALA:HB1	1:G:493:VAL:HA	1.97	0.45
1:G:516:GLU:O	1:G:520:GLN:HG2	2.15	0.45
2:H:96:HIS:CD2	2:H:384:GLY:HA3	2.51	0.45
1:A:445:ALA:O	1:A:453:GLY:HA3	2.16	0.45
2:B:171:PHE:HA	2:B:174:GLN:HB3	1.98	0.45
1:C:59:PRO:HG2	1:C:76:ASP:HB3	1.98	0.45
1:C:240:THR:HG22	1:C:315:HIS:HB3	1.97	0.45
2:D:116:PHE:CZ	2:D:151:GLN:HG2	2.52	0.45
1:E:361:HIS:CD2	1:E:505:ILE:HG23	2.52	0.45
2:F:104:LYS:HZ2	2:F:194:GLU:HA	1.81	0.45
2:F:171:PHE:CZ	2:F:205:LEU:HB2	2.51	0.45
1:G:115:TYR:O	1:G:117:SER:N	2.50	0.45
1:G:175:ASN:ND2	1:G:201:LYS:NZ	2.64	0.45
1:A:240:THR:HG22	1:A:315:HIS:HB3	1.97	0.45
2:B:96:HIS:CD2	2:B:384:GLY:HA3	2.51	0.45
1:C:329:ILE:HA	1:C:338:THR:O	2.17	0.45
1:C:345:PRO:HG2	1:G:326:ILE:HD11	1.84	0.45
1:C:361:HIS:CD2	1:C:505:ILE:HG23	2.52	0.45
1:C:445:ALA:O	1:C:453:GLY:HA3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:10:VAL:HG11	2:D:153:TRP:HH2	1.81	0.45
2:D:96:HIS:CD2	2:D:384:GLY:HA3	2.51	0.45
2:D:171:PHE:CZ	2:D:205:LEU:HB2	2.51	0.45
1:G:326:ILE:CB	1:G:342:TYR:HE1	2.28	0.45
1:G:357:MET:SD	1:G:362:THR:OG1	2.71	0.45
1:G:361:HIS:CD2	1:G:505:ILE:HG23	2.52	0.45
1:G:445:ALA:O	1:G:453:GLY:HA3	2.16	0.45
1:G:537:PRO:HB2	1:G:540:LYS:HD2	1.97	0.45
2:H:24:TRP:HZ3	2:H:61:PHE:CB	2.28	0.45
1:A:361:HIS:CD2	1:A:505:ILE:HG23	2.52	0.45
2:B:171:PHE:CZ	2:B:205:LEU:HB2	2.51	0.45
1:C:115:TYR:O	1:C:117:SER:N	2.50	0.45
1:C:418:ASN:C	1:C:418:ASN:ND2	2.74	0.45
2:D:390:LYS:HA	2:D:415:GLU:O	2.16	0.45
1:E:445:ALA:O	1:E:453:GLY:HA3	2.16	0.45
1:E:503:LEU:O	1:E:507:GLN:HG2	2.16	0.45
2:F:10:VAL:HG11	2:F:153:TRP:HH2	1.81	0.45
2:F:116:PHE:CZ	2:F:151:GLN:HG2	2.52	0.45
2:F:255:ASN:HA	2:F:258:GLN:HB2	1.98	0.45
2:H:116:PHE:CZ	2:H:151:GLN:HG2	2.52	0.45
1:A:34:LEU:HD21	1:A:62:ALA:HB2	1.99	0.45
1:A:46:LYS:HG3	1:A:116:PHE:HD2	1.81	0.45
1:A:329:ILE:HA	1:A:338:THR:O	2.17	0.45
2:B:195:ILE:O	2:B:199:ARG:HG3	2.17	0.45
1:G:503:LEU:O	1:G:507:GLN:HG2	2.16	0.45
1:G:546:GLU:O	1:G:549:ASP:HB3	2.17	0.45
2:H:195:ILE:O	2:H:199:ARG:HG3	2.17	0.45
2:H:345:PRO:O	2:H:346:PHE:HB2	2.15	0.45
1:A:85:GLN:O	1:A:85:GLN:CG	2.55	0.45
1:A:148:VAL:HG12	1:A:149:LEU:N	2.31	0.45
1:A:357:MET:SD	1:A:362:THR:OG1	2.71	0.45
2:D:195:ILE:O	2:D:199:ARG:HG3	2.17	0.45
1:E:191:SER:OG	1:E:198:HIS:HD2	1.98	0.45
1:G:241:VAL:HB	1:G:314:VAL:HG22	1.98	0.45
1:G:327:ALA:HA	1:G:340:GLN:O	2.17	0.45
2:H:135:ILE:H	2:H:135:ILE:HG12	1.38	0.45
2:H:171:PHE:CZ	2:H:205:LEU:HB2	2.51	0.45
2:H:259:LYS:HE3	2:H:263:LYS:HZ1	1.81	0.45
1:A:410:TRP:HZ3	2:B:401:TRP:CZ2	2.35	0.45
2:B:10:VAL:HG11	2:B:153:TRP:HH2	1.81	0.45
2:B:120:LEU:O	2:B:125:ARG:CZ	2.65	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:248:GLU:CG	1:C:307:ARG:HH21	2.28	0.45
1:C:516:GLU:O	1:C:520:GLN:HG2	2.15	0.45
1:E:57:ASN:OD1	1:E:130:PHE:HA	2.17	0.45
2:F:297:GLU:HA	2:F:300:GLU:HB3	1.98	0.45
2:H:104:LYS:HZ3	2:H:194:GLU:HA	1.80	0.45
2:H:193:LEU:CD1	2:H:201:LYS:HG3	2.47	0.45
2:H:249:LYS:HZ3	2:H:256:ASP:CG	2.25	0.45
2:H:390:LYS:HA	2:H:415:GLU:O	2.16	0.45
2:H:390:LYS:HG2	2:H:415:GLU:OE1	2.17	0.45
1:A:248:GLU:CG	1:A:307:ARG:HH21	2.28	0.45
1:C:78:ARG:NH1	1:C:287:LYS:O	2.39	0.45
1:C:148:VAL:HG12	1:C:149:LEU:N	2.31	0.45
1:C:410:TRP:HZ3	2:D:401:TRP:CZ2	2.35	0.45
2:D:108:VAL:HG11	2:D:188:TYR:CE2	2.52	0.45
2:D:365:VAL:HG12	2:D:405:TYR:HE2	1.80	0.45
2:D:376:THR:HG22	2:D:389:PHE:HE1	1.80	0.45
2:F:72:ARG:HH22	2:F:409:THR:HB	1.81	0.45
2:F:241:VAL:O	2:F:243:PRO:HD3	2.17	0.45
1:G:57:ASN:OD1	1:G:130:PHE:HA	2.17	0.45
2:H:72:ARG:HH22	2:H:409:THR:HB	1.81	0.45
1:A:115:TYR:O	1:A:117:SER:N	2.50	0.45
1:C:46:LYS:HG3	1:C:116:PHE:HD2	1.81	0.45
1:C:326:ILE:CB	1:C:342:TYR:HE1	2.28	0.45
1:C:440:PHE:CE2	1:C:457:TYR:CE2	3.05	0.45
2:D:78:ARG:O	2:D:82:LYS:HG3	2.17	0.45
2:D:120:LEU:O	2:D:125:ARG:CZ	2.65	0.45
1:E:54:ASN:HA	1:E:55:PRO:HD3	1.78	0.45
1:E:326:ILE:CB	1:E:342:TYR:HE1	2.28	0.45
1:E:442:VAL:HG12	1:E:481:ALA:CB	2.46	0.45
2:F:195:ILE:O	2:F:199:ARG:HG3	2.17	0.45
1:G:34:LEU:HD21	1:G:62:ALA:HB2	1.99	0.45
1:G:167:ILE:O	1:G:208:HIS:CE1	2.66	0.45
1:G:329:ILE:HA	1:G:338:THR:O	2.17	0.45
2:H:123:ASP:HA	2:H:126:LYS:HZ2	1.78	0.45
1:A:440:PHE:CE2	1:A:457:TYR:CE2	3.05	0.44
1:A:546:GLU:O	1:A:549:ASP:HB3	2.17	0.44
2:B:108:VAL:HG11	2:B:188:TYR:CE2	2.52	0.44
1:C:10:VAL:HG11	1:C:153:TRP:CZ2	2.52	0.44
2:D:193:LEU:CD1	2:D:201:LYS:HG3	2.47	0.44
1:E:10:VAL:HG11	1:E:153:TRP:CZ2	2.52	0.44
2:F:78:ARG:O	2:F:82:LYS:HG3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:120:LEU:O	2:F:125:ARG:CZ	2.65	0.44
1:G:410:TRP:HZ3	2:H:401:TRP:CZ2	2.35	0.44
2:H:241:VAL:O	2:H:243:PRO:HD3	2.17	0.44
1:A:57:ASN:OD1	1:A:130:PHE:HA	2.17	0.44
1:A:78:ARG:NH1	1:A:287:LYS:O	2.39	0.44
1:A:160:PHE:CZ	1:A:164:MET:CG	3.01	0.44
1:A:229:TRP:CH2	1:A:230:MET:CE	3.01	0.44
1:A:379:SER:HB3	1:A:383:TRP:HD1	1.82	0.44
1:A:439:THR:HG22	1:A:441:TYR:HE1	1.82	0.44
2:B:162:SER:O	2:B:166:LYS:HG2	2.17	0.44
2:B:193:LEU:CD1	2:B:201:LYS:HG3	2.47	0.44
2:B:390:LYS:HG2	2:B:415:GLU:OE1	2.17	0.44
1:C:379:SER:HB3	1:C:383:TRP:HD1	1.83	0.44
2:D:255:ASN:HA	2:D:258:GLN:HB2	1.99	0.44
1:E:155:GLY:O	1:E:156:SER:C	2.60	0.44
1:E:329:ILE:HA	1:E:338:THR:O	2.17	0.44
2:F:171:PHE:HA	2:F:174:GLN:HB3	1.98	0.44
2:F:292:VAL:HG12	2:F:293:ILE:N	2.33	0.44
1:G:160:PHE:CZ	1:G:164:MET:CG	3.01	0.44
2:H:297:GLU:HA	2:H:300:GLU:HB3	1.98	0.44
1:A:10:VAL:HG11	1:A:153:TRP:CZ2	2.52	0.44
1:A:155:GLY:O	1:A:156:SER:C	2.60	0.44
1:C:95:PRO:HG3	1:C:230:MET:HE1	1.96	0.44
1:C:546:GLU:O	1:C:549:ASP:HB3	2.17	0.44
1:E:546:GLU:O	1:E:549:ASP:HB3	2.17	0.44
2:F:100:LEU:HD23	2:F:100:LEU:HA	1.81	0.44
2:F:390:LYS:HG2	2:F:415:GLU:OE1	2.17	0.44
1:A:327:ALA:HA	1:A:340:GLN:O	2.17	0.44
2:B:78:ARG:O	2:B:82:LYS:HG3	2.17	0.44
1:E:115:TYR:O	1:E:117:SER:N	2.50	0.44
1:E:148:VAL:HG12	1:E:149:LEU:N	2.31	0.44
1:E:327:ALA:HA	1:E:340:GLN:O	2.17	0.44
1:E:379:SER:HB3	1:E:383:TRP:HD1	1.83	0.44
2:F:108:VAL:HG11	2:F:188:TYR:CE2	2.53	0.44
2:B:157:PRO:CG	2:B:158:ALA:N	2.79	0.44
1:C:57:ASN:OD1	1:C:130:PHE:HA	2.17	0.44
1:C:327:ALA:HA	1:C:340:GLN:O	2.17	0.44
1:C:451:LYS:O	1:C:471:ASN:N	2.51	0.44
1:E:160:PHE:CZ	1:E:164:MET:CG	3.01	0.44
1:E:241:VAL:HB	1:E:314:VAL:HG22	1.98	0.44
1:E:410:TRP:HZ3	2:F:401:TRP:CZ2	2.35	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:441:TYR:O	1:E:548:VAL:HG21	2.18	0.44
1:G:95:PRO:HG3	1:G:230:MET:HE1	1.96	0.44
1:G:412:PRO:HG2	1:G:413:GLU:H	1.83	0.44
1:G:451:LYS:O	1:G:471:ASN:N	2.51	0.44
2:H:78:ARG:O	2:H:82:LYS:HG3	2.17	0.44
1:A:451:LYS:O	1:A:471:ASN:N	2.51	0.44
2:B:292:VAL:HG12	2:B:293:ILE:N	2.33	0.44
1:C:229:TRP:CH2	1:C:230:MET:CE	3.01	0.44
2:D:104:LYS:HZ1	2:D:194:GLU:HA	1.82	0.44
2:D:157:PRO:CG	2:D:158:ALA:N	2.79	0.44
2:D:162:SER:O	2:D:166:LYS:HG2	2.17	0.44
2:D:292:VAL:HG12	2:D:293:ILE:N	2.33	0.44
2:D:390:LYS:HG2	2:D:415:GLU:OE1	2.17	0.44
1:E:229:TRP:CH2	1:E:230:MET:CE	3.01	0.44
2:F:395:LYS:HG3	2:F:416:PHE:HE2	1.78	0.44
1:G:155:GLY:O	1:G:156:SER:C	2.60	0.44
2:H:292:VAL:HG12	2:H:293:ILE:N	2.33	0.44
2:H:354:TYR:CE1	2:H:374:LYS:HD3	2.53	0.44
1:A:326:ILE:CB	1:A:342:TYR:HE1	2.28	0.44
2:B:255:ASN:HA	2:B:258:GLN:HB2	1.99	0.44
1:C:160:PHE:CZ	1:C:164:MET:CG	3.00	0.44
1:C:417:VAL:HG21	1:G:346:PHE:CG	2.53	0.44
2:D:47:ILE:HG22	2:D:48:SER:N	2.30	0.44
1:G:229:TRP:CH2	1:G:230:MET:CE	3.01	0.44
1:G:379:SER:HB3	1:G:383:TRP:HD1	1.83	0.44
2:H:120:LEU:O	2:H:125:ARG:CZ	2.65	0.44
2:H:162:SER:O	2:H:166:LYS:HG2	2.17	0.44
2:H:319:TYR:O	2:H:321:PRO:HD3	2.18	0.44
1:A:540:LYS:NZ	2:B:261:VAL:HG12	2.31	0.44
2:B:249:LYS:HB2	2:B:252:TRP:CZ2	2.52	0.44
2:B:354:TYR:CE1	2:B:374:LYS:HD3	2.53	0.44
1:C:155:GLY:O	1:C:156:SER:C	2.60	0.44
1:C:194:GLU:C	1:C:196:GLY:N	2.76	0.44
2:D:24:TRP:CZ3	2:D:61:PHE:CB	3.00	0.44
2:D:249:LYS:HB2	2:D:252:TRP:CZ2	2.52	0.44
1:E:540:LYS:HB2	1:E:542:ILE:HG13	2.00	0.44
2:F:24:TRP:CZ3	2:F:61:PHE:CB	3.01	0.44
2:F:365:VAL:HG12	2:F:405:TYR:HE2	1.81	0.44
2:F:376:THR:HG22	2:F:389:PHE:HE1	1.80	0.44
2:F:420:PRO:HB2	2:F:421:PRO:CD	2.42	0.44
1:G:1:PRO:HG2	1:G:1:PRO:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:10:VAL:HG11	1:G:153:TRP:CZ2	2.53	0.44
2:H:108:VAL:HG11	2:H:188:TYR:CE2	2.52	0.44
2:H:255:ASN:HA	2:H:258:GLN:HB2	1.99	0.44
2:H:336:GLN:C	2:H:337:TRP:CD1	2.96	0.44
1:A:441:TYR:O	1:A:548:VAL:HG21	2.18	0.44
2:B:241:VAL:O	2:B:243:PRO:HD3	2.17	0.44
2:B:286:THR:HG22	2:B:286:THR:O	2.18	0.44
2:B:336:GLN:C	2:B:337:TRP:CD1	2.96	0.44
1:C:439:THR:HG22	1:C:441:TYR:HE1	1.82	0.44
2:D:286:THR:HG22	2:D:286:THR:O	2.18	0.44
1:E:88:TRP:CH2	2:F:57:ASN:CB	3.01	0.44
1:E:114:ALA:HB1	1:E:160:PHE:CE1	2.52	0.44
1:E:440:PHE:CE2	1:E:457:TYR:CE2	3.05	0.44
1:E:451:LYS:O	1:E:471:ASN:N	2.51	0.44
2:F:38:CYS:SG	2:F:132:ILE:HD11	2.58	0.44
2:B:376:THR:HG22	2:B:389:PHE:HE1	1.80	0.43
1:C:363:ASN:OD1	1:C:365:VAL:N	2.50	0.43
1:E:412:PRO:HG2	1:E:413:GLU:H	1.83	0.43
1:G:440:PHE:CE2	1:G:457:TYR:CE2	3.05	0.43
1:G:441:TYR:O	1:G:548:VAL:HG21	2.18	0.43
1:C:441:TYR:O	1:C:548:VAL:HG21	2.18	0.43
2:D:336:GLN:C	2:D:337:TRP:CD1	2.96	0.43
1:E:336:GLN:HG2	1:E:355:ALA:CB	2.48	0.43
2:F:286:THR:O	2:F:286:THR:HG22	2.18	0.43
1:G:132:ILE:HD11	1:G:144:TYR:CE2	2.54	0.43
2:H:286:THR:O	2:H:286:THR:HG22	2.18	0.43
1:A:536:VAL:HB	1:A:542:ILE:HD13	2.01	0.43
1:C:167:ILE:O	1:C:208:HIS:CE1	2.66	0.43
2:D:100:LEU:HA	2:D:100:LEU:HD23	1.81	0.43
2:D:319:TYR:O	2:D:321:PRO:HD3	2.18	0.43
1:E:368:LEU:HD11	1:E:391:LEU:HD22	2.00	0.43
1:E:536:VAL:HB	1:E:542:ILE:HD13	2.01	0.43
2:F:122:GLU:C	2:F:124:PHE:H	2.27	0.43
2:F:193:LEU:CD1	2:F:201:LYS:HG3	2.47	0.43
2:F:354:TYR:CE1	2:F:374:LYS:HD3	2.53	0.43
1:G:148:VAL:HG12	1:G:149:LEU:N	2.31	0.43
2:B:324:ASP:O	2:B:343:GLN:HG2	2.19	0.43
2:D:395:LYS:HE2	2:D:399:GLU:OE1	2.18	0.43
1:E:34:LEU:HD21	1:E:62:ALA:HB2	1.99	0.43
1:E:467:VAL:HG12	1:E:468:PRO:O	2.18	0.43
2:F:162:SER:O	2:F:166:LYS:HG2	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:540:LYS:HB2	1:G:542:ILE:HG13	2.00	0.43
2:H:38:CYS:SG	2:H:132:ILE:HD11	2.58	0.43
2:B:319:TYR:O	2:B:321:PRO:HD3	2.18	0.43
1:C:320:ASP:HA	1:C:321:PRO:HD2	1.85	0.43
2:D:241:VAL:O	2:D:243:PRO:HD3	2.17	0.43
2:F:312:GLU:HA	2:F:313:PRO:HD3	1.72	0.43
1:G:88:TRP:CH2	2:H:57:ASN:CB	3.01	0.43
2:H:320:ASP:HA	2:H:321:PRO:HD3	1.84	0.43
2:H:324:ASP:O	2:H:343:GLN:HG2	2.19	0.43
1:A:12:LEU:HD23	1:A:124:PHE:HE2	1.83	0.43
1:A:88:TRP:CH2	2:B:57:ASN:CB	3.01	0.43
1:A:412:PRO:HG2	1:A:413:GLU:H	1.83	0.43
2:B:38:CYS:SG	2:B:132:ILE:HD11	2.58	0.43
1:C:188:TYR:HB2	1:C:229:TRP:CD1	2.54	0.43
2:F:324:ASP:O	2:F:343:GLN:HG2	2.19	0.43
2:F:395:LYS:HE2	2:F:399:GLU:OE1	2.18	0.43
1:G:84:THR:CG2	1:G:154:LYS:HE2	2.49	0.43
1:A:114:ALA:HB1	1:A:160:PHE:CE1	2.52	0.43
1:A:188:TYR:HB2	1:A:229:TRP:CD1	2.54	0.43
1:A:467:VAL:HG12	1:A:468:PRO:O	2.18	0.43
1:A:476:LYS:O	1:A:480:GLN:HG2	2.19	0.43
2:B:395:LYS:HE2	2:B:399:GLU:OE1	2.18	0.43
1:C:114:ALA:HB1	1:C:160:PHE:CE1	2.52	0.43
1:C:412:PRO:HG2	1:C:413:GLU:H	1.83	0.43
1:E:14:PRO:HG2	1:E:14:PRO:O	2.18	0.43
1:E:391:LEU:HA	1:E:392:PRO:HD3	1.72	0.43
1:G:114:ALA:HB1	1:G:160:PHE:CE1	2.52	0.43
1:G:188:TYR:HB2	1:G:229:TRP:CD1	2.54	0.43
1:G:194:GLU:O	1:G:195:ILE:C	2.62	0.43
2:H:54:ASN:C	2:H:54:ASN:ND2	2.76	0.43
2:H:395:LYS:HE2	2:H:399:GLU:OE1	2.18	0.43
2:H:420:PRO:HB2	2:H:421:PRO:CD	2.42	0.43
1:A:14:PRO:O	1:A:14:PRO:HG2	2.18	0.43
1:A:50:ILE:HD13	1:A:145:GLN:HB2	2.01	0.43
1:A:84:THR:CG2	1:A:154:LYS:HE2	2.49	0.43
1:A:356:ARG:HH21	1:A:358:ARG:CZ	2.32	0.43
2:B:24:TRP:CZ3	2:B:61:PHE:CB	3.00	0.43
1:C:12:LEU:HD23	1:C:124:PHE:HE2	1.83	0.43
1:C:132:ILE:HD11	1:C:144:TYR:CE2	2.54	0.43
2:D:108:VAL:CG1	2:D:188:TYR:CE2	3.02	0.43
2:D:324:ASP:O	2:D:343:GLN:HG2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:354:TYR:CE1	2:D:374:LYS:HD3	2.53	0.43
1:E:132:ILE:HD11	1:E:144:TYR:CE2	2.54	0.43
1:E:194:GLU:C	1:E:196:GLY:N	2.76	0.43
2:F:108:VAL:CG1	2:F:188:TYR:CE2	3.02	0.43
2:F:319:TYR:O	2:F:321:PRO:HD3	2.18	0.43
1:G:476:LYS:O	1:G:480:GLN:HG2	2.19	0.43
2:H:108:VAL:CG1	2:H:188:TYR:CE2	3.02	0.43
2:B:61:PHE:CZ	2:B:411:ILE:HD11	2.54	0.43
2:B:160:PHE:O	2:B:160:PHE:CD1	2.72	0.43
1:C:50:ILE:HD13	1:C:145:GLN:HB2	2.01	0.43
1:C:357:MET:SD	1:C:362:THR:OG1	2.71	0.43
1:C:368:LEU:HD11	1:C:391:LEU:HD22	2.00	0.43
1:C:467:VAL:HG12	1:C:468:PRO:O	2.18	0.43
1:C:536:VAL:HB	1:C:542:ILE:HD13	2.01	0.43
1:G:238:LYS:HE3	1:G:315:HIS:CG	2.54	0.43
1:G:536:VAL:HB	1:G:542:ILE:HD13	2.01	0.43
1:A:132:ILE:HD11	1:A:144:TYR:CE2	2.54	0.43
1:C:356:ARG:HH21	1:C:358:ARG:CZ	2.32	0.43
2:D:38:CYS:SG	2:D:132:ILE:HD11	2.58	0.43
2:D:72:ARG:HH12	2:D:409:THR:CG2	2.29	0.43
1:E:1:PRO:HG2	1:E:1:PRO:O	2.18	0.43
1:E:188:TYR:HB2	1:E:229:TRP:CD1	2.54	0.43
2:F:336:GLN:C	2:F:337:TRP:CD1	2.96	0.43
1:G:194:GLU:C	1:G:196:GLY:N	2.76	0.43
1:G:336:GLN:HG2	1:G:355:ALA:CB	2.48	0.43
2:H:120:LEU:HB3	2:H:125:ARG:NH1	2.34	0.43
2:H:376:THR:HG22	2:H:389:PHE:HE1	1.80	0.43
1:A:175:ASN:HB3	1:A:178:ILE:HD12	2.00	0.42
1:A:336:GLN:HG2	1:A:355:ALA:CB	2.48	0.42
1:A:540:LYS:HB2	1:A:542:ILE:HG13	2.00	0.42
2:B:38:CYS:HA	2:B:41:MET:HE3	2.01	0.42
1:C:84:THR:CG2	1:C:154:LYS:HE2	2.49	0.42
1:C:476:LYS:O	1:C:480:GLN:HG2	2.19	0.42
2:D:61:PHE:CZ	2:D:411:ILE:HD11	2.54	0.42
2:D:160:PHE:CD1	2:D:160:PHE:O	2.72	0.42
1:E:238:LYS:HE3	1:E:315:HIS:CG	2.54	0.42
2:F:38:CYS:HA	2:F:41:MET:HE3	2.01	0.42
1:G:356:ARG:HH21	1:G:358:ARG:CZ	2.32	0.42
1:A:90:VAL:CG1	2:B:141:GLY:H	2.29	0.42
2:B:78:ARG:HD3	2:B:411:ILE:O	2.20	0.42
2:D:78:ARG:HD3	2:D:411:ILE:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:175:ASN:CB	1:E:178:ILE:HD12	2.49	0.42
1:E:363:ASN:OD1	1:E:365:VAL:N	2.50	0.42
2:F:61:PHE:CZ	2:F:411:ILE:HD11	2.54	0.42
2:F:363:ASN:O	2:F:364:ASP:C	2.62	0.42
1:G:12:LEU:HD23	1:G:124:PHE:HE2	1.83	0.42
1:G:104:LYS:N	1:G:192:ASP:OD1	2.52	0.42
1:G:175:ASN:HB3	1:G:178:ILE:HD12	2.00	0.42
1:A:325:LEU:C	1:A:326:ILE:HG13	2.44	0.42
1:A:368:LEU:HD11	1:A:391:LEU:HD22	2.00	0.42
1:A:408:ALA:HB2	2:B:337:TRP:HH2	1.85	0.42
2:B:47:ILE:HG22	2:B:48:SER:N	2.30	0.42
1:C:90:VAL:CG1	2:D:141:GLY:H	2.29	0.42
1:C:540:LYS:HB2	1:C:542:ILE:HG13	2.00	0.42
2:D:38:CYS:HA	2:D:41:MET:HE3	2.01	0.42
2:D:97:PRO:C	2:D:99:GLY:N	2.77	0.42
2:F:204:GLU:O	2:F:208:HIS:CD2	2.72	0.42
2:F:316:GLY:O	2:F:318:TYR:CD1	2.66	0.42
1:G:287:LYS:O	1:G:288:ALA:C	2.62	0.42
1:G:467:VAL:HG12	1:G:468:PRO:O	2.18	0.42
2:B:262:GLY:O	2:B:265:ASN:HB3	2.20	0.42
1:C:325:LEU:C	1:C:326:ILE:HG13	2.44	0.42
1:C:345:PRO:HB3	1:G:342:TYR:CE1	2.54	0.42
1:C:408:ALA:HB2	2:D:337:TRP:HH2	1.85	0.42
1:E:84:THR:CG2	1:E:154:LYS:HE2	2.49	0.42
1:E:325:LEU:C	1:E:326:ILE:HG13	2.44	0.42
1:E:357:MET:SD	1:E:362:THR:OG1	2.71	0.42
1:G:14:PRO:O	1:G:14:PRO:HG2	2.18	0.42
1:G:363:ASN:OD1	1:G:365:VAL:N	2.50	0.42
2:H:249:LYS:HB2	2:H:252:TRP:CZ2	2.52	0.42
1:A:23:GLN:NE2	1:A:131:THR:H	2.18	0.42
1:A:175:ASN:CB	1:A:178:ILE:HD12	2.49	0.42
1:A:346:PHE:HE1	1:E:342:TYR:OH	2.02	0.42
2:B:108:VAL:CG1	2:B:188:TYR:CE2	3.02	0.42
2:B:204:GLU:O	2:B:208:HIS:CD2	2.72	0.42
1:C:14:PRO:HG2	1:C:14:PRO:O	2.18	0.42
1:C:44:GLU:HB2	1:C:46:LYS:HG2	2.02	0.42
1:C:336:GLN:HG2	1:C:355:ALA:CB	2.48	0.42
1:E:483:TYR:O	1:E:486:LEU:HB2	2.20	0.42
2:F:47:ILE:HG21	2:F:47:ILE:HD13	1.82	0.42
1:G:50:ILE:HD13	1:G:145:GLN:HB2	2.01	0.42
1:G:368:LEU:HD11	1:G:391:LEU:HD22	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:432:GLU:HB3	1:G:433:PRO:HD2	2.01	0.42
2:H:38:CYS:HA	2:H:41:MET:HE3	2.01	0.42
2:H:204:GLU:O	2:H:208:HIS:CD2	2.72	0.42
2:H:246:LEU:HD13	2:H:260:LEU:HD11	2.02	0.42
1:C:1:PRO:O	1:C:1:PRO:HG2	2.18	0.42
1:C:23:GLN:NE2	1:C:131:THR:H	2.18	0.42
1:C:175:ASN:HB3	1:C:178:ILE:HD12	2.00	0.42
2:D:122:GLU:C	2:D:124:PHE:H	2.27	0.42
2:D:204:GLU:O	2:D:208:HIS:CD2	2.72	0.42
2:D:262:GLY:O	2:D:265:ASN:HB3	2.20	0.42
1:E:175:ASN:HB3	1:E:178:ILE:HD12	2.00	0.42
2:F:160:PHE:CD1	2:F:160:PHE:O	2.72	0.42
2:F:278:GLN:OE1	2:F:278:GLN:HA	2.20	0.42
1:G:23:GLN:NE2	1:G:131:THR:H	2.18	0.42
1:G:325:LEU:C	1:G:326:ILE:HG13	2.44	0.42
1:G:363:ASN:HB3	1:G:366:LYS:HB2	2.02	0.42
2:H:122:GLU:C	2:H:124:PHE:H	2.27	0.42
2:B:97:PRO:C	2:B:99:GLY:N	2.77	0.42
1:C:96:HIS:ND1	1:C:98:ALA:HB3	2.35	0.42
1:C:175:ASN:CB	1:C:178:ILE:HD12	2.49	0.42
1:C:238:LYS:HE3	1:C:315:HIS:CG	2.54	0.42
1:E:23:GLN:NE2	1:E:131:THR:H	2.18	0.42
1:E:432:GLU:HB3	1:E:433:PRO:HD2	2.01	0.42
1:E:476:LYS:O	1:E:480:GLN:HG2	2.19	0.42
2:F:5:ILE:HG22	2:F:6:GLU:H	1.85	0.42
2:F:249:LYS:HB2	2:F:252:TRP:CZ2	2.52	0.42
2:F:262:GLY:O	2:F:265:ASN:HB3	2.20	0.42
2:F:380:ILE:O	2:F:384:GLY:HA2	2.20	0.42
1:G:175:ASN:CB	1:G:178:ILE:HD12	2.50	0.42
1:G:232:TYR:CD1	1:G:241:VAL:HG22	2.53	0.42
2:H:61:PHE:CZ	2:H:411:ILE:HD11	2.54	0.42
2:H:72:ARG:HH12	2:H:409:THR:CG2	2.29	0.42
2:H:380:ILE:O	2:H:384:GLY:HA2	2.20	0.42
1:A:104:LYS:N	1:A:192:ASP:OD1	2.52	0.42
1:A:483:TYR:O	1:A:486:LEU:HB2	2.20	0.42
2:B:122:GLU:C	2:B:124:PHE:H	2.27	0.42
1:C:54:ASN:HA	1:C:55:PRO:HD3	1.77	0.42
1:C:104:LYS:N	1:C:192:ASP:OD1	2.52	0.42
1:C:194:GLU:O	1:C:195:ILE:C	2.62	0.42
1:C:483:TYR:O	1:C:486:LEU:HB2	2.20	0.42
2:D:363:ASN:O	2:D:364:ASP:C	2.62	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:194:GLU:O	1:E:195:ILE:C	2.62	0.42
1:E:275:LYS:C	1:E:277:ARG:H	2.28	0.42
2:F:120:LEU:HB3	2:F:125:ARG:NH1	2.34	0.42
2:F:271:TYR:CD1	2:F:271:TYR:N	2.88	0.42
1:G:275:LYS:C	1:G:277:ARG:H	2.28	0.42
2:H:47:ILE:HG22	2:H:48:SER:N	2.30	0.42
1:A:1:PRO:O	1:A:1:PRO:HG2	2.18	0.42
1:A:96:HIS:ND1	1:A:98:ALA:HB3	2.35	0.42
1:A:194:GLU:O	1:A:195:ILE:C	2.62	0.42
1:A:194:GLU:C	1:A:196:GLY:N	2.76	0.42
1:A:432:GLU:HB3	1:A:433:PRO:HD2	2.01	0.42
2:B:278:GLN:HA	2:B:278:GLN:OE1	2.20	0.42
2:B:420:PRO:HB2	2:B:421:PRO:CD	2.43	0.42
1:C:88:TRP:CH2	2:D:57:ASN:CB	3.01	0.42
1:C:225:PRO:N	1:C:226:PRO:HD2	2.35	0.42
1:C:363:ASN:HB3	1:C:366:LYS:HB2	2.02	0.42
1:C:421:PRO:HG2	1:C:421:PRO:O	2.20	0.42
2:D:393:ILE:HG12	2:D:394:GLN:N	2.35	0.42
1:E:132:ILE:N	1:E:142:ILE:O	2.52	0.42
1:E:356:ARG:HH21	1:E:358:ARG:CZ	2.32	0.42
1:E:439:THR:HG22	1:E:441:TYR:HE1	1.82	0.42
2:F:28:GLU:O	2:F:32:LYS:HG3	2.20	0.42
1:G:331:LYS:O	1:G:331:LYS:HG2	2.20	0.42
2:H:262:GLY:O	2:H:265:ASN:HB3	2.20	0.42
1:A:44:GLU:HB2	1:A:46:LYS:HG2	2.02	0.42
1:A:175:ASN:ND2	1:A:201:LYS:HZ1	2.18	0.42
1:A:312:GLU:HA	1:A:313:PRO:HD2	1.89	0.42
1:C:96:HIS:CD2	1:C:97:PRO:HD2	2.55	0.42
1:C:287:LYS:O	1:C:288:ALA:C	2.62	0.42
1:C:342:TYR:CZ	1:G:345:PRO:HB3	2.54	0.42
1:E:18:GLY:HA3	1:E:127:TYR:HD1	1.85	0.42
1:E:50:ILE:HD13	1:E:145:GLN:HB2	2.01	0.42
1:G:96:HIS:ND1	1:G:98:ALA:HB3	2.35	0.42
1:G:116:PHE:N	1:G:116:PHE:CD1	2.88	0.42
1:G:483:TYR:O	1:G:486:LEU:HB2	2.20	0.42
2:H:109:LEU:O	2:H:186:ASP:HA	2.20	0.42
2:H:160:PHE:O	2:H:160:PHE:CD1	2.72	0.42
2:H:271:TYR:CD1	2:H:271:TYR:N	2.88	0.42
2:H:278:GLN:OE1	2:H:278:GLN:HA	2.20	0.42
1:A:427:TYR:CD1	1:A:427:TYR:N	2.88	0.41
2:B:24:TRP:HZ3	2:B:61:PHE:CG	2.38	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:363:ASN:O	2:B:364:ASP:C	2.62	0.41
2:B:395:LYS:O	2:B:399:GLU:N	2.48	0.41
1:C:232:TYR:CD1	1:C:241:VAL:HG22	2.53	0.41
2:D:28:GLU:O	2:D:32:LYS:HG3	2.20	0.41
2:D:120:LEU:HB3	2:D:125:ARG:NH1	2.34	0.41
1:G:8:VAL:HA	1:G:9:PRO:HD2	1.78	0.41
1:G:38:CYS:HB3	1:G:144:TYR:CE2	2.55	0.41
1:G:96:HIS:CD2	1:G:97:PRO:HD2	2.55	0.41
1:G:201:LYS:HD3	1:G:201:LYS:HA	1.85	0.41
1:G:439:THR:CG2	1:G:441:TYR:HE1	2.33	0.41
2:H:78:ARG:HD3	2:H:411:ILE:O	2.20	0.41
2:H:365:VAL:HG12	2:H:405:TYR:HE2	1.81	0.41
2:H:393:ILE:HG12	2:H:394:GLN:N	2.35	0.41
1:A:249:LYS:CG	1:A:250:ASP:N	2.83	0.41
1:A:275:LYS:C	1:A:277:ARG:H	2.28	0.41
2:B:28:GLU:O	2:B:32:LYS:HG3	2.20	0.41
2:B:120:LEU:HB3	2:B:125:ARG:NH1	2.34	0.41
2:B:380:ILE:O	2:B:384:GLY:HA2	2.20	0.41
1:C:38:CYS:HB3	1:C:144:TYR:CE2	2.55	0.41
1:C:275:LYS:C	1:C:277:ARG:H	2.28	0.41
1:C:427:TYR:N	1:C:427:TYR:CD1	2.88	0.41
1:E:77:PHE:CE2	1:E:150:PRO:HB3	2.55	0.41
1:E:96:HIS:ND1	1:E:98:ALA:HB3	2.35	0.41
1:E:427:TYR:N	1:E:427:TYR:CD1	2.88	0.41
1:E:439:THR:CG2	1:E:441:TYR:HE1	2.33	0.41
2:F:18:GLY:HA3	2:F:127:TYR:CD1	2.56	0.41
2:F:78:ARG:HD3	2:F:411:ILE:O	2.19	0.41
2:F:246:LEU:HD13	2:F:260:LEU:HD11	2.02	0.41
1:G:18:GLY:HA3	1:G:127:TYR:HD1	1.85	0.41
1:G:77:PHE:CE2	1:G:150:PRO:HB3	2.55	0.41
1:G:116:PHE:N	1:G:116:PHE:HD1	2.18	0.41
1:G:320:ASP:HA	1:G:321:PRO:HD2	1.85	0.41
1:G:439:THR:HG22	1:G:441:TYR:HE1	1.82	0.41
2:H:336:GLN:HG2	2:H:355:ALA:HB1	2.02	0.41
2:B:72:ARG:HH12	2:B:409:THR:CG2	2.29	0.41
1:E:408:ALA:HB2	2:F:337:TRP:HH2	1.85	0.41
1:A:38:CYS:HB3	1:A:144:TYR:CE2	2.55	0.41
1:A:363:ASN:HB3	1:A:366:LYS:HB2	2.02	0.41
2:B:99:GLY:O	2:B:100:LEU:C	2.64	0.41
2:B:100:LEU:HD23	2:B:100:LEU:HA	1.81	0.41
1:C:77:PHE:CE2	1:C:150:PRO:HB3	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:116:PHE:HD1	1:C:116:PHE:N	2.18	0.41
1:C:432:GLU:HB3	1:C:433:PRO:HD2	2.01	0.41
2:D:24:TRP:HZ3	2:D:61:PHE:CG	2.38	0.41
2:D:246:LEU:HD13	2:D:260:LEU:HD11	2.02	0.41
1:E:116:PHE:N	1:E:116:PHE:HD1	2.18	0.41
1:E:456:GLY:HA3	1:E:466:VAL:HA	2.02	0.41
1:G:409:THR:O	1:G:410:TRP:HB2	2.21	0.41
1:G:427:TYR:N	1:G:427:TYR:CD1	2.88	0.41
2:H:10:VAL:HA	2:H:85:GLN:OE1	2.20	0.41
1:A:238:LYS:HE3	1:A:315:HIS:CG	2.54	0.41
2:B:109:LEU:O	2:B:186:ASP:HA	2.20	0.41
2:B:136:ASN:O	2:B:137:ASN:HB2	2.21	0.41
1:C:10:VAL:HG11	1:C:153:TRP:HZ2	1.86	0.41
1:C:331:LYS:O	1:C:331:LYS:HG2	2.20	0.41
2:D:278:GLN:OE1	2:D:278:GLN:HA	2.20	0.41
1:E:12:LEU:HD23	1:E:124:PHE:HE2	1.83	0.41
1:E:78:ARG:NH1	1:E:287:LYS:O	2.39	0.41
1:E:116:PHE:N	1:E:116:PHE:CD1	2.88	0.41
1:E:153:TRP:CD1	1:E:154:LYS:H	2.39	0.41
1:E:249:LYS:CG	1:E:250:ASP:N	2.83	0.41
2:F:136:ASN:O	2:F:137:ASN:HB2	2.21	0.41
1:G:53:GLU:N	1:G:53:GLU:OE2	2.54	0.41
1:G:344:GLU:HA	1:G:345:PRO:HD2	1.81	0.41
1:G:421:PRO:O	1:G:421:PRO:HG2	2.20	0.41
2:B:391:LEU:HD12	2:B:416:PHE:HE1	1.86	0.41
1:C:53:GLU:N	1:C:53:GLU:OE2	2.54	0.41
1:C:349:LEU:HA	1:C:349:LEU:HD23	1.84	0.41
2:D:136:ASN:O	2:D:137:ASN:HB2	2.21	0.41
2:D:395:LYS:O	2:D:399:GLU:N	2.48	0.41
1:E:225:PRO:N	1:E:226:PRO:HD2	2.35	0.41
2:F:10:VAL:HA	2:F:85:GLN:OE1	2.20	0.41
2:F:109:LEU:O	2:F:186:ASP:HA	2.20	0.41
2:F:153:TRP:CE3	2:F:155:GLY:CA	3.03	0.41
2:F:193:LEU:HD12	2:F:201:LYS:HG3	2.03	0.41
2:F:393:ILE:HG12	2:F:394:GLN:N	2.35	0.41
1:G:44:GLU:HB2	1:G:46:LYS:HG2	2.02	0.41
1:G:225:PRO:N	1:G:226:PRO:HD2	2.35	0.41
1:G:408:ALA:HB2	2:H:337:TRP:HH2	1.85	0.41
2:H:363:ASN:O	2:H:364:ASP:C	2.62	0.41
1:A:18:GLY:HA3	1:A:127:TYR:HD1	1.85	0.41
1:A:88:TRP:CZ2	2:B:57:ASN:CG	2.99	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:456:GLY:HA3	1:A:466:VAL:HA	2.02	0.41
2:B:61:PHE:CD2	2:B:403:THR:HG22	2.56	0.41
2:B:108:VAL:CG1	2:B:188:TYR:CD2	3.04	0.41
2:B:246:LEU:HD13	2:B:260:LEU:HD11	2.02	0.41
2:B:393:ILE:HG12	2:B:394:GLN:N	2.35	0.41
1:C:88:TRP:CZ2	2:D:57:ASN:CG	2.99	0.41
1:C:409:THR:O	1:C:410:TRP:HB2	2.21	0.41
2:D:61:PHE:CD2	2:D:403:THR:HG22	2.56	0.41
2:D:103:LYS:HB3	2:D:191:SER:O	2.21	0.41
2:D:156:SER:HB2	2:D:157:PRO:CD	2.51	0.41
2:D:336:GLN:HG2	2:D:355:ALA:HB1	2.02	0.41
2:D:380:ILE:O	2:D:384:GLY:HA2	2.20	0.41
1:E:10:VAL:HG11	1:E:153:TRP:HZ2	1.86	0.41
1:E:38:CYS:HB3	1:E:144:TYR:CE2	2.55	0.41
1:E:472:THR:HB	1:E:476:LYS:HB2	2.03	0.41
2:F:24:TRP:HZ3	2:F:61:PHE:CG	2.38	0.41
2:F:104:LYS:O	2:F:235:HIS:CD2	2.74	0.41
1:A:96:HIS:CD2	1:A:97:PRO:HD2	2.55	0.41
1:A:116:PHE:HD1	1:A:116:PHE:N	2.18	0.41
1:A:225:PRO:N	1:A:226:PRO:HD2	2.35	0.41
1:A:439:THR:CG2	1:A:441:TYR:HE1	2.33	0.41
2:B:58:THR:HG21	2:B:77:PHE:CD1	2.56	0.41
2:B:94:ILE:H	2:B:94:ILE:HG13	1.54	0.41
2:B:156:SER:HB2	2:B:157:PRO:CD	2.51	0.41
1:C:57:ASN:HB2	1:C:143:ARG:HH21	1.86	0.41
1:C:116:PHE:N	1:C:116:PHE:CD1	2.88	0.41
1:C:118:VAL:HA	1:C:119:PRO:HD2	1.71	0.41
1:C:249:LYS:CG	1:C:250:ASP:N	2.83	0.41
1:C:442:VAL:CG1	1:C:481:ALA:CB	2.96	0.41
2:D:18:GLY:HA3	2:D:127:TYR:CD1	2.56	0.41
2:D:99:GLY:O	2:D:100:LEU:C	2.64	0.41
1:E:44:GLU:HB2	1:E:46:LYS:HG2	2.02	0.41
1:E:53:GLU:N	1:E:53:GLU:OE2	2.54	0.41
1:E:440:PHE:HD2	1:E:457:TYR:CD2	2.39	0.41
2:F:202:ILE:O	2:F:206:ARG:N	2.54	0.41
1:G:88:TRP:CZ2	2:H:57:ASN:CG	2.99	0.41
1:G:90:VAL:CG1	2:H:141:GLY:H	2.29	0.41
1:G:391:LEU:HA	1:G:392:PRO:HD3	1.73	0.41
1:G:440:PHE:HD2	1:G:457:TYR:CD2	2.39	0.41
2:H:61:PHE:CD2	2:H:403:THR:HG22	2.56	0.41
2:H:108:VAL:CG1	2:H:188:TYR:CD2	3.04	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:175:ASN:O	2:H:177:ASP:N	2.54	0.41
1:A:10:VAL:HG11	1:A:153:TRP:HZ2	1.86	0.41
1:A:53:GLU:N	1:A:53:GLU:OE2	2.54	0.41
1:A:54:ASN:O	1:A:143:ARG:NH1	2.54	0.41
1:A:57:ASN:HB2	1:A:143:ARG:HH21	1.86	0.41
1:A:77:PHE:CE2	1:A:150:PRO:HB3	2.55	0.41
1:A:116:PHE:N	1:A:116:PHE:CD1	2.88	0.41
1:A:132:ILE:CD1	1:A:144:TYR:HE2	2.34	0.41
1:A:287:LYS:O	1:A:288:ALA:C	2.62	0.41
1:A:320:ASP:HA	1:A:321:PRO:HD2	1.85	0.41
1:A:320:ASP:C	1:A:322:SER:H	2.29	0.41
1:A:331:LYS:O	1:A:331:LYS:HG2	2.20	0.41
1:A:388:LYS:HA	1:A:413:GLU:HB2	2.03	0.41
1:A:416:PHE:CD1	1:A:416:PHE:C	2.98	0.41
1:A:463:ARG:HG3	1:A:463:ARG:NH1	2.35	0.41
1:A:484:LEU:O	1:A:487:GLN:N	2.54	0.41
2:B:11:LYS:N	2:B:85:GLN:OE1	2.49	0.41
2:B:103:LYS:HB3	2:B:191:SER:O	2.21	0.41
2:B:153:TRP:CE3	2:B:155:GLY:CA	3.03	0.41
2:B:175:ASN:O	2:B:177:ASP:N	2.54	0.41
2:B:193:LEU:HD12	2:B:201:LYS:HG3	2.03	0.41
1:C:116:PHE:HA	1:C:148:VAL:HG11	2.03	0.41
1:C:320:ASP:C	1:C:322:SER:H	2.29	0.41
1:C:417:VAL:HG21	1:G:346:PHE:CD1	2.56	0.41
1:C:420:PRO:CG	1:C:421:PRO:HD2	2.35	0.41
1:C:463:ARG:HG3	1:C:463:ARG:NH1	2.35	0.41
1:C:484:LEU:O	1:C:487:GLN:N	2.54	0.41
2:D:58:THR:HG21	2:D:77:PHE:CD1	2.56	0.41
2:D:63:ILE:HG12	2:D:64:LYS:H	1.86	0.41
2:D:271:TYR:CD1	2:D:271:TYR:N	2.88	0.41
2:D:391:LEU:HD12	2:D:416:PHE:HE1	1.86	0.41
1:E:96:HIS:CD2	1:E:97:PRO:HD2	2.55	0.41
1:E:287:LYS:O	1:E:288:ALA:C	2.62	0.41
1:E:320:ASP:C	1:E:322:SER:H	2.29	0.41
1:E:323:LYS:O	1:E:343:GLN:NE2	2.52	0.41
1:E:388:LYS:HA	1:E:413:GLU:HB2	2.03	0.41
1:E:418:ASN:C	1:E:418:ASN:ND2	2.74	0.41
1:E:421:PRO:O	1:E:421:PRO:HG2	2.20	0.41
1:E:484:LEU:O	1:E:487:GLN:N	2.54	0.41
2:F:99:GLY:O	2:F:100:LEU:C	2.64	0.41
2:F:252:TRP:CH2	2:F:260:LEU:HD22	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:336:GLN:HG2	2:F:355:ALA:HB1	2.02	0.41
1:G:132:ILE:CD1	1:G:144:TYR:HE2	2.33	0.41
1:G:317:VAL:CG2	1:G:347:LYS:HB3	2.41	0.41
1:G:472:THR:HB	1:G:476:LYS:HB2	2.03	0.41
2:H:18:GLY:HA3	2:H:127:TYR:CD1	2.56	0.41
2:H:24:TRP:HZ3	2:H:61:PHE:CG	2.38	0.41
2:H:74:LEU:HD12	2:H:74:LEU:HA	1.83	0.41
2:H:100:LEU:HA	2:H:100:LEU:HD23	1.81	0.41
2:H:104:LYS:O	2:H:235:HIS:CD2	2.74	0.41
2:H:136:ASN:O	2:H:137:ASN:HB2	2.21	0.41
2:H:153:TRP:CE3	2:H:155:GLY:CA	3.04	0.41
2:H:156:SER:HB2	2:H:157:PRO:CD	2.51	0.41
2:H:193:LEU:HD12	2:H:201:LYS:HG3	2.03	0.41
2:H:252:TRP:CH2	2:H:260:LEU:HD22	2.56	0.41
2:H:391:LEU:HD12	2:H:416:PHE:HE1	1.86	0.41
1:A:409:THR:O	1:A:410:TRP:HB2	2.21	0.41
2:B:10:VAL:HA	2:B:85:GLN:OE1	2.20	0.41
2:B:37:ILE:HG13	2:B:37:ILE:H	1.69	0.41
2:B:271:TYR:CD1	2:B:271:TYR:N	2.88	0.41
2:B:336:GLN:HG2	2:B:355:ALA:HB1	2.02	0.41
1:C:8:VAL:HA	1:C:9:PRO:HD2	1.78	0.41
1:C:54:ASN:O	1:C:143:ARG:NH1	2.54	0.41
1:C:439:THR:CG2	1:C:441:TYR:HE1	2.33	0.41
1:C:540:LYS:O	1:C:542:ILE:N	2.53	0.41
2:D:175:ASN:O	2:D:177:ASP:N	2.54	0.41
2:D:420:PRO:HB2	2:D:421:PRO:CD	2.43	0.41
1:E:116:PHE:HA	1:E:148:VAL:HG11	2.03	0.41
1:E:331:LYS:O	1:E:331:LYS:HG2	2.20	0.41
1:E:363:ASN:HB3	1:E:366:LYS:HB2	2.02	0.41
2:F:156:SER:HB2	2:F:157:PRO:CD	2.51	0.41
2:F:175:ASN:O	2:F:177:ASP:N	2.54	0.41
1:G:116:PHE:HA	1:G:148:VAL:HG11	2.03	0.41
1:G:320:ASP:C	1:G:322:SER:H	2.29	0.41
2:H:34:LEU:HD23	2:H:34:LEU:HA	1.92	0.41
2:H:52:PRO:HG2	2:H:53:GLU:N	2.36	0.41
2:H:274:ILE:HG13	2:H:306:ASN:OD1	2.21	0.41
1:A:116:PHE:HA	1:A:148:VAL:HG11	2.03	0.40
2:B:104:LYS:O	2:B:235:HIS:CD2	2.74	0.40
1:C:18:GLY:HA3	1:C:127:TYR:HD1	1.85	0.40
1:C:456:GLY:HA3	1:C:466:VAL:HA	2.02	0.40
2:D:108:VAL:CG1	2:D:188:TYR:CD2	3.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:153:TRP:CE3	2:D:155:GLY:CA	3.03	0.40
2:D:274:ILE:HG13	2:D:306:ASN:OD1	2.21	0.40
2:F:61:PHE:CD2	2:F:403:THR:HG22	2.56	0.40
2:F:259:LYS:HE3	2:F:263:LYS:HZ1	1.85	0.40
1:G:153:TRP:CD1	1:G:154:LYS:H	2.39	0.40
1:G:312:GLU:HA	1:G:313:PRO:HD2	1.89	0.40
1:G:377:THR:O	1:G:380:ILE:N	2.54	0.40
1:G:536:VAL:HA	1:G:537:PRO:HD3	1.77	0.40
1:A:132:ILE:N	1:A:142:ILE:O	2.52	0.40
1:C:153:TRP:CD1	1:C:154:LYS:H	2.39	0.40
1:C:252:TRP:HA	1:C:252:TRP:CE3	2.56	0.40
1:C:331:LYS:O	1:C:333:GLY:N	2.54	0.40
1:C:402:TRP:CE3	1:C:402:TRP:O	2.74	0.40
2:D:419:THR:HA	2:D:420:PRO:HD2	1.96	0.40
1:E:88:TRP:CZ2	2:F:57:ASN:CG	2.99	0.40
1:E:232:TYR:CD1	1:E:241:VAL:HG22	2.53	0.40
2:F:63:ILE:HG12	2:F:64:LYS:H	1.86	0.40
1:G:349:LEU:HA	1:G:349:LEU:HD23	1.84	0.40
2:H:28:GLU:O	2:H:32:LYS:HG3	2.20	0.40
2:H:47:ILE:HG21	2:H:47:ILE:HD13	1.82	0.40
1:A:153:TRP:CD1	1:A:154:LYS:H	2.39	0.40
1:A:232:TYR:CD1	1:A:241:VAL:HG22	2.53	0.40
1:A:246:LEU:O	1:A:307:ARG:NH1	2.54	0.40
1:A:252:TRP:HA	1:A:252:TRP:CE3	2.56	0.40
1:A:402:TRP:CE3	1:A:402:TRP:O	2.74	0.40
1:A:440:PHE:HD2	1:A:457:TYR:CD2	2.39	0.40
2:D:104:LYS:O	2:D:235:HIS:CD2	2.74	0.40
2:D:109:LEU:O	2:D:186:ASP:HA	2.20	0.40
1:E:252:TRP:HA	1:E:252:TRP:CE3	2.56	0.40
1:E:326:ILE:CG2	1:E:342:TYR:HE1	2.35	0.40
1:E:344:GLU:HA	1:E:345:PRO:HD2	1.82	0.40
1:E:377:THR:O	1:E:380:ILE:N	2.55	0.40
2:F:72:ARG:HH12	2:F:409:THR:CA	2.35	0.40
2:F:274:ILE:HG13	2:F:306:ASN:OD1	2.21	0.40
1:G:452:LEU:HD22	1:G:470:THR:HA	2.04	0.40
1:G:456:GLY:HA3	1:G:466:VAL:HA	2.02	0.40
1:A:472:THR:HB	1:A:476:LYS:HB2	2.03	0.40
2:B:7:THR:HG22	2:B:119:PRO:HG2	2.04	0.40
2:B:18:GLY:HA3	2:B:127:TYR:CD1	2.56	0.40
1:C:30:LYS:HB3	1:C:62:ALA:HB3	2.04	0.40
1:C:132:ILE:CD1	1:C:144:TYR:HE2	2.33	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:239:TRP:N	1:C:318:TYR:HE1	2.20	0.40
1:C:246:LEU:O	1:C:307:ARG:NH1	2.54	0.40
1:C:388:LYS:HA	1:C:413:GLU:HB2	2.03	0.40
1:C:472:THR:HB	1:C:476:LYS:HB2	2.03	0.40
2:D:7:THR:HG22	2:D:119:PRO:HG2	2.04	0.40
2:D:10:VAL:HA	2:D:85:GLN:OE1	2.20	0.40
2:D:193:LEU:HD12	2:D:201:LYS:HG3	2.03	0.40
2:D:252:TRP:CH2	2:D:260:LEU:HD22	2.56	0.40
1:E:132:ILE:CD1	1:E:144:TYR:HE2	2.34	0.40
1:E:228:LEU:CD2	1:E:233:GLU:HG2	2.51	0.40
1:E:243:PRO:HD3	1:E:313:PRO:HB3	2.04	0.40
1:E:246:LEU:O	1:E:307:ARG:NH1	2.54	0.40
1:E:312:GLU:HA	1:E:313:PRO:HD2	1.90	0.40
1:E:452:LEU:HD22	1:E:470:THR:HA	2.04	0.40
2:F:28:GLU:HG3	2:F:135:ILE:HD13	2.02	0.40
2:F:52:PRO:HG2	2:F:53:GLU:N	2.36	0.40
2:F:58:THR:HG21	2:F:77:PHE:CD1	2.56	0.40
2:F:97:PRO:C	2:F:99:GLY:N	2.77	0.40
2:F:103:LYS:HB3	2:F:191:SER:O	2.21	0.40
2:F:108:VAL:CG1	2:F:188:TYR:CD2	3.04	0.40
2:F:391:LEU:HD12	2:F:416:PHE:HE1	1.86	0.40
1:G:10:VAL:HG11	1:G:153:TRP:HZ2	1.86	0.40
1:G:239:TRP:N	1:G:318:TYR:HE1	2.20	0.40
1:G:244:ILE:HD12	1:G:267:ALA:CB	2.40	0.40
2:H:7:THR:HG22	2:H:119:PRO:HG2	2.03	0.40
1:A:27:THR:O	1:A:28:GLU:C	2.65	0.40
2:B:252:TRP:CH2	2:B:260:LEU:HD22	2.56	0.40
2:B:316:GLY:O	2:B:318:TYR:CD1	2.65	0.40
1:C:201:LYS:HD3	1:C:201:LYS:HA	1.85	0.40
1:C:442:VAL:HG12	1:C:481:ALA:CB	2.46	0.40
1:E:104:LYS:N	1:E:192:ASP:OD1	2.52	0.40
2:F:135:ILE:C	2:F:137:ASN:N	2.80	0.40
2:F:330:GLN:HB2	2:F:338:THR:OG1	2.22	0.40
1:G:377:THR:OG1	1:G:378:GLU:N	2.55	0.40
1:G:484:LEU:O	1:G:487:GLN:N	2.54	0.40
2:H:103:LYS:HB3	2:H:191:SER:O	2.21	0.40
2:H:395:LYS:HG2	2:H:399:GLU:OE1	2.21	0.40

All (34) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:54:ASN:CA	2:H:88:TRP:CZ2[3_445]	0.68	1.52
1:C:53:GLU:O	2:H:88:TRP:NE1[3_445]	0.72	1.48
2:D:88:TRP:NE1	1:G:54:ASN:N[3_445]	0.91	1.29
1:C:53:GLU:O	2:H:88:TRP:CD1[3_445]	1.03	1.17
1:C:53:GLU:C	2:H:88:TRP:NE1[3_445]	1.08	1.12
2:B:200:THR:CG2	1:C:211:ARG:NH2[2_657]	1.33	0.87
1:C:54:ASN:N	2:H:88:TRP:CE2[3_445]	1.35	0.85
1:C:464:GLN:NE2	1:G:464:GLN:NE2[2_657]	1.36	0.84
1:C:54:ASN:CA	2:H:88:TRP:CE2[3_445]	1.39	0.81
2:B:200:THR:CG2	1:C:211:ARG:CZ[2_657]	1.45	0.75
2:D:88:TRP:NE1	1:G:54:ASN:CA[3_445]	1.49	0.71
2:B:200:THR:CG2	1:C:211:ARG:NE[2_657]	1.54	0.66
1:C:54:ASN:CB	2:H:88:TRP:CZ2[3_445]	1.55	0.65
1:C:54:ASN:N	2:H:88:TRP:CZ2[3_445]	1.58	0.62
2:D:88:TRP:CD1	1:G:53:GLU:C[3_445]	1.69	0.51
1:C:54:ASN:N	2:H:88:TRP:NE1[3_445]	1.72	0.48
1:C:464:GLN:O	1:G:464:GLN:O[2_657]	1.73	0.47
1:C:53:GLU:C	2:H:88:TRP:CE2[3_445]	1.74	0.46
2:D:88:TRP:CD1	1:G:54:ASN:N[3_445]	1.77	0.43
1:C:53:GLU:C	2:H:88:TRP:CD1[3_445]	1.80	0.40
1:A:212:TRP:CZ2	2:H:211:ARG:NE[4_647]	1.90	0.30
2:D:88:TRP:NE1	1:G:53:GLU:C[3_445]	1.91	0.29
1:C:54:ASN:CA	2:H:88:TRP:CH2[3_445]	2.03	0.17
1:C:53:GLU:O	2:H:88:TRP:CE2[3_445]	2.04	0.16
2:D:208:HIS:O	1:E:211:ARG:NE[2_657]	2.04	0.16
2:B:200:THR:CB	1:C:211:ARG:NE[2_657]	2.09	0.11
1:C:54:ASN:C	2:H:88:TRP:NE1[3_445]	2.14	0.06
2:D:211:ARG:O	1:E:207:GLN:OE1[2_657]	2.14	0.06
1:A:212:TRP:CH2	2:H:211:ARG:CZ[4_647]	2.15	0.05
1:C:54:ASN:C	2:H:88:TRP:CZ2[3_445]	2.15	0.05
2:D:88:TRP:CE2	1:G:54:ASN:CA[3_445]	2.15	0.05
1:C:54:ASN:CB	2:H:88:TRP:CH2[3_445]	2.16	0.04
1:C:54:ASN:CA	2:H:88:TRP:NE1[3_445]	2.17	0.03
1:C:54:ASN:C	2:H:88:TRP:CE2[3_445]	2.17	0.03

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	530/560 (95%)	439 (83%)	74 (14%)	17 (3%)	3	21
1	C	530/560 (95%)	438 (83%)	75 (14%)	17 (3%)	3	21
1	E	530/560 (95%)	439 (83%)	74 (14%)	17 (3%)	3	21
1	G	530/560 (95%)	439 (83%)	74 (14%)	17 (3%)	3	21
2	B	389/440 (88%)	320 (82%)	57 (15%)	12 (3%)	3	22
2	D	389/440 (88%)	320 (82%)	57 (15%)	12 (3%)	3	22
2	F	389/440 (88%)	320 (82%)	57 (15%)	12 (3%)	3	22
2	H	389/440 (88%)	320 (82%)	57 (15%)	12 (3%)	3	22
All	All	3676/4000 (92%)	3035 (83%)	525 (14%)	116 (3%)	3	21

All (116) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	222	GLN
1	A	345	PRO
2	B	94	ILE
1	C	222	GLN
1	C	345	PRO
2	D	94	ILE
1	E	222	GLN
1	E	345	PRO
2	F	94	ILE
1	G	222	GLN
1	G	345	PRO
2	H	94	ILE
1	A	85	GLN
1	A	273	GLY
1	A	412	PRO
1	C	85	GLN
1	C	273	GLY
1	C	412	PRO
1	E	85	GLN
1	E	273	GLY
1	E	412	PRO
1	G	85	GLN
1	G	273	GLY
1	G	412	PRO

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Mol	Chain	Res	Type
1	A	123	ASP
1	A	156	SER
1	A	296	THR
1	A	420	PRO
2	B	28	GLU
2	B	123	ASP
2	B	176	PRO
2	B	286	THR
1	C	123	ASP
1	C	156	SER
1	C	296	THR
1	C	420	PRO
2	D	28	GLU
2	D	123	ASP
2	D	176	PRO
2	D	286	THR
1	E	123	ASP
1	E	156	SER
1	E	296	THR
1	E	420	PRO
2	F	28	GLU
2	F	123	ASP
2	F	176	PRO
2	F	286	THR
1	G	123	ASP
1	G	156	SER
1	G	296	THR
1	G	420	PRO
2	H	28	GLU
2	H	123	ASP
2	H	176	PRO
2	H	286	THR
1	A	114	ALA
1	A	116	PHE
1	A	195	ILE
1	A	274	ILE
1	A	275	LYS
2	B	277	ARG
2	B	316	GLY
1	C	114	ALA
1	C	116	PHE
1	C	195	ILE

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Mol	Chain	Res	Type
1	C	274	ILE
1	C	275	LYS
2	D	277	ARG
2	D	316	GLY
1	E	114	ALA
1	E	116	PHE
1	E	195	ILE
1	E	274	ILE
1	E	275	LYS
2	F	277	ARG
2	F	316	GLY
1	G	114	ALA
1	G	116	PHE
1	G	195	ILE
1	G	274	ILE
1	G	275	LYS
2	H	277	ARG
2	H	316	GLY
1	A	357	MET
2	B	77	PHE
2	B	88	TRP
1	C	357	MET
2	D	77	PHE
2	D	88	TRP
1	E	357	MET
2	F	77	PHE
2	F	88	TRP
1	G	276	VAL
1	G	357	MET
2	H	77	PHE
2	H	88	TRP
1	A	276	VAL
1	A	462	GLY
2	B	55	PRO
1	C	276	VAL
1	C	462	GLY
2	D	55	PRO
1	E	276	VAL
1	E	462	GLY
2	F	55	PRO
1	G	462	GLY
2	H	55	PRO

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Mol	Chain	Res	Type
2	B	170	PRO
2	D	170	PRO
2	F	170	PRO
2	H	170	PRO
2	B	420	PRO
2	D	420	PRO
2	F	420	PRO
2	H	420	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	431/500 (86%)	410 (95%)	21 (5%)	22	55
1	C	431/500 (86%)	410 (95%)	21 (5%)	22	55
1	E	431/500 (86%)	410 (95%)	21 (5%)	22	55
1	G	431/500 (86%)	410 (95%)	21 (5%)	22	55
2	B	343/400 (86%)	323 (94%)	20 (6%)	18	51
2	D	343/400 (86%)	323 (94%)	20 (6%)	18	51
2	F	343/400 (86%)	323 (94%)	20 (6%)	18	51
2	H	343/400 (86%)	323 (94%)	20 (6%)	18	51
All	All	3096/3600 (86%)	2932 (95%)	164 (5%)	20	53

All (164) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	PRO
1	A	4	PRO
1	A	14	PRO
1	A	19	PRO
1	A	58	THR
1	A	91	GLN
1	A	169	GLU

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Mol	Chain	Res	Type
1	A	170	PRO
1	A	217	PRO
1	A	236	PRO
1	A	252	TRP
1	A	318	TYR
1	A	342	TYR
1	A	402	TRP
1	A	414	TRP
1	A	415	GLU
1	A	418	ASN
1	A	426	TRP
1	A	497	THR
1	A	507	GLN
1	A	510	PRO
2	B	24	TRP
2	B	25	PRO
2	B	52	PRO
2	B	54	ASN
2	B	55	PRO
2	B	59	PRO
2	B	60	VAL
2	B	63	ILE
2	B	88	TRP
2	B	97	PRO
2	B	135	ILE
2	B	148	VAL
2	B	170	PRO
2	B	176	PRO
2	B	266	TRP
2	B	313	PRO
2	B	321	PRO
2	B	392	PRO
2	B	402	TRP
2	B	412	PRO
1	C	1	PRO
1	C	4	PRO
1	C	14	PRO
1	C	19	PRO
1	C	58	THR
1	C	91	GLN
1	C	169	GLU
1	C	170	PRO

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Mol	Chain	Res	Type
1	C	217	PRO
1	C	236	PRO
1	C	252	TRP
1	C	318	TYR
1	C	342	TYR
1	C	402	TRP
1	C	414	TRP
1	C	415	GLU
1	C	418	ASN
1	C	426	TRP
1	C	497	THR
1	C	507	GLN
1	C	510	PRO
2	D	24	TRP
2	D	25	PRO
2	D	52	PRO
2	D	54	ASN
2	D	55	PRO
2	D	59	PRO
2	D	60	VAL
2	D	63	ILE
2	D	88	TRP
2	D	97	PRO
2	D	135	ILE
2	D	148	VAL
2	D	170	PRO
2	D	176	PRO
2	D	266	TRP
2	D	313	PRO
2	D	321	PRO
2	D	392	PRO
2	D	402	TRP
2	D	412	PRO
1	E	1	PRO
1	E	4	PRO
1	E	14	PRO
1	E	19	PRO
1	E	58	THR
1	E	91	GLN
1	E	169	GLU
1	E	170	PRO
1	E	217	PRO

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Mol	Chain	Res	Type
1	E	236	PRO
1	E	252	TRP
1	E	318	TYR
1	E	342	TYR
1	E	402	TRP
1	E	414	TRP
1	E	415	GLU
1	E	418	ASN
1	E	426	TRP
1	E	497	THR
1	E	507	GLN
1	E	510	PRO
2	F	24	TRP
2	F	25	PRO
2	F	52	PRO
2	F	54	ASN
2	F	55	PRO
2	F	59	PRO
2	F	60	VAL
2	F	63	ILE
2	F	88	TRP
2	F	97	PRO
2	F	135	ILE
2	F	148	VAL
2	F	170	PRO
2	F	176	PRO
2	F	266	TRP
2	F	313	PRO
2	F	321	PRO
2	F	392	PRO
2	F	402	TRP
2	F	412	PRO
1	G	1	PRO
1	G	4	PRO
1	G	14	PRO
1	G	19	PRO
1	G	58	THR
1	G	91	GLN
1	G	169	GLU
1	G	170	PRO
1	G	217	PRO
1	G	236	PRO

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Mol	Chain	Res	Type
1	G	252	TRP
1	G	318	TYR
1	G	342	TYR
1	G	402	TRP
1	G	414	TRP
1	G	415	GLU
1	G	418	ASN
1	G	426	TRP
1	G	497	THR
1	G	507	GLN
1	G	510	PRO
2	H	24	TRP
2	H	25	PRO
2	H	52	PRO
2	H	54	ASN
2	H	55	PRO
2	H	59	PRO
2	H	60	VAL
2	H	63	ILE
2	H	88	TRP
2	H	97	PRO
2	H	135	ILE
2	H	148	VAL
2	H	170	PRO
2	H	176	PRO
2	H	266	TRP
2	H	313	PRO
2	H	321	PRO
2	H	392	PRO
2	H	402	TRP
2	H	412	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (99) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	GLN
1	A	91	GLN
1	A	145	GLN
1	A	174	GLN
1	A	175	ASN
1	A	198	HIS
1	A	208	HIS

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Mol	Chain	Res	Type
1	A	315	HIS
1	A	373	GLN
1	A	407	GLN
1	A	418	ASN
1	A	471	ASN
1	A	474	ASN
1	A	507	GLN
2	B	54	ASN
2	B	57	ASN
2	B	96	HIS
2	B	145	GLN
2	B	147	ASN
2	B	151	GLN
2	B	208	HIS
2	B	235	HIS
2	B	394	GLN
2	B	418	ASN
1	C	23	GLN
1	C	91	GLN
1	C	145	GLN
1	C	174	GLN
1	C	175	ASN
1	C	198	HIS
1	C	208	HIS
1	C	315	HIS
1	C	373	GLN
1	C	407	GLN
1	C	418	ASN
1	C	471	ASN
1	C	474	ASN
2	D	54	ASN
2	D	57	ASN
2	D	96	HIS
2	D	145	GLN
2	D	147	ASN
2	D	151	GLN
2	D	208	HIS
2	D	235	HIS
2	D	394	GLN
2	D	418	ASN
1	E	23	GLN
1	E	91	GLN

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Mol	Chain	Res	Type
1	E	145	GLN
1	E	174	GLN
1	E	175	ASN
1	E	198	HIS
1	E	208	HIS
1	E	315	HIS
1	E	330	GLN
1	E	340	GLN
1	E	373	GLN
1	E	407	GLN
1	E	418	ASN
1	E	471	ASN
1	E	474	ASN
2	F	54	ASN
2	F	57	ASN
2	F	96	HIS
2	F	145	GLN
2	F	147	ASN
2	F	151	GLN
2	F	208	HIS
2	F	235	HIS
2	F	336	GLN
2	F	394	GLN
2	F	418	ASN
1	G	23	GLN
1	G	91	GLN
1	G	145	GLN
1	G	174	GLN
1	G	175	ASN
1	G	198	HIS
1	G	208	HIS
1	G	315	HIS
1	G	361	HIS
1	G	373	GLN
1	G	407	GLN
1	G	418	ASN
1	G	471	ASN
1	G	474	ASN
2	H	54	ASN
2	H	57	ASN
2	H	96	HIS
2	H	145	GLN

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Mol	Chain	Res	Type
2	H	147	ASN
2	H	151	GLN
2	H	174	GLN
2	H	208	HIS
2	H	235	HIS
2	H	336	GLN
2	H	394	GLN
2	H	418	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.