Full wwPDB X-ray Structure Validation Report ⓘ

Aug 10, 2020 – 04:40 AM BST

PDB ID	:	1SIE
Title	:	MURINE POLYOMAVIRUS COMPLEXED WITH A DISIALYLATED OLIGOSACCHARIDE
Authors	:	Stehle, T.; Harrison, S.C.
Deposited on	:	1995-12-12
Resolution	:	3.65 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 following versions of software and data (see references ⓘ) were used in the production of this report:

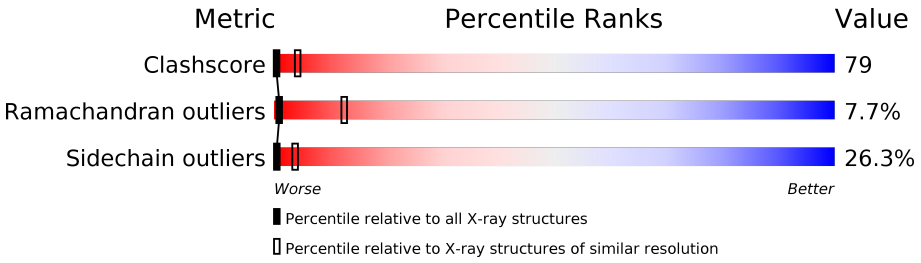
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.65 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	141614	1037 (3.80-3.52)
Ramachandran outliers	138981	1004 (3.80-3.52)
Sidechain outliers	138945	1002 (3.80-3.52)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria 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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	383	20% 52% 20%
1	B	383	21% 49% 23%
1	C	383	22% 48% 20% 7%
1	D	383	19% 46% 20% 11%
1	E	383	17% 48% 27%
1	F	383	20% 46% 23% 8%
2	G	4	50% 50%
2	H	4	50% 50%

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Mol	Chain	Length	Quality of chain
2	I	4	100%
2	J	4	75% 25%
2	K	4	50% 50%
2	L	4	50% 50%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 17141 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.

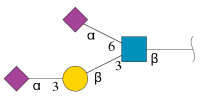
- Molecule 1 is a protein called POLYOMAVIRUS COAT PROTEIN VP1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	366	Total	C	N	O	S	0	0	0
			2849	1804	479	550	16			
1	B	367	Total	C	N	O	S	0	0	0
			2857	1808	481	552	16			
1	C	357	Total	C	N	O	S	0	0	0
			2784	1761	468	539	16			
1	D	340	Total	C	N	O	S	0	0	0
			2645	1674	445	511	15			
1	E	367	Total	C	N	O	S	0	0	0
			2857	1808	481	552	16			
1	F	354	Total	C	N	O	S	0	0	0
			2753	1740	461	536	16			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	6	ALA	SER	conflict	UNP P49302
B	6	ALA	SER	conflict	UNP P49302
C	6	ALA	SER	conflict	UNP P49302
D	6	ALA	SER	conflict	UNP P49302
E	6	ALA	SER	conflict	UNP P49302
F	6	ALA	SER	conflict	UNP P49302

- Molecule 2 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galacto pyranose-(1-3)-[N-acetyl-alpha-neuraminic acid-(2-6)]2-acetamido-2-deoxy-beta-D-glucopyr anose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	G	4	Total	C	N	O	0	0	0
			66	36	3	27			
2	H	4	Total	C	N	O	0	0	0
			66	36	3	27			
2	I	4	Total	C	N	O	0	0	0
			66	36	3	27			
2	J	4	Total	C	N	O	0	0	0
			66	36	3	27			
2	K	4	Total	C	N	O	0	0	0
			66	36	3	27			
2	L	4	Total	C	N	O	0	0	0
			66	36	3	27			

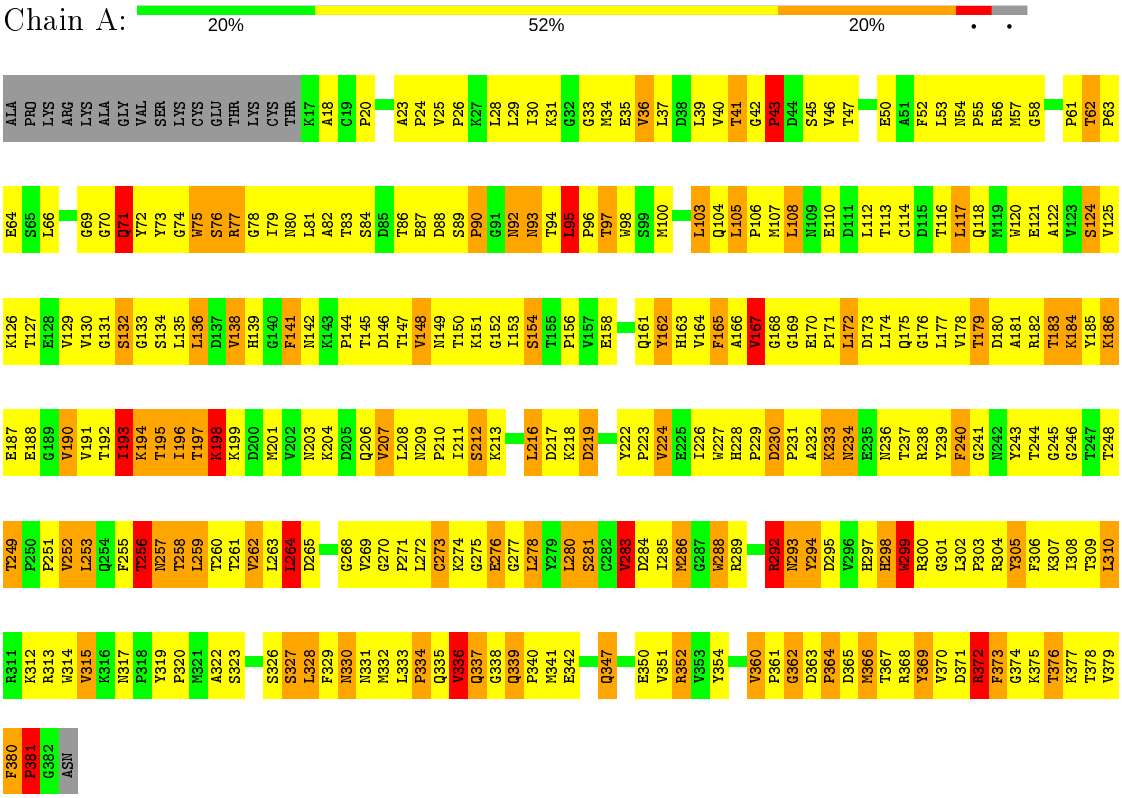
3 Residue-property plots (i)

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.

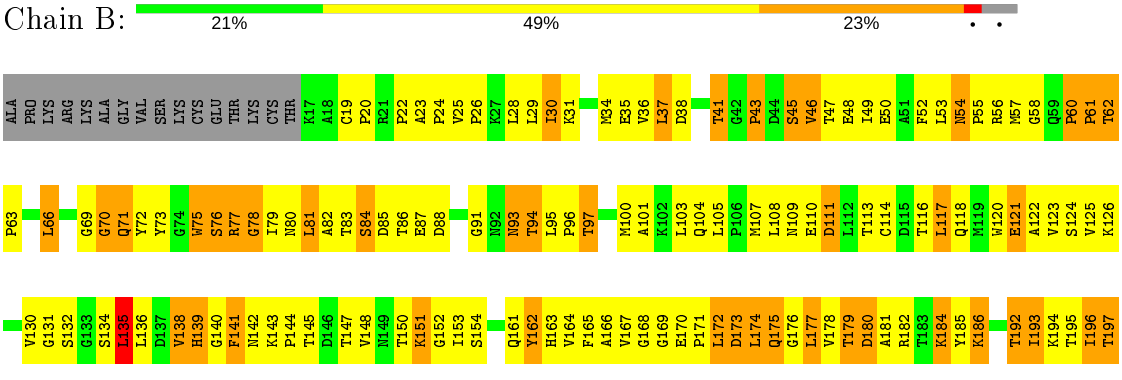
- Molecule 1: POLYOMAVIRUS COAT PROTEIN VP1

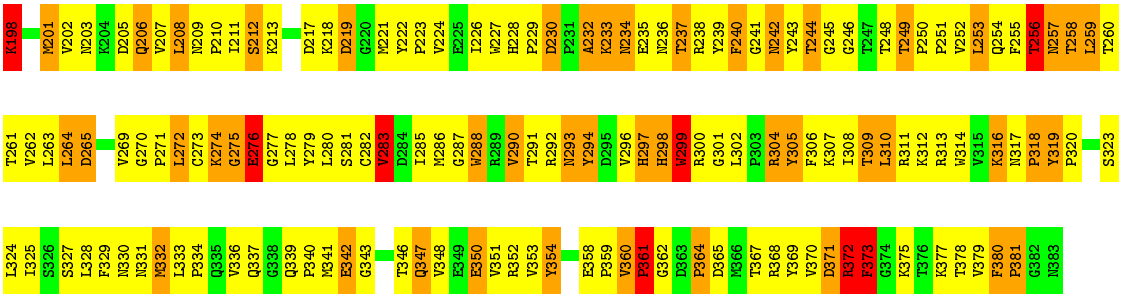
Chain A:



- Molecule 1: POLYOMAVIRUS COAT PROTEIN VP1

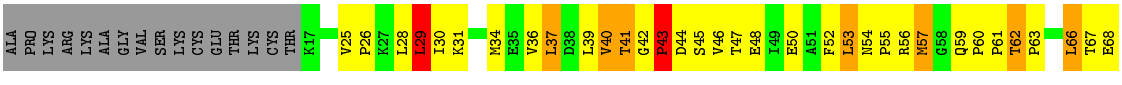
Chain B:

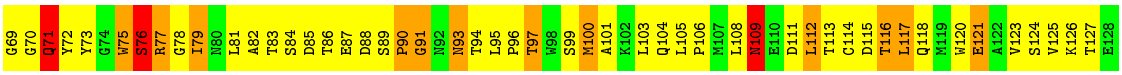


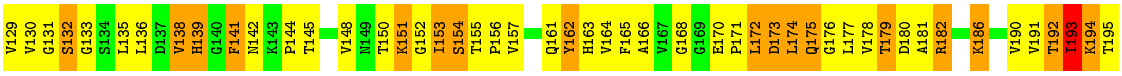


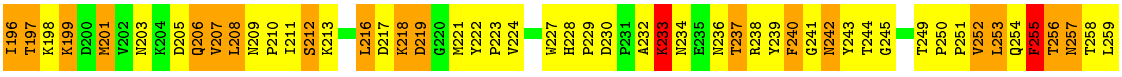
• Molecule 1: POLYOMAVIRUS COAT PROTEIN VP1

Chain C:



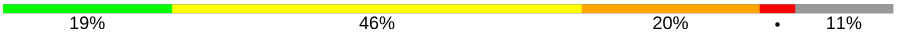


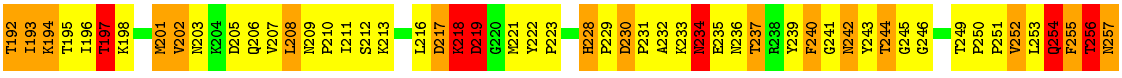


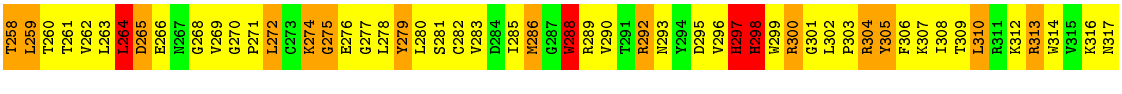


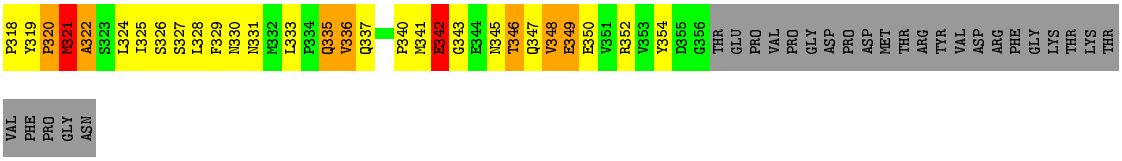
• Molecule 1: POLYOMAVIRUS COAT PROTEIN VP1

Chain D:



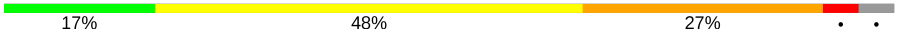


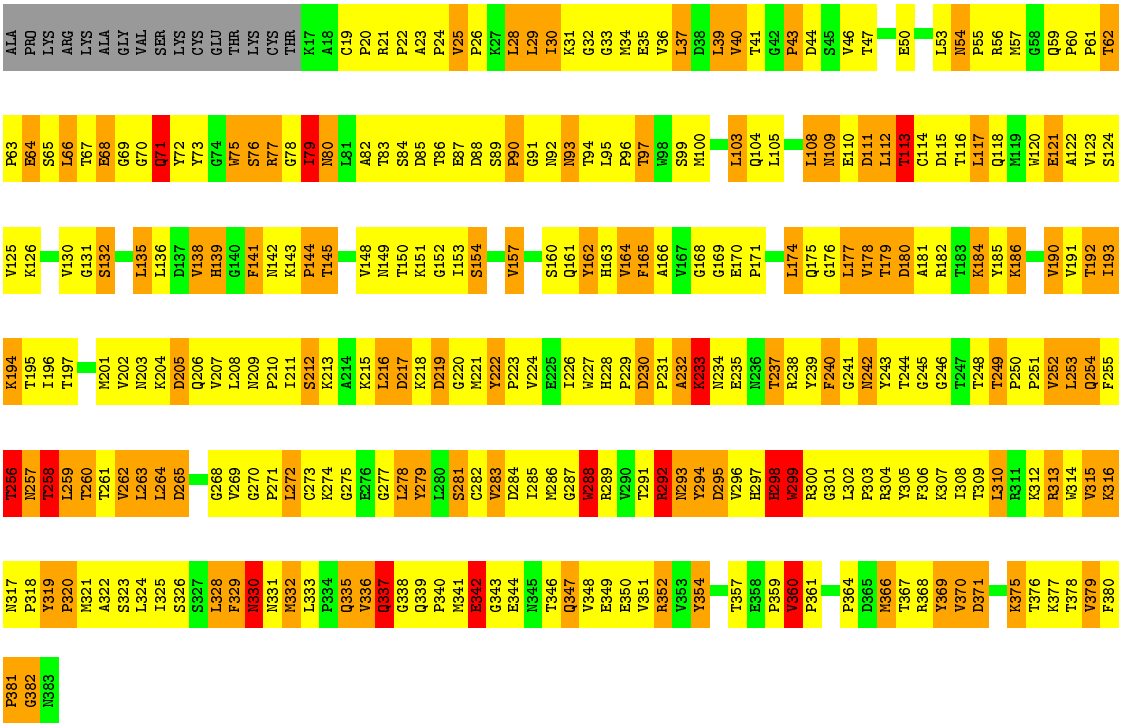




• Molecule 1: POLYOMAVIRUS COAT PROTEIN VP1

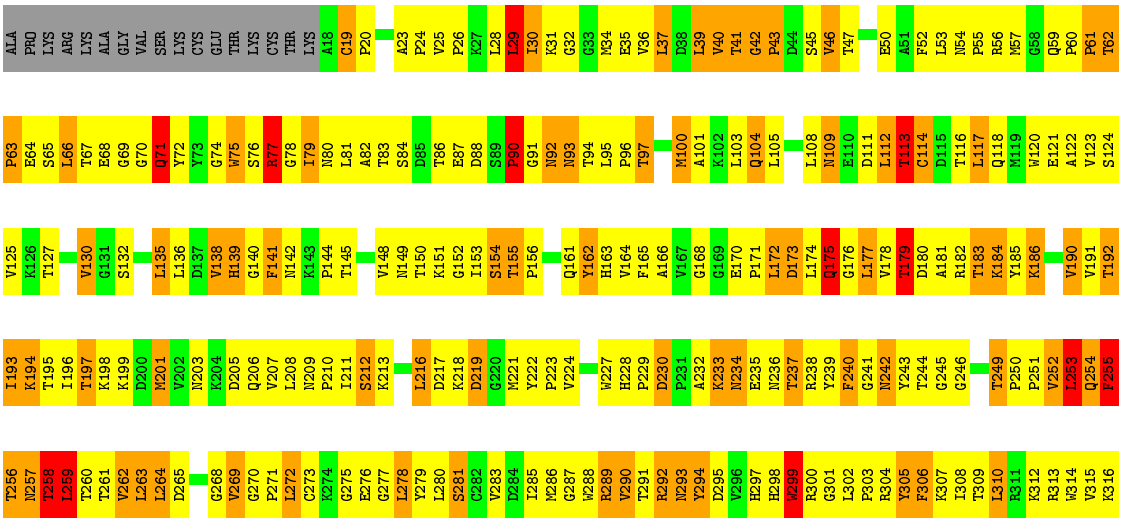
Chain E:

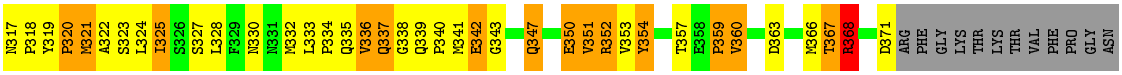




• Molecule 1: POLYOMAVIRUS COAT PROTEIN VP1

Chain F:





• Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-3)-[N-acetyl-alpha -neuraminic acid-(2-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

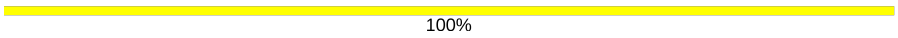
Chain G:

• Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-3)-[N-acetyl-alpha -neuraminic acid-(2-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:

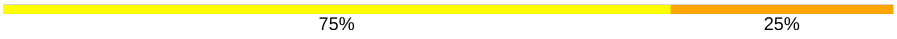
• Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-3)-[N-acetyl-alpha -neuraminic acid-(2-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:



• Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-3)-[N-acetyl-alpha -neuraminic acid-(2-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:



• Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-3)-[N-acetyl-alpha -neuraminic acid-(2-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:

• Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-3)-[N-acetyl-alpha -neuraminic acid-(2-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain L:

4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	I 2 3	Depositor
Cell constants a, b, c, α, β, γ	570.00Å 570.00Å 570.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	12.00 – 3.65	Depositor
% Data completeness (in resolution range)	74.0 (12.00-3.65)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.244 , 0.264	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	17141	wwPDB-VP
Average B, all atoms (Å^2)	82.0	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: SIA, GAL, NAG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	1.00	3/2920 (0.1%)	1.32	19/3981 (0.5%)
1	B	1.00	0/2927	1.29	21/3989 (0.5%)
1	C	1.00	1/2852 (0.0%)	1.30	23/3888 (0.6%)
1	D	1.02	2/2708 (0.1%)	1.27	17/3690 (0.5%)
1	E	1.00	2/2928 (0.1%)	1.32	31/3992 (0.8%)
1	F	1.00	1/2820 (0.0%)	1.28	23/3847 (0.6%)
All	All	1.00	9/17155 (0.1%)	1.30	134/23387 (0.6%)

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	5
1	B	0	3
1	C	0	2
1	D	0	4
1	E	0	2
1	F	0	2
All	All	0	18

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	299	TRP	CB-CG	6.41	1.61	1.50
1	E	336	VAL	C-N	-6.36	1.19	1.34
1	A	262	VAL	CA-CB	-5.91	1.42	1.54
1	D	288	TRP	CB-CG	-5.70	1.40	1.50
1	F	234	ASN	CB-CG	5.69	1.64	1.51
1	A	165	PHE	CB-CG	-5.60	1.41	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	165	PHE	CB-CG	-5.49	1.42	1.51
1	D	234	ASN	CB-CG	5.26	1.63	1.51
1	C	360	VAL	CA-CB	-5.10	1.44	1.54

All (134) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	336	VAL	O-C-N	-18.34	93.36	122.70
1	C	29	LEU	CA-CB-CG	-12.06	87.55	115.30
1	A	336	VAL	CA-C-N	-11.21	92.54	117.20
1	F	264	LEU	CA-CB-CG	-10.79	90.49	115.30
1	E	336	VAL	O-C-N	10.50	139.51	122.70
1	F	29	LEU	CA-CB-CG	-9.95	92.42	115.30
1	C	275	GLY	N-CA-C	-9.91	88.31	113.10
1	B	275	GLY	N-CA-C	-9.88	88.41	113.10
1	E	29	LEU	CA-CB-CG	-9.83	92.69	115.30
1	A	264	LEU	CA-CB-CG	-9.52	93.41	115.30
1	C	264	LEU	CA-CB-CG	-9.37	93.76	115.30
1	B	299	TRP	CA-CB-CG	9.12	131.02	113.70
1	E	299	TRP	CA-CB-CG	9.06	130.92	113.70
1	A	299	TRP	CA-CB-CG	8.59	130.03	113.70
1	D	29	LEU	CA-CB-CG	-8.59	95.55	115.30
1	E	336	VAL	CA-C-N	-8.20	99.16	117.20
1	A	258	THR	N-CA-C	8.17	133.05	111.00
1	F	275	GLY	N-CA-C	-7.79	93.63	113.10
1	D	264	LEU	CA-CB-CG	-7.74	97.49	115.30
1	A	136	LEU	CA-CB-CG	-7.72	97.55	115.30
1	E	263	LEU	CA-CB-CG	-7.71	97.56	115.30
1	A	259	LEU	CA-CB-CG	7.70	133.00	115.30
1	B	264	LEU	CA-CB-CG	-7.51	98.03	115.30
1	D	256	THR	N-CA-C	7.48	131.19	111.00
1	A	95	LEU	CA-CB-CG	-7.41	98.25	115.30
1	E	256	THR	N-CA-C	7.24	130.56	111.00
1	E	259	LEU	N-CA-C	7.12	130.21	111.00
1	E	71	GLN	CA-C-N	-7.07	101.66	117.20
1	E	292	ARG	N-CA-C	-7.03	92.02	111.00
1	F	39	LEU	CA-CB-CG	-7.03	99.13	115.30
1	F	197	THR	N-CA-C	-6.97	92.17	111.00
1	C	208	LEU	CA-CB-CG	-6.84	99.56	115.30
1	A	256	THR	CA-C-N	-6.84	102.16	117.20
1	D	272	LEU	CA-CB-CG	-6.83	99.58	115.30
1	F	177	LEU	CA-CB-CG	-6.83	99.58	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	258	THR	N-CA-C	6.80	129.36	111.00
1	A	71	GLN	CA-C-N	-6.78	102.28	117.20
1	D	254	GLN	N-CA-C	6.77	129.27	111.00
1	E	259	LEU	CA-CB-CG	-6.76	99.76	115.30
1	F	254	GLN	N-CA-C	6.72	129.16	111.00
1	C	292	ARG	N-CA-C	-6.67	92.98	111.00
1	B	256	THR	N-CA-C	6.64	128.92	111.00
1	C	259	LEU	CA-CB-CG	6.62	130.54	115.30
1	B	177	LEU	CA-CB-CG	-6.55	100.23	115.30
1	C	95	LEU	CA-CB-CG	-6.54	100.26	115.30
1	D	259	LEU	N-CA-C	6.50	128.56	111.00
1	D	298	HIS	N-CA-C	6.50	128.56	111.00
1	C	95	LEU	N-CA-C	6.46	128.44	111.00
1	E	258	THR	N-CA-C	6.44	128.38	111.00
1	C	263	LEU	CA-CB-CG	-6.43	100.52	115.30
1	D	78	GLY	N-CA-C	-6.37	97.19	113.10
1	E	220	GLY	N-CA-C	-6.36	97.21	113.10
1	E	40	VAL	CB-CA-C	-6.34	99.35	111.40
1	B	362	GLY	N-CA-C	-6.33	97.28	113.10
1	C	153	ILE	CB-CA-C	-6.32	98.97	111.60
1	B	259	LEU	CA-CB-CG	-6.26	100.90	115.30
1	B	360	VAL	CB-CA-C	-6.25	99.53	111.40
1	D	297	HIS	N-CA-C	6.24	127.86	111.00
1	E	264	LEU	CA-CB-CG	-6.22	100.99	115.30
1	B	377	LYS	N-CA-C	-6.20	94.25	111.00
1	F	42	GLY	N-CA-C	-6.18	97.64	113.10
1	F	256	THR	N-CA-C	6.18	127.68	111.00
1	E	28	LEU	CA-CB-CG	-6.11	101.26	115.30
1	A	257	ASN	N-CA-CB	-6.03	99.74	110.60
1	D	275	GLY	N-CA-C	-6.01	98.08	113.10
1	B	208	LEU	CA-CB-CG	-5.99	101.53	115.30
1	A	283	VAL	CB-CA-C	-5.99	100.03	111.40
1	C	256	THR	N-CA-C	5.92	126.99	111.00
1	F	256	THR	CA-C-N	-5.88	104.25	117.20
1	D	71	GLN	CA-C-N	-5.85	104.33	117.20
1	C	109	ASN	N-CA-C	5.82	126.72	111.00
1	C	362	GLY	N-CA-C	-5.82	98.54	113.10
1	A	256	THR	N-CA-C	5.82	126.71	111.00
1	E	76	SER	N-CA-C	-5.79	95.36	111.00
1	E	178	VAL	CB-CA-C	-5.78	100.41	111.40
1	F	292	ARG	N-CA-C	-5.78	95.39	111.00
1	F	114	CYS	N-CA-C	-5.78	95.41	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	81	LEU	CA-CB-CG	-5.74	102.11	115.30
1	F	253	LEU	CA-CB-CG	-5.72	102.14	115.30
1	A	336	VAL	C-N-CA	5.72	135.99	121.70
1	E	272	LEU	CA-CB-CG	-5.71	102.16	115.30
1	E	254	GLN	N-CA-C	5.70	126.39	111.00
1	B	19	CYS	N-CA-C	-5.69	95.63	111.00
1	E	298	HIS	N-CA-C	5.69	126.36	111.00
1	F	259	LEU	N-CA-C	5.69	126.36	111.00
1	B	78	GLY	N-CA-C	-5.64	99.00	113.10
1	B	259	LEU	N-CA-C	5.63	126.21	111.00
1	E	274	LYS	N-CA-C	-5.61	95.86	111.00
1	F	289	ARG	N-CA-C	-5.59	95.90	111.00
1	A	292	ARG	N-CA-C	-5.57	95.97	111.00
1	B	298	HIS	N-CA-C	5.55	125.99	111.00
1	C	40	VAL	CB-CA-C	-5.54	100.87	111.40
1	E	370	VAL	N-CA-C	-5.54	96.05	111.00
1	E	382	GLY	N-CA-C	-5.49	99.37	113.10
1	D	197	THR	N-CA-C	-5.48	96.20	111.00
1	E	319	TYR	N-CA-C	5.47	125.77	111.00
1	B	274	LYS	N-CA-C	-5.45	96.29	111.00
1	C	272	LEU	CA-CB-CG	-5.43	102.80	115.30
1	B	350	GLU	N-CA-C	5.39	125.56	111.00
1	C	348	VAL	N-CA-C	-5.39	96.44	111.00
1	E	232	ALA	N-CA-C	-5.39	96.43	111.00
1	A	167	VAL	CB-CA-C	-5.38	101.17	111.40
1	D	274	LYS	N-CA-C	-5.36	96.52	111.00
1	C	327	SER	N-CA-C	-5.29	96.72	111.00
1	F	263	LEU	CA-CB-CG	-5.29	103.13	115.30
1	F	257	ASN	N-CA-CB	-5.29	101.08	110.60
1	D	324	LEU	CA-CB-CG	5.29	127.46	115.30
1	E	256	THR	CA-C-N	-5.28	105.58	117.20
1	B	94	THR	N-CA-C	-5.28	96.76	111.00
1	D	170	GLU	N-CA-C	-5.27	96.76	111.00
1	E	275	GLY	N-CA-C	-5.27	99.92	113.10
1	D	296	VAL	N-CA-C	-5.26	96.79	111.00
1	E	139	HIS	N-CA-C	-5.26	96.79	111.00
1	E	288	TRP	N-CA-C	5.26	125.20	111.00
1	B	283	VAL	CB-CA-C	-5.25	101.43	111.40
1	A	105	LEU	CA-CB-CG	-5.24	103.24	115.30
1	F	299	TRP	CA-CB-CG	5.24	123.66	113.70
1	B	76	SER	N-CA-C	-5.24	96.85	111.00
1	C	78	GLY	N-CA-C	-5.22	100.05	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	232	ALA	N-CA-C	-5.20	96.97	111.00
1	C	76	SER	N-CA-C	-5.20	96.97	111.00
1	F	272	LEU	CA-CB-CG	-5.20	103.35	115.30
1	F	71	GLN	CA-C-N	-5.17	105.83	117.20
1	E	315	VAL	CB-CA-C	-5.16	101.59	111.40
1	C	42	GLY	N-CA-C	-5.13	100.28	113.10
1	D	31	LYS	N-CA-C	-5.13	97.16	111.00
1	C	216	LEU	CA-CB-CG	-5.12	103.53	115.30
1	A	376	THR	N-CA-C	5.12	124.81	111.00
1	C	91	GLY	N-CA-C	-5.11	100.32	113.10
1	E	164	VAL	CB-CA-C	-5.11	101.69	111.40
1	F	299	TRP	N-CA-C	5.10	124.78	111.00
1	A	360	VAL	CB-CA-C	-5.09	101.73	111.40
1	C	360	VAL	CB-CA-C	-5.08	101.75	111.40
1	F	175	GLN	N-CA-C	-5.04	97.40	111.00

There are no chirality outliers.

All (18) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	162	TYR	Sidechain
1	A	305	TYR	Sidechain
1	A	336	VAL	Mainchain,Peptide
1	A	71	GLN	Mainchain
1	B	162	TYR	Sidechain
1	B	305	TYR	Sidechain
1	B	319	TYR	Sidechain
1	C	162	TYR	Sidechain
1	C	305	TYR	Sidechain
1	D	162	TYR	Sidechain
1	D	305	TYR	Sidechain
1	D	354	TYR	Sidechain
1	D	71	GLN	Mainchain
1	E	162	TYR	Sidechain
1	E	71	GLN	Mainchain
1	F	162	TYR	Sidechain
1	F	305	TYR	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2849	0	2815	535	1
1	B	2857	0	2820	503	0
1	C	2784	0	2743	444	0
1	D	2645	0	2616	433	0
1	E	2857	0	2820	514	0
1	F	2753	0	2710	461	0
2	G	66	0	56	2	0
2	H	66	0	56	2	0
2	I	66	0	56	0	0
2	J	66	0	56	1	0
2	K	66	0	56	3	0
2	L	66	0	56	5	0
All	All	17141	0	16860	2673	1

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 79.

All (2673) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:336:VAL:CG2	1:A:337:GLN:HA	1.27	1.61
1:A:328:LEU:CD2	1:A:333:LEU:HD21	1.37	1.54
1:A:328:LEU:CD1	1:A:332:MET:HE1	1.32	1.53
1:A:328:LEU:HD12	1:A:332:MET:CE	1.44	1.44
1:A:336:VAL:HG23	1:A:337:GLN:CA	0.98	1.44
1:A:328:LEU:HD21	1:A:333:LEU:CD2	1.51	1.40
1:A:328:LEU:HD11	1:A:333:LEU:CD2	1.58	1.33
1:A:328:LEU:CD1	1:A:332:MET:CE	2.00	1.31
1:A:336:VAL:CG2	1:A:337:GLN:CA	1.90	1.29
1:A:336:VAL:HG23	1:A:337:GLN:N	1.30	1.27
1:A:328:LEU:HD23	1:A:328:LEU:O	1.46	1.15
1:A:203:ASN:HB3	1:E:71:GLN:HG3	1.18	1.15
1:A:328:LEU:HG	1:A:332:MET:HE2	1.28	1.13
1:E:177:LEU:HD21	1:E:206:GLN:O	1.45	1.11
1:D:71:GLN:HG3	1:E:203:ASN:HB3	1.34	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:84:SER:HB3	1:A:86:THR:HG22	1.32	1.10
1:B:336:VAL:HA	1:B:337:GLN:N	1.66	1.10
1:C:71:GLN:HG3	1:D:203:ASN:HB3	1.33	1.09
1:B:175:GLN:HB2	1:B:230:ASP:HB2	1.35	1.08
1:F:168:GLY:HA3	1:F:237:THR:HG23	1.38	1.06
1:A:71:GLN:HG3	1:B:203:ASN:HB3	1.36	1.06
1:F:175:GLN:HB2	1:F:230:ASP:HB2	1.33	1.05
1:A:328:LEU:CD1	1:A:333:LEU:CD2	2.34	1.05
1:A:336:VAL:CG2	1:A:337:GLN:N	1.95	1.04
1:E:121:GLU:HG3	1:E:313:ARG:HD3	1.40	1.04
1:D:336:VAL:CA	1:D:337:GLN:OE1	2.05	1.04
1:A:336:VAL:HG21	1:A:337:GLN:HA	1.34	1.03
1:A:328:LEU:CD1	1:A:333:LEU:HD23	1.87	1.03
1:A:328:LEU:CG	1:A:332:MET:HE2	1.90	1.01
1:A:328:LEU:CG	1:A:332:MET:CE	2.38	1.01
1:B:177:LEU:HD13	1:B:207:VAL:O	1.57	1.01
1:C:168:GLY:HA3	1:C:237:THR:HG23	1.40	1.00
1:B:54:ASN:HD21	1:C:208:LEU:H	1.08	1.00
1:C:350:GLU:HG3	1:F:233:LYS:HG2	1.43	1.00
1:A:208:LEU:H	1:E:54:ASN:HD21	1.09	0.98
1:D:336:VAL:C	1:D:337:GLN:OE1	2.01	0.98
1:B:257:ASN:HD22	1:B:257:ASN:H	1.02	0.98
1:B:71:GLN:HG3	1:C:203:ASN:HB3	1.45	0.97
1:D:336:VAL:HA	1:D:337:GLN:OE1	1.63	0.96
1:A:328:LEU:HD11	1:A:333:LEU:HD23	0.95	0.95
1:F:205:ASP:HA	1:F:209:ASN:HB2	1.48	0.95
1:A:176:GLY:O	1:A:177:LEU:HD23	1.66	0.95
1:D:114:CYS:HB2	1:D:116:THR:HG22	1.49	0.94
1:D:192:THR:HB	1:D:194:LYS:HD3	1.50	0.94
1:D:346:THR:HG22	1:D:348:VAL:HB	1.47	0.94
1:A:251:PRO:HG2	1:B:245:GLY:HA3	1.50	0.94
1:E:305:TYR:HE1	1:E:307:LYS:HB2	1.34	0.93
1:F:192:THR:HB	1:F:194:LYS:HD3	1.49	0.93
1:A:69:GLY:HA3	1:A:71:GLN:HE22	1.35	0.92
1:B:30:ILE:HD13	1:B:36:VAL:HG13	1.48	0.92
1:A:372:ARG:HH11	1:A:372:ARG:HB2	1.33	0.92
1:B:336:VAL:O	1:B:337:GLN:HA	1.70	0.91
1:A:328:LEU:CG	1:A:333:LEU:HD21	1.99	0.91
1:F:175:GLN:HG2	1:F:213:LYS:HD3	1.49	0.91
1:B:346:THR:CG2	1:B:348:VAL:HG12	2.01	0.91
1:B:346:THR:HG21	1:B:348:VAL:HG12	1.50	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:122:ALA:HB3	1:F:271:PRO:HD2	1.50	0.90
1:D:138:VAL:HB	1:D:153:ILE:HD12	1.54	0.90
1:A:308:ILE:HG22	1:A:310:LEU:HD12	1.52	0.89
1:B:22:PRO:HB2	1:F:360:VAL:HG23	1.52	0.89
1:B:192:THR:HB	1:B:194:LYS:HG2	1.55	0.89
1:B:79:ILE:HD11	1:B:298:HIS:HA	1.52	0.89
1:E:258:THR:HB	1:E:259:LEU:HD22	1.55	0.89
1:F:177:LEU:HD13	1:F:207:VAL:O	1.73	0.89
1:F:258:THR:HB	1:F:259:LEU:HD13	1.52	0.89
1:F:262:VAL:HG12	1:F:264:LEU:H	1.37	0.89
1:B:262:VAL:HG12	1:B:264:LEU:H	1.38	0.88
1:D:168:GLY:HA3	1:D:237:THR:HG23	1.54	0.88
1:C:138:VAL:HB	1:C:153:ILE:HG23	1.51	0.88
1:B:177:LEU:HD21	1:B:208:LEU:HA	1.54	0.88
1:D:19:CYS:SG	1:E:112:LEU:HD22	2.14	0.88
1:A:328:LEU:HG	1:A:332:MET:CE	2.02	0.88
1:A:341:MET:HE1	1:A:347:GLN:HB2	1.54	0.88
1:B:233:LYS:HG2	1:B:234:ASN:N	1.89	0.87
1:C:62:THR:OG1	1:C:63:PRO:HD3	1.73	0.87
1:E:342:GLU:N	1:E:346:THR:HG23	1.89	0.87
1:A:328:LEU:HD21	1:A:333:LEU:CG	2.04	0.87
1:F:104:GLN:HE22	1:F:276:GLU:HB2	1.37	0.87
1:A:141:PHE:CE1	1:A:292:ARG:HG3	2.10	0.87
1:F:90:PRO:HB3	1:F:95:LEU:HD11	1.56	0.87
1:D:218:LYS:O	1:D:219:ASP:HB3	1.73	0.86
1:F:30:ILE:HD13	1:F:36:VAL:HG13	1.57	0.86
1:A:328:LEU:O	1:A:328:LEU:CD2	2.24	0.86
1:C:172:LEU:HD22	1:C:173:ASP:N	1.91	0.86
1:C:350:GLU:HB3	1:F:233:LYS:HB3	1.55	0.86
1:B:141:PHE:HE1	1:B:144:PRO:HG3	1.40	0.86
1:E:62:THR:OG1	1:E:63:PRO:HD3	1.76	0.85
1:A:83:THR:HB	1:A:87:GLU:HB3	1.56	0.85
1:C:191:VAL:HG21	1:C:222:TYR:CD2	2.10	0.85
1:A:340:PRO:HG2	1:A:347:GLN:HE22	1.42	0.85
1:E:112:LEU:HB3	1:E:116:THR:HG23	1.55	0.85
1:A:328:LEU:CD1	1:A:333:LEU:HD21	2.04	0.85
1:F:288:TRP:HZ3	1:F:299:TRP:CE2	1.95	0.84
1:A:192:THR:HG22	1:A:193:ILE:CD1	2.07	0.84
1:C:97:THR:HA	1:C:223:PRO:HA	1.59	0.84
1:B:97:THR:HA	1:B:223:PRO:HA	1.59	0.84
1:A:163:HIS:HA	1:A:283:VAL:O	1.75	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:117:LEU:HD12	1:B:117:LEU:H	1.40	0.84
1:A:233:LYS:HA	1:E:50:GLU:HG2	1.57	0.84
1:F:111:ASP:HB3	1:F:116:THR:HG22	1.59	0.84
1:F:172:LEU:HD22	1:F:173:ASP:N	1.93	0.84
1:F:233:LYS:HE2	1:F:234:ASN:ND2	1.93	0.84
1:E:117:LEU:HD13	1:E:118:GLN:H	1.42	0.84
1:D:292:ARG:HH11	1:D:292:ARG:HB3	1.41	0.83
1:C:192:THR:HB	1:C:194:LYS:HD3	1.58	0.83
1:E:253:LEU:HD23	1:E:254:GLN:H	1.42	0.83
1:E:141:PHE:CE1	1:E:292:ARG:HG3	2.12	0.83
1:C:50:GLU:CD	1:D:233:LYS:HA	1.98	0.83
1:A:103:LEU:HB2	1:A:278:LEU:HB3	1.60	0.83
1:E:122:ALA:HB3	1:E:271:PRO:HD2	1.59	0.83
1:B:308:ILE:N	1:B:308:ILE:HD12	1.94	0.83
1:A:192:THR:HG22	1:A:193:ILE:HD12	1.60	0.83
1:E:83:THR:HB	1:E:87:GLU:HB3	1.59	0.83
1:E:175:GLN:HG3	1:E:213:LYS:HG2	1.60	0.83
1:E:288:TRP:HB3	1:E:299:TRP:HB3	1.57	0.83
1:E:222:TYR:HB3	1:E:227:TRP:CD1	2.14	0.83
1:F:97:THR:HA	1:F:223:PRO:HA	1.61	0.83
1:B:328:LEU:O	1:B:332:MET:SD	2.37	0.82
1:C:308:ILE:HD12	1:C:308:ILE:H	1.44	0.82
1:E:142:ASN:O	1:E:292:ARG:HG2	1.78	0.82
1:E:91:GLY:H	1:E:186:LYS:HE3	1.43	0.82
1:A:262:VAL:HG12	1:A:264:LEU:H	1.42	0.82
1:D:286:MET:CE	1:D:286:MET:HA	2.10	0.82
1:E:163:HIS:HA	1:E:283:VAL:O	1.79	0.82
1:D:286:MET:HA	1:D:286:MET:HE3	1.61	0.82
1:B:177:LEU:CD1	1:B:207:VAL:O	2.27	0.82
1:C:233:LYS:NZ	1:F:350:GLU:HG2	1.95	0.82
1:D:257:ASN:HB3	1:E:239:TYR:CE2	2.14	0.82
1:A:336:VAL:HG23	1:A:337:GLN:CB	2.09	0.82
1:B:71:GLN:HE21	1:B:73:TYR:HB2	1.44	0.81
1:F:65:SER:HB3	1:F:68:GLU:HG2	1.62	0.81
1:A:138:VAL:HB	1:A:153:ILE:HG23	1.63	0.81
1:E:193:ILE:HG12	1:E:201:MET:HE3	1.62	0.81
1:B:258:THR:HB	1:B:259:LEU:HD22	1.60	0.81
1:C:208:LEU:O	1:C:210:PRO:HD3	1.81	0.81
1:D:114:CYS:HB2	1:D:116:THR:CG2	2.09	0.81
1:F:138:VAL:HB	1:F:153:ILE:HG23	1.59	0.81
1:A:122:ALA:HA	1:A:310:LEU:HB3	1.62	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:186:LYS:HE2	1:B:186:LYS:H	1.45	0.81
1:F:161:GLN:HE22	1:F:251:PRO:HA	1.45	0.81
1:C:144:PRO:HD3	1:C:292:ARG:HG2	1.63	0.81
1:B:22:PRO:HG2	1:F:359:PRO:HB3	1.62	0.81
1:B:54:ASN:ND2	1:C:207:VAL:HB	1.95	0.81
1:E:168:GLY:HA3	1:E:237:THR:HG23	1.60	0.81
1:F:178:VAL:HG22	1:F:179:THR:H	1.47	0.80
1:F:30:ILE:HG12	1:F:31:LYS:N	1.94	0.80
1:F:57:MET:HB2	1:F:96:PRO:HB3	1.63	0.80
1:E:103:LEU:HB2	1:E:278:LEU:HB3	1.63	0.80
1:E:82:ALA:HB1	1:E:88:ASP:HA	1.62	0.80
1:F:203:ASN:O	1:F:206:GLN:HB3	1.81	0.80
1:A:125:VAL:HG12	1:A:263:LEU:HD21	1.63	0.80
1:C:233:LYS:HD3	1:C:234:ASN:N	1.95	0.80
1:B:125:VAL:HB	1:B:263:LEU:HD11	1.63	0.80
1:C:336:VAL:O	1:C:337:GLN:HA	1.81	0.80
1:E:233:LYS:HD2	1:E:234:ASN:H	1.46	0.80
1:E:115:ASP:O	1:E:316:LYS:HA	1.82	0.80
1:C:175:GLN:HE21	1:C:176:GLY:N	1.80	0.80
1:B:304:ARG:HD3	1:B:306:PHE:CZ	2.17	0.80
1:B:276:GLU:HG2	1:C:370:VAL:HG21	1.64	0.79
1:A:90:PRO:HG2	1:A:185:TYR:HA	1.64	0.79
1:B:276:GLU:HG2	1:C:370:VAL:CG2	2.13	0.79
1:D:257:ASN:ND2	1:E:239:TYR:H	1.81	0.79
1:E:75:TRP:CZ2	1:E:300:ARG:HD2	2.17	0.79
1:F:317:ASN:HD22	1:F:318:PRO:HD2	1.43	0.79
1:D:175:GLN:HB2	1:D:230:ASP:HB2	1.62	0.79
1:F:177:LEU:HD21	1:F:208:LEU:HA	1.64	0.79
1:B:296:VAL:HG11	2:H:3:SIA:H32	1.64	0.79
1:B:138:VAL:HB	1:B:153:ILE:HG23	1.63	0.79
1:E:265:ASP:H	1:E:270:GLY:H	1.27	0.79
1:D:186:LYS:H	1:D:186:LYS:HD2	1.47	0.79
1:F:76:SER:O	1:F:298:HIS:HB2	1.83	0.79
1:F:308:ILE:HD12	1:F:308:ILE:N	1.98	0.79
1:B:34:MET:O	1:B:37:LEU:HB2	1.83	0.79
1:C:126:LYS:HG3	1:C:260:THR:HG23	1.62	0.79
1:C:163:HIS:HA	1:C:283:VAL:O	1.81	0.79
1:E:286:MET:HE3	1:E:286:MET:HA	1.65	0.78
1:A:135:LEU:N	1:A:135:LEU:HD12	1.97	0.78
1:D:153:ILE:HG12	1:E:297:HIS:ND1	1.99	0.78
1:E:350:GLU:HG2	1:E:351:VAL:N	1.97	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:55:PRO:O	1:E:56:ARG:HG3	1.83	0.78
1:F:286:MET:HA	1:F:286:MET:HE3	1.64	0.78
1:D:262:VAL:HG12	1:D:264:LEU:H	1.48	0.78
1:E:259:LEU:HD22	1:E:259:LEU:N	1.98	0.78
1:B:77:ARG:HB2	1:B:93:ASN:HB2	1.66	0.78
1:D:71:GLN:HG3	1:E:203:ASN:CB	2.13	0.78
1:F:144:PRO:HD3	1:F:292:ARG:HG2	1.64	0.78
1:B:257:ASN:ND2	1:B:257:ASN:H	1.76	0.78
1:D:346:THR:CG2	1:D:348:VAL:HB	2.14	0.78
1:B:251:PRO:HD2	1:C:245:GLY:HA3	1.65	0.78
1:D:168:GLY:CA	1:D:237:THR:HG23	2.12	0.78
1:D:342:GLU:N	1:D:346:THR:HG23	1.99	0.78
1:A:41:THR:O	1:A:45:SER:HB3	1.83	0.78
1:A:52:PHE:CE2	1:B:208:LEU:HD22	2.19	0.78
1:D:180:ASP:OD2	1:D:182:ARG:HD3	1.83	0.78
1:A:180:ASP:HA	1:A:206:GLN:HE21	1.46	0.78
1:D:96:PRO:HD3	1:D:299:TRP:CZ3	2.19	0.78
1:A:203:ASN:CB	1:E:71:GLN:HG3	2.07	0.78
1:F:34:MET:O	1:F:37:LEU:HB2	1.83	0.78
1:D:71:GLN:CG	1:E:203:ASN:HB3	2.12	0.77
1:B:332:MET:N	1:B:332:MET:SD	2.57	0.77
1:D:304:ARG:HD3	1:D:306:PHE:CZ	2.19	0.77
1:A:198:LYS:N	1:A:198:LYS:HE2	1.99	0.77
1:B:186:LYS:HE2	1:B:186:LYS:N	1.99	0.77
1:C:308:ILE:HD12	1:C:308:ILE:N	2.00	0.77
1:B:103:LEU:HD22	1:F:341:MET:HG3	1.67	0.77
1:D:122:ALA:HB3	1:D:271:PRO:HD2	1.64	0.77
1:E:233:LYS:HD3	1:E:234:ASN:ND2	1.99	0.77
1:C:350:GLU:CB	1:F:233:LYS:HB3	2.13	0.77
1:F:81:LEU:HG	1:F:82:ALA:H	1.50	0.77
1:C:256:THR:HA	1:D:239:TYR:CE1	2.20	0.77
1:B:203:ASN:O	1:B:206:GLN:HB3	1.83	0.77
1:F:288:TRP:HZ3	1:F:299:TRP:CD2	2.02	0.77
1:A:350:GLU:HG2	1:A:351:VAL:N	2.00	0.76
1:B:208:LEU:O	1:B:210:PRO:HD3	1.86	0.76
1:A:76:SER:O	1:A:298:HIS:HB3	1.85	0.76
1:E:90:PRO:HD2	1:E:186:LYS:NZ	2.01	0.76
1:C:142:ASN:HD21	1:C:289:ARG:HG3	1.51	0.76
1:A:239:TYR:CD1	1:E:257:ASN:HB2	2.20	0.76
1:F:182:ARG:HG3	1:F:183:THR:H	1.50	0.76
1:F:259:LEU:HD22	1:F:259:LEU:H	1.50	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:336:VAL:HG23	1:A:337:GLN:HA	0.80	0.76
1:F:208:LEU:O	1:F:210:PRO:HD3	1.85	0.76
1:C:304:ARG:HD3	1:C:306:PHE:CZ	2.21	0.76
1:F:341:MET:HE1	1:F:347:GLN:HB2	1.68	0.76
1:A:257:ASN:ND2	1:B:238:ARG:HA	2.00	0.76
1:A:170:GLU:HB2	1:A:171:PRO:HD2	1.67	0.76
1:A:87:GLU:HA	1:A:184:LYS:NZ	1.99	0.76
1:B:117:LEU:HD12	1:B:117:LEU:N	2.00	0.76
1:B:194:LYS:HG3	1:B:195:THR:H	1.50	0.76
1:D:62:THR:OG1	1:D:63:PRO:HD3	1.86	0.76
1:E:255:PHE:O	1:E:256:THR:HB	1.86	0.76
1:A:233:LYS:HG3	1:A:234:ASN:N	2.01	0.76
1:E:186:LYS:HE2	1:E:186:LYS:N	2.01	0.76
1:C:175:GLN:HE21	1:C:176:GLY:H	1.34	0.75
1:B:192:THR:HB	1:B:194:LYS:CG	2.15	0.75
1:C:256:THR:HA	1:D:239:TYR:HE1	1.51	0.75
1:E:233:LYS:HD2	1:E:234:ASN:N	2.01	0.75
1:C:125:VAL:HB	1:C:263:LEU:HD11	1.69	0.75
1:C:197:THR:O	1:C:199:LYS:HE3	1.86	0.75
1:C:175:GLN:OE1	1:C:208:LEU:HD11	1.86	0.75
1:D:164:VAL:CG2	1:D:241:GLY:HA3	2.17	0.75
1:D:143:LYS:HA	1:D:292:ARG:HG2	1.67	0.75
1:F:122:ALA:HA	1:F:310:LEU:HB3	1.68	0.75
1:E:177:LEU:CD2	1:E:206:GLN:O	2.32	0.75
1:F:150:THR:O	1:F:150:THR:HG22	1.85	0.75
1:C:175:GLN:HB2	1:C:230:ASP:HB2	1.68	0.75
1:F:238:ARG:NH2	1:F:265:ASP:HB3	2.01	0.75
1:A:328:LEU:HD21	1:A:333:LEU:HD21	0.76	0.75
1:C:181:ALA:H	1:C:206:GLN:NE2	1.85	0.75
1:C:257:ASN:HD22	1:C:257:ASN:H	1.32	0.75
1:E:243:TYR:CZ	1:E:245:GLY:HA2	2.22	0.75
1:B:192:THR:HG22	1:B:193:ILE:CD1	2.16	0.74
1:C:336:VAL:C	1:C:337:GLN:HA	2.07	0.74
1:D:211:ILE:HD12	1:D:211:ILE:N	2.01	0.74
1:A:313:ARG:HD3	1:E:23:ALA:HB2	1.68	0.74
1:F:130:VAL:HG23	1:F:303:PRO:HG2	1.68	0.74
1:B:198:LYS:CE	1:B:198:LYS:H	2.01	0.74
1:B:25:VAL:HG21	1:F:360:VAL:HG13	1.69	0.74
1:C:257:ASN:HD21	1:D:239:TYR:H	1.35	0.74
1:C:103:LEU:HB2	1:C:278:LEU:HB3	1.68	0.74
1:F:108:LEU:HB3	1:F:118:GLN:HE21	1.52	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:269:VAL:HG12	1:F:270:GLY:O	1.87	0.74
1:B:259:LEU:N	1:B:259:LEU:HD22	2.02	0.74
1:B:104:GLN:HE22	1:B:276:GLU:HB2	1.52	0.74
1:A:71:GLN:HG3	1:B:203:ASN:CB	2.16	0.74
1:A:336:VAL:CG2	1:A:337:GLN:H	2.00	0.74
1:A:71:GLN:CG	1:B:203:ASN:HB3	2.16	0.74
1:F:125:VAL:CG1	1:F:263:LEU:HD21	2.18	0.74
1:D:164:VAL:HG22	1:D:241:GLY:HA3	1.69	0.74
1:A:84:SER:HB3	1:A:86:THR:CG2	2.17	0.73
1:A:298:HIS:H	1:A:298:HIS:CD2	2.03	0.73
1:F:321:MET:O	1:F:324:LEU:HG	1.89	0.73
1:A:175:GLN:HG2	1:A:212:SER:O	1.89	0.73
1:A:50:GLU:HG2	1:B:233:LYS:HA	1.70	0.73
1:D:178:VAL:HG22	1:D:179:THR:N	2.02	0.73
1:D:265:ASP:H	1:D:270:GLY:H	1.36	0.73
1:F:238:ARG:HH21	1:F:265:ASP:HB3	1.54	0.73
1:B:272:LEU:HD12	1:B:272:LEU:N	2.02	0.73
1:C:138:VAL:HB	1:C:153:ILE:CG2	2.19	0.73
1:E:335:GLN:HA	1:E:335:GLN:OE1	1.87	0.73
1:F:62:THR:OG1	1:F:63:PRO:HD3	1.88	0.73
1:A:278:LEU:HD22	1:A:280:LEU:CD2	2.18	0.73
1:B:162:TYR:HB3	1:B:285:ILE:HD13	1.69	0.73
1:C:28:LEU:HD23	1:C:29:LEU:N	2.03	0.73
1:E:135:LEU:HD12	1:E:157:VAL:HG21	1.71	0.73
1:C:352:ARG:NH2	1:F:233:LYS:O	2.22	0.73
1:A:257:ASN:HD22	1:B:239:TYR:H	1.34	0.72
1:A:175:GLN:CB	1:A:230:ASP:HB2	2.19	0.72
1:A:306:PHE:HB3	1:A:308:ILE:HD11	1.71	0.72
1:D:141:PHE:CE1	1:D:292:ARG:HG3	2.24	0.72
1:E:313:ARG:CG	1:E:313:ARG:HH11	2.02	0.72
1:A:192:THR:HB	1:A:194:LYS:HE2	1.70	0.72
1:B:75:TRP:NE1	1:B:300:ARG:HB2	2.03	0.72
1:C:50:GLU:OE2	1:D:233:LYS:HA	1.90	0.72
1:E:209:ASN:OD1	1:E:211:ILE:HD13	1.90	0.72
1:F:163:HIS:HA	1:F:283:VAL:O	1.88	0.72
1:A:57:MET:SD	1:A:301:GLY:HA3	2.29	0.72
1:A:304:ARG:HD3	1:A:306:PHE:CZ	2.25	0.71
1:A:328:LEU:HD11	1:A:332:MET:CE	2.19	0.71
1:E:121:GLU:HG3	1:E:313:ARG:CD	2.20	0.71
1:E:144:PRO:HD3	1:E:292:ARG:HD3	1.71	0.71
1:B:125:VAL:HG12	1:B:263:LEU:HD21	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:228:HIS:HB3	1:E:229:PRO:HD2	1.72	0.71
1:F:288:TRP:HE3	1:F:299:TRP:HB3	1.55	0.71
1:B:50:GLU:HG2	1:C:233:LYS:HA	1.72	0.71
1:C:141:PHE:CE1	1:C:292:ARG:HG3	2.25	0.71
1:D:72:TYR:HE2	1:D:77:ARG:HH21	1.38	0.71
1:F:161:GLN:HE22	1:F:251:PRO:CA	2.03	0.71
1:A:240:PHE:CD1	1:A:240:PHE:N	2.57	0.71
1:D:240:PHE:CD1	1:D:240:PHE:N	2.57	0.71
1:E:177:LEU:HD23	1:E:178:VAL:N	2.05	0.71
1:B:265:ASP:H	1:B:270:GLY:H	1.37	0.71
1:A:327:SER:O	1:A:329:PHE:N	2.24	0.71
1:A:62:THR:OG1	1:A:63:PRO:HD3	1.89	0.71
1:B:30:ILE:HG12	1:B:31:LYS:N	2.06	0.71
1:C:55:PRO:HD3	1:C:303:PRO:CA	2.21	0.71
1:B:217:ASP:O	1:F:336:VAL:HG13	1.91	0.71
1:A:308:ILE:HD12	1:A:308:ILE:N	2.05	0.71
1:E:240:PHE:N	1:E:240:PHE:CD1	2.59	0.71
1:B:161:GLN:HE22	1:B:251:PRO:HA	1.56	0.70
1:B:342:GLU:HG2	1:B:343:GLY:N	2.06	0.70
1:A:265:ASP:H	1:A:270:GLY:H	1.37	0.70
1:E:317:ASN:HD22	1:E:318:PRO:HD2	1.54	0.70
1:F:287:GLY:O	1:F:299:TRP:HB2	1.91	0.70
1:B:141:PHE:CE1	1:B:292:ARG:HG3	2.27	0.70
1:B:222:TYR:HB3	1:B:227:TRP:CD1	2.26	0.70
1:C:108:LEU:HD11	1:C:120:TRP:CE2	2.27	0.70
1:F:209:ASN:ND2	1:F:211:ILE:HB	2.06	0.70
1:B:256:THR:HG23	1:B:258:THR:H	1.56	0.70
1:C:53:LEU:HD21	1:C:306:PHE:CE1	2.26	0.70
1:D:209:ASN:OD1	1:D:211:ILE:HD13	1.92	0.70
1:D:100:MET:HG3	1:D:219:ASP:HB2	1.73	0.70
1:A:39:LEU:HD12	1:A:40:VAL:H	1.56	0.70
1:F:83:THR:HB	1:F:87:GLU:HB3	1.73	0.70
1:A:84:SER:HA	1:E:141:PHE:CD2	2.27	0.70
1:D:269:VAL:HG12	1:D:270:GLY:O	1.91	0.70
1:A:124:SER:HA	1:A:263:LEU:HG	1.73	0.69
1:B:163:HIS:HA	1:B:283:VAL:O	1.92	0.69
1:D:205:ASP:HA	1:D:209:ASN:HB2	1.74	0.69
1:D:28:LEU:HG	1:D:29:LEU:N	2.06	0.69
1:C:121:GLU:HG2	1:C:271:PRO:O	1.92	0.69
1:C:180:ASP:OD2	1:C:182:ARG:HD3	1.92	0.69
1:C:288:TRP:HA	1:C:299:TRP:HA	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:380:PHE:H	1:B:380:PHE:HD1	1.39	0.69
1:C:79:ILE:HB	1:C:297:HIS:O	1.92	0.69
1:E:88:ASP:H	1:E:184:LYS:HD3	1.57	0.69
1:E:208:LEU:O	1:E:208:LEU:HD23	1.92	0.69
1:B:324:LEU:H	1:B:324:LEU:HD22	1.57	0.69
1:C:265:ASP:HB3	1:C:270:GLY:H	1.56	0.69
1:C:55:PRO:HD3	1:C:303:PRO:HA	1.74	0.69
1:C:52:PHE:CE2	1:D:208:LEU:HD22	2.27	0.69
1:F:288:TRP:HA	1:F:299:TRP:HB3	1.73	0.69
1:E:178:VAL:HG22	1:E:179:THR:N	2.06	0.69
1:E:193:ILE:HG12	1:E:201:MET:CE	2.22	0.69
1:F:320:PRO:O	1:F:323:SER:HB3	1.92	0.69
1:A:82:ALA:HB1	1:A:87:GLU:O	1.92	0.69
1:B:192:THR:HG22	1:B:193:ILE:HD12	1.74	0.69
1:B:232:ALA:HB3	1:B:234:ASN:O	1.91	0.69
1:C:174:LEU:N	1:C:174:LEU:HD12	2.07	0.69
1:C:273:CYS:HB3	1:C:277:GLY:O	1.92	0.69
1:C:104:GLN:HE22	1:C:276:GLU:HB2	1.58	0.69
1:D:39:LEU:HD12	1:D:40:VAL:N	2.08	0.69
1:E:150:THR:O	1:E:150:THR:HG22	1.93	0.69
1:E:145:THR:HB	1:E:152:GLY:HA3	1.73	0.69
1:E:88:ASP:O	1:E:184:LYS:HB2	1.93	0.69
1:F:168:GLY:CA	1:F:237:THR:HG23	2.20	0.69
1:B:168:GLY:HA3	1:B:237:THR:HG23	1.74	0.69
1:C:191:VAL:HG21	1:C:222:TYR:CG	2.28	0.69
1:C:76:SER:HG	1:C:299:TRP:HE3	1.40	0.69
1:E:245:GLY:O	1:E:249:THR:HG21	1.93	0.69
1:E:285:ILE:N	1:E:285:ILE:HD12	2.08	0.69
1:A:298:HIS:N	1:A:298:HIS:CD2	2.61	0.69
1:C:174:LEU:HD23	1:C:227:TRP:HB3	1.73	0.69
1:C:142:ASN:C	1:C:292:ARG:HB2	2.13	0.69
1:D:208:LEU:HD23	1:D:208:LEU:O	1.93	0.69
1:A:336:VAL:CB	1:A:337:GLN:CA	2.71	0.69
1:B:105:LEU:HB2	1:B:276:GLU:O	1.92	0.69
1:C:100:MET:SD	1:C:101:ALA:N	2.66	0.69
1:C:108:LEU:HD11	1:C:120:TRP:NE1	2.08	0.69
1:D:192:THR:HG21	1:D:194:LYS:HE2	1.75	0.69
1:E:272:LEU:N	1:E:272:LEU:HD12	2.07	0.69
1:F:265:ASP:OD1	1:F:269:VAL:HB	1.93	0.69
1:F:317:ASN:ND2	1:F:318:PRO:HD2	2.08	0.69
1:A:126:LYS:HG2	1:A:260:THR:HA	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:79:ILE:HD11	1:A:298:HIS:HA	1.74	0.68
1:A:328:LEU:CG	1:A:333:LEU:CD2	2.64	0.68
1:A:328:LEU:HD23	1:A:328:LEU:C	2.13	0.68
1:D:106:PRO:HD2	1:D:120:TRP:HE1	1.58	0.68
1:A:297:HIS:HE1	1:E:145:THR:HG21	1.58	0.68
1:F:161:GLN:NE2	1:F:251:PRO:HA	2.06	0.68
1:C:209:ASN:OD1	1:C:211:ILE:HD13	1.92	0.68
1:D:112:LEU:H	1:D:112:LEU:HD12	1.57	0.68
1:E:125:VAL:HA	1:E:307:LYS:O	1.93	0.68
1:F:104:GLN:HE21	1:F:105:LEU:N	1.91	0.68
1:F:180:ASP:HB3	1:F:182:ARG:CG	2.23	0.68
1:B:177:LEU:HD21	1:B:208:LEU:CA	2.23	0.68
1:D:340:PRO:HG2	1:D:347:GLN:HG3	1.75	0.68
1:D:83:THR:O	1:D:84:SER:HB2	1.92	0.68
1:B:161:GLN:OE1	1:B:251:PRO:HA	1.94	0.68
1:E:77:ARG:O	1:E:298:HIS:HB3	1.93	0.68
1:F:185:TYR:HB2	1:F:194:LYS:HE2	1.74	0.68
1:F:19:CYS:HB3	1:F:20:PRO:HD2	1.76	0.68
1:A:204:LYS:O	1:A:209:ASN:HB2	1.94	0.68
1:B:291:THR:HB	1:B:293:ASN:HB3	1.76	0.68
1:D:108:LEU:HB3	1:D:118:GLN:HE21	1.59	0.68
1:D:251:PRO:HD2	1:E:245:GLY:HA3	1.75	0.68
1:B:25:VAL:CG2	1:F:360:VAL:HG13	2.24	0.68
1:C:115:ASP:O	1:C:317:ASN:HB2	1.94	0.68
1:D:193:ILE:N	1:D:193:ILE:HD12	2.08	0.68
1:E:105:LEU:HD12	1:E:105:LEU:N	2.09	0.68
1:A:105:LEU:HB3	1:A:120:TRP:NE1	2.08	0.68
1:A:184:LYS:HD2	1:A:184:LYS:N	2.08	0.68
1:A:50:GLU:HA	1:A:306:PHE:O	1.94	0.68
1:C:360:VAL:HG12	1:C:361:PRO:HD2	1.76	0.68
1:D:54:ASN:HD21	1:E:208:LEU:CB	2.07	0.68
1:E:71:GLN:NE2	1:E:73:TYR:HB2	2.08	0.68
1:F:308:ILE:HD12	1:F:308:ILE:H	1.57	0.68
1:C:100:MET:C	1:C:100:MET:SD	2.72	0.68
1:F:259:LEU:HD13	1:F:259:LEU:N	2.08	0.68
1:E:305:TYR:CE1	1:E:307:LYS:HB2	2.23	0.68
1:B:178:VAL:HG22	1:B:179:THR:N	2.09	0.67
1:C:105:LEU:N	1:C:105:LEU:HD12	2.09	0.67
1:C:313:ARG:HG2	1:C:314:TRP:N	2.09	0.67
1:D:149:ASN:O	1:D:151:LYS:HE2	1.92	0.67
1:D:177:LEU:HD23	1:D:178:VAL:N	2.09	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:240:PHE:N	1:F:240:PHE:CD1	2.56	0.67
1:A:369:TYR:N	1:A:369:TYR:CD1	2.62	0.67
1:A:56:ARG:NH1	1:A:56:ARG:HB2	2.09	0.67
1:B:76:SER:OG	1:B:299:TRP:CE3	2.44	0.67
1:D:185:TYR:HB2	1:D:194:LYS:HE2	1.76	0.67
1:F:178:VAL:HG22	1:F:179:THR:N	2.07	0.67
1:B:71:GLN:NE2	1:B:71:GLN:HA	1.98	0.67
1:D:193:ILE:HD11	1:D:201:MET:SD	2.34	0.67
1:A:341:MET:CE	1:A:347:GLN:HB2	2.25	0.67
1:A:52:PHE:CZ	1:B:208:LEU:HD22	2.29	0.67
1:E:194:LYS:H	1:E:194:LYS:HD2	1.60	0.67
1:A:39:LEU:HD12	1:A:40:VAL:N	2.10	0.67
1:B:257:ASN:N	1:B:257:ASN:HD22	1.84	0.67
1:B:275:GLY:O	1:B:277:GLY:N	2.28	0.67
1:C:263:LEU:O	1:C:270:GLY:HA2	1.95	0.67
1:E:117:LEU:HD13	1:E:118:GLN:N	2.10	0.67
1:A:141:PHE:CD2	1:B:84:SER:HA	2.30	0.67
1:D:76:SER:OG	1:D:299:TRP:HB2	1.94	0.67
1:D:30:ILE:CD1	1:D:36:VAL:HG13	2.25	0.67
1:E:194:LYS:HD3	1:E:195:THR:H	1.60	0.67
1:C:240:PHE:N	1:C:240:PHE:CD1	2.61	0.67
1:C:300:ARG:HH21	1:D:177:LEU:HD21	1.58	0.67
1:E:109:ASN:HD22	1:E:110:GLU:H	1.43	0.67
1:A:243:TYR:HE2	1:E:251:PRO:HB2	1.60	0.67
1:C:191:VAL:CG2	1:C:222:TYR:HA	2.24	0.67
1:D:193:ILE:CD1	1:D:201:MET:SD	2.83	0.67
1:D:285:ILE:N	1:D:285:ILE:HD12	2.10	0.67
1:E:320:PRO:HG2	1:E:323:SER:CB	2.25	0.67
1:E:90:PRO:HB3	1:E:95:LEU:HD11	1.75	0.67
1:A:328:LEU:CD2	1:A:333:LEU:CD2	2.30	0.67
1:A:69:GLY:CA	1:A:71:GLN:HE22	2.05	0.67
1:D:30:ILE:HD13	1:D:36:VAL:HG13	1.76	0.67
1:A:203:ASN:HB3	1:E:71:GLN:CG	2.11	0.66
1:E:138:VAL:HB	1:E:153:ILE:HG23	1.75	0.66
1:E:169:GLY:HA3	1:E:272:LEU:O	1.95	0.66
1:E:194:LYS:HA	1:E:197:THR:O	1.95	0.66
1:F:288:TRP:CZ3	1:F:299:TRP:CD2	2.82	0.66
1:B:124:SER:HA	1:B:261:THR:O	1.95	0.66
1:B:269:VAL:HA	1:B:313:ARG:NH2	2.11	0.66
1:B:30:ILE:CD1	1:B:36:VAL:HG13	2.23	0.66
1:B:71:GLN:HG3	1:C:203:ASN:CB	2.23	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:318:PRO:HG2	1:D:319:TYR:CD2	2.30	0.66
1:B:105:LEU:HB3	1:B:120:TRP:CD1	2.31	0.66
1:C:341:MET:CE	1:C:347:GLN:HB2	2.25	0.66
1:E:109:ASN:OD1	1:E:117:LEU:HA	1.96	0.66
1:E:191:VAL:HG23	1:E:221:MET:HG3	1.77	0.66
1:B:265:ASP:HB3	1:B:270:GLY:H	1.60	0.66
1:C:316:LYS:NZ	1:F:359:PRO:HD2	2.10	0.66
1:F:81:LEU:HG	1:F:82:ALA:N	2.10	0.66
1:A:35:GLU:HG2	1:A:36:VAL:N	2.11	0.66
1:C:105:LEU:HB3	1:C:120:TRP:CD1	2.29	0.66
1:C:286:MET:HE3	1:C:286:MET:HA	1.76	0.66
1:B:192:THR:HG23	1:B:226:ILE:HD13	1.77	0.66
1:B:161:GLN:NE2	1:B:251:PRO:HA	2.11	0.66
1:B:341:MET:C	1:B:346:THR:HG23	2.16	0.66
1:D:192:THR:H	1:D:195:THR:CB	2.08	0.66
1:E:180:ASP:OD1	1:E:182:ARG:HG2	1.95	0.66
1:B:161:GLN:HE22	1:B:251:PRO:CA	2.08	0.66
1:C:82:ALA:HB1	1:C:88:ASP:HA	1.76	0.66
1:D:132:SER:O	1:D:135:LEU:HD23	1.96	0.66
1:F:150:THR:CG2	1:F:292:ARG:HH21	2.09	0.66
1:A:264:LEU:HD23	1:A:268:GLY:HA2	1.78	0.66
1:A:37:LEU:HD23	1:A:106:PRO:HD3	1.78	0.66
1:B:318:PRO:HG2	1:B:319:TYR:H	1.60	0.66
1:C:112:LEU:H	1:C:112:LEU:HD22	1.61	0.66
1:E:66:LEU:HD23	1:E:66:LEU:H	1.58	0.66
1:F:75:TRP:NE1	1:F:300:ARG:HB2	2.11	0.66
1:A:340:PRO:HG2	1:A:347:GLN:NE2	2.09	0.66
1:A:350:GLU:CG	1:A:351:VAL:N	2.58	0.66
1:B:164:VAL:HA	1:B:241:GLY:HA3	1.78	0.66
1:B:263:LEU:O	1:B:270:GLY:HA2	1.96	0.66
1:B:286:MET:HE3	1:B:286:MET:HA	1.76	0.66
1:A:217:ASP:OD1	1:A:218:LYS:HD3	1.96	0.66
1:A:97:THR:HA	1:A:223:PRO:HA	1.76	0.66
1:E:367:THR:HG22	1:E:368:ARG:N	2.09	0.66
1:F:92:ASN:OD1	1:F:186:LYS:HD2	1.96	0.66
1:A:57:MET:HB2	1:A:96:PRO:HB3	1.78	0.65
1:C:54:ASN:HD21	1:D:208:LEU:HB3	1.61	0.65
1:D:72:TYR:HE2	1:D:77:ARG:NH2	1.94	0.65
1:E:378:THR:HG22	1:E:379:VAL:O	1.94	0.65
1:F:30:ILE:HG23	1:F:36:VAL:HG13	1.78	0.65
1:A:79:ILE:HG13	1:A:297:HIS:HB2	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:172:LEU:HD22	1:C:173:ASP:H	1.61	0.65
1:E:118:GLN:HB2	1:E:314:TRP:CZ3	2.30	0.65
1:E:28:LEU:HG	1:E:29:LEU:N	2.09	0.65
1:A:208:LEU:N	1:E:54:ASN:HD21	1.89	0.65
1:F:103:LEU:HB2	1:F:278:LEU:HB3	1.76	0.65
1:A:269:VAL:HG12	1:A:270:GLY:O	1.97	0.65
1:B:177:LEU:CD2	1:B:208:LEU:HA	2.24	0.65
1:B:275:GLY:C	1:B:277:GLY:H	1.99	0.65
1:B:273:CYS:HB3	1:B:277:GLY:O	1.96	0.65
1:E:112:LEU:O	1:E:116:THR:HG22	1.96	0.65
1:E:218:LYS:N	1:E:218:LYS:HD2	2.10	0.65
1:F:341:MET:CE	1:F:347:GLN:HB2	2.26	0.65
1:A:328:LEU:HD21	1:A:333:LEU:CD1	2.27	0.65
1:A:371:ASP:O	1:A:373:PHE:N	2.29	0.65
1:B:83:THR:HB	1:B:87:GLU:HB3	1.79	0.65
1:F:108:LEU:HD11	1:F:120:TRP:CZ2	2.32	0.65
1:A:175:GLN:HB3	1:A:230:ASP:HB2	1.78	0.65
1:A:30:ILE:HG12	1:A:36:VAL:HG13	1.79	0.65
1:D:172:LEU:HD22	1:D:173:ASP:N	2.10	0.65
1:E:82:ALA:CB	1:E:88:ASP:HA	2.26	0.65
1:F:177:LEU:CD2	1:F:208:LEU:HA	2.25	0.65
1:F:324:LEU:HD12	1:F:325:ILE:N	2.11	0.65
1:B:84:SER:O	1:B:86:THR:N	2.29	0.65
1:D:105:LEU:HB2	1:D:276:GLU:O	1.96	0.65
1:D:105:LEU:HD23	1:D:120:TRP:CG	2.32	0.65
1:F:177:LEU:HD22	1:F:205:ASP:O	1.97	0.65
1:A:135:LEU:N	1:A:135:LEU:CD1	2.58	0.65
1:A:88:ASP:H	1:A:184:LYS:HD3	1.62	0.65
1:A:239:TYR:CE1	1:E:257:ASN:HB2	2.31	0.65
1:D:216:LEU:O	1:D:218:LYS:N	2.29	0.65
1:F:318:PRO:HG2	1:F:319:TYR:CD2	2.32	0.65
1:F:72:TYR:O	1:F:75:TRP:HB2	1.97	0.65
1:A:108:LEU:HD11	1:A:120:TRP:CE2	2.31	0.65
1:A:369:TYR:N	1:A:369:TYR:HD1	1.94	0.65
1:C:126:LYS:HG3	1:C:260:THR:CG2	2.27	0.65
1:F:19:CYS:HB3	1:F:20:PRO:CD	2.27	0.65
1:F:233:LYS:HD3	1:F:234:ASN:N	2.12	0.65
1:B:209:ASN:OD1	1:B:211:ILE:HD13	1.98	0.64
1:B:255:PHE:O	1:B:256:THR:HB	1.95	0.64
1:B:308:ILE:H	1:B:308:ILE:HD12	1.61	0.64
1:C:193:ILE:HG12	1:C:201:MET:CE	2.27	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:175:GLN:HG2	1:E:212:SER:O	1.97	0.64
1:E:191:VAL:HA	1:E:195:THR:HG21	1.80	0.64
2:L:2:GAL:H3	2:L:3:SIA:O1B	1.96	0.64
1:A:194:LYS:HD3	1:A:195:THR:H	1.62	0.64
1:B:192:THR:HG23	1:B:226:ILE:CD1	2.27	0.64
1:B:371:ASP:C	1:B:373:PHE:H	1.99	0.64
1:D:32:GLY:HA3	1:D:36:VAL:CG2	2.27	0.64
1:F:288:TRP:HA	1:F:299:TRP:CB	2.27	0.64
1:F:90:PRO:HD2	1:F:184:LYS:O	1.97	0.64
1:B:278:LEU:HD23	1:B:279:TYR:N	2.12	0.64
1:B:193:ILE:HG12	1:B:201:MET:HE3	1.80	0.64
1:B:194:LYS:HG3	1:B:195:THR:N	2.13	0.64
1:C:135:LEU:N	1:C:135:LEU:HD22	2.13	0.64
1:D:111:ASP:HB3	1:D:116:THR:HG23	1.78	0.64
1:D:327:SER:OG	1:D:328:LEU:N	2.30	0.64
1:A:174:LEU:HD13	1:A:227:TRP:HB3	1.80	0.64
1:A:231:PRO:HB2	1:E:305:TYR:CE2	2.33	0.64
1:C:233:LYS:HE2	1:F:352:ARG:NH1	2.13	0.64
1:E:317:ASN:ND2	1:E:318:PRO:HD2	2.12	0.64
1:F:306:PHE:N	1:F:306:PHE:CD1	2.63	0.64
1:A:117:LEU:HD22	1:A:317:ASN:HA	1.79	0.64
1:B:193:ILE:HG22	1:B:212:SER:HB3	1.80	0.64
1:D:322:ALA:O	1:D:325:ILE:HB	1.98	0.64
1:E:164:VAL:HA	1:E:241:GLY:HA3	1.80	0.64
1:E:304:ARG:HD3	1:E:306:PHE:CZ	2.33	0.64
1:A:319:TYR:N	1:A:320:PRO:HD2	2.12	0.64
1:B:211:ILE:N	1:B:211:ILE:HD12	2.13	0.64
1:B:76:SER:HG	1:B:299:TRP:HE3	1.40	0.64
1:F:108:LEU:HD11	1:F:120:TRP:CE2	2.33	0.64
1:F:218:LYS:HB2	1:F:222:TYR:CE1	2.33	0.64
1:B:29:LEU:HB3	1:B:30:ILE:HG22	1.80	0.64
1:C:211:ILE:N	1:C:211:ILE:HD12	2.12	0.64
1:D:97:THR:HA	1:D:223:PRO:HA	1.80	0.64
1:A:233:LYS:HG3	1:A:234:ASN:H	1.61	0.64
1:B:180:ASP:HB3	1:B:182:ARG:HG2	1.79	0.64
1:B:104:GLN:NE2	1:B:276:GLU:HB2	2.13	0.64
1:D:292:ARG:NH1	1:D:292:ARG:HB3	2.13	0.64
1:D:75:TRP:CE2	1:D:300:ARG:HD2	2.33	0.64
1:E:317:ASN:HD21	1:E:319:TYR:HB2	1.63	0.64
1:A:197:THR:O	1:A:198:LYS:HG2	1.99	0.63
1:B:240:PHE:N	1:B:240:PHE:CD1	2.65	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:84:SER:O	1:C:86:THR:N	2.31	0.63
1:C:194:LYS:O	1:C:198:LYS:N	2.30	0.63
1:C:71:GLN:HA	1:C:71:GLN:NE2	2.00	0.63
1:C:79:ILE:HD13	1:C:94:THR:HG23	1.79	0.63
1:F:111:ASP:HB3	1:F:116:THR:CG2	2.29	0.63
1:F:150:THR:HG21	1:F:292:ARG:NH2	2.13	0.63
1:A:232:ALA:HB3	1:A:234:ASN:O	1.97	0.63
1:B:54:ASN:HD21	1:C:207:VAL:HB	1.62	0.63
1:A:380:PHE:CG	1:A:381:PRO:HD2	2.33	0.63
1:A:82:ALA:HB1	1:A:88:ASP:HA	1.81	0.63
1:D:233:LYS:HG3	1:D:234:ASN:HD22	1.64	0.63
1:F:135:LEU:HD22	1:F:135:LEU:H	1.64	0.63
1:F:125:VAL:HG11	1:F:263:LEU:HD21	1.79	0.63
1:A:197:THR:C	1:A:198:LYS:HG2	2.19	0.63
1:B:23:ALA:O	1:F:359:PRO:HA	1.98	0.63
1:C:256:THR:HB	1:D:240:PHE:HA	1.80	0.63
1:D:341:MET:SD	1:D:348:VAL:HG23	2.39	0.63
1:D:35:GLU:HG2	1:D:36:VAL:N	2.13	0.63
1:F:112:LEU:HD12	1:F:112:LEU:N	2.14	0.63
1:F:177:LEU:CD1	1:F:207:VAL:O	2.47	0.63
1:C:153:ILE:HD11	1:D:297:HIS:CG	2.34	0.63
1:C:71:GLN:HE21	1:C:73:TYR:H	1.44	0.63
1:D:103:LEU:N	1:D:103:LEU:HD22	2.13	0.63
1:D:97:THR:HG22	1:D:222:TYR:C	2.18	0.63
1:F:272:LEU:HD12	1:F:272:LEU:N	2.13	0.63
1:F:288:TRP:CZ3	1:F:299:TRP:CE2	2.83	0.63
1:A:174:LEU:CD1	1:A:227:TRP:HB3	2.28	0.63
1:D:32:GLY:HA3	1:D:36:VAL:HG21	1.80	0.63
1:F:79:ILE:HD13	1:F:94:THR:HG23	1.81	0.63
1:C:141:PHE:CD1	1:C:292:ARG:HG3	2.34	0.63
1:E:150:THR:CG2	1:E:292:ARG:HH21	2.12	0.63
1:F:269:VAL:HA	1:F:313:ARG:HH21	1.64	0.63
1:F:62:THR:O	1:F:64:GLU:N	2.31	0.63
1:C:39:LEU:HD12	1:C:40:VAL:H	1.63	0.63
1:D:257:ASN:HD22	1:E:239:TYR:H	1.44	0.63
1:E:192:THR:HG22	1:E:193:ILE:HD12	1.80	0.63
1:E:166:ALA:HA	1:E:238:ARG:O	1.98	0.63
1:F:228:HIS:HB3	1:F:229:PRO:HD2	1.79	0.63
1:A:34:MET:O	1:A:37:LEU:HD13	1.99	0.62
1:A:79:ILE:HA	1:A:94:THR:HG23	1.81	0.62
1:B:46:VAL:O	1:F:353:VAL:HA	1.98	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:79:ILE:HD11	1:B:298:HIS:CA	2.26	0.62
1:C:352:ARG:HG3	1:C:354:TYR:HE1	1.63	0.62
1:E:318:PRO:HG2	1:E:319:TYR:CD2	2.35	0.62
1:A:178:VAL:HG22	1:A:179:THR:N	2.14	0.62
1:B:285:ILE:HD12	1:B:285:ILE:N	2.14	0.62
1:B:324:LEU:O	1:B:328:LEU:HD23	1.98	0.62
1:D:45:SER:OG	1:D:312:LYS:HD2	1.98	0.62
1:F:222:TYR:HB3	1:F:227:TRP:CD1	2.34	0.62
1:F:57:MET:SD	1:F:301:GLY:HA3	2.39	0.62
1:B:177:LEU:HD22	1:B:207:VAL:C	2.20	0.62
1:B:48:GLU:O	1:F:351:VAL:HA	1.99	0.62
1:D:55:PRO:HD3	1:D:303:PRO:CA	2.29	0.62
1:E:192:THR:HB	1:E:194:LYS:HD3	1.82	0.62
1:E:370:VAL:HG22	1:E:375:LYS:HA	1.81	0.62
1:B:257:ASN:ND2	1:C:239:TYR:O	2.33	0.62
1:D:66:LEU:HD23	1:D:66:LEU:N	2.14	0.62
1:E:192:THR:O	1:E:195:THR:HB	2.00	0.62
1:E:232:ALA:O	1:E:234:ASN:N	2.31	0.62
1:A:257:ASN:HB2	1:B:239:TYR:CE2	2.35	0.62
1:B:262:VAL:CG1	1:B:264:LEU:HB2	2.29	0.62
1:B:346:THR:HG21	1:B:348:VAL:CG1	2.27	0.62
1:C:342:GLU:N	1:C:346:THR:HG23	2.14	0.62
1:C:50:GLU:OE1	1:D:233:LYS:HA	1.99	0.62
1:D:278:LEU:HD23	1:D:279:TYR:N	2.15	0.62
1:E:243:TYR:OH	1:E:245:GLY:HA2	2.00	0.62
1:F:264:LEU:HD23	1:F:268:GLY:HA2	1.81	0.62
1:D:181:ALA:HA	1:D:201:MET:HE2	1.82	0.62
1:A:164:VAL:HG23	1:A:283:VAL:HG23	1.82	0.62
1:B:261:THR:HG22	1:B:262:VAL:N	2.14	0.62
1:B:28:LEU:HD12	1:F:353:VAL:O	2.00	0.62
1:E:233:LYS:HD3	1:E:234:ASN:HD22	1.62	0.62
1:F:174:LEU:HD12	1:F:174:LEU:N	2.14	0.62
1:F:208:LEU:HD23	1:F:208:LEU:O	2.00	0.62
1:A:286:MET:HA	1:A:286:MET:HE3	1.82	0.62
1:A:118:GLN:HB2	1:A:314:TRP:CZ3	2.34	0.62
1:B:172:LEU:HD22	1:B:173:ASP:N	2.15	0.62
1:B:165:PHE:CZ	1:B:240:PHE:CE1	2.87	0.62
1:B:243:TYR:CZ	1:B:245:GLY:HA2	2.35	0.62
1:D:71:GLN:HE21	1:D:73:TYR:HB2	1.64	0.62
1:B:262:VAL:HG12	1:B:264:LEU:HB2	1.81	0.62
1:C:192:THR:HG21	1:C:194:LYS:HE2	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:46:VAL:HG12	1:E:47:THR:N	2.14	0.62
1:F:233:LYS:HD3	1:F:234:ASN:H	1.65	0.62
1:A:57:MET:SD	1:A:301:GLY:CA	2.88	0.61
1:D:335:GLN:NE2	1:D:335:GLN:HA	2.14	0.61
1:E:305:TYR:CD1	1:E:306:PHE:N	2.68	0.61
1:F:142:ASN:N	1:F:292:ARG:HB2	2.15	0.61
1:B:56:ARG:NH2	1:F:339:GLN:HG3	2.14	0.61
1:E:78:GLY:HA3	2:K:2:GAL:O4	2.01	0.61
1:A:288:TRP:HB3	1:A:297:HIS:O	2.00	0.61
1:A:86:THR:HG23	1:A:87:GLU:N	2.15	0.61
1:B:341:MET:HE3	1:B:346:THR:HG22	1.81	0.61
1:C:152:GLY:HA2	1:D:295:ASP:HB3	1.82	0.61
1:D:177:LEU:HD23	1:D:177:LEU:C	2.19	0.61
1:E:180:ASP:HA	1:E:206:GLN:HE21	1.65	0.61
1:B:29:LEU:HB2	1:F:353:VAL:HG23	1.81	0.61
1:A:257:ASN:HD22	1:B:239:TYR:N	1.99	0.61
1:B:380:PHE:CD1	1:B:380:PHE:N	2.68	0.61
1:C:228:HIS:HB3	1:C:229:PRO:HD2	1.81	0.61
1:C:57:MET:HB3	1:C:96:PRO:HB3	1.82	0.61
1:E:177:LEU:HD23	1:E:178:VAL:H	1.65	0.61
1:A:222:TYR:HB3	1:A:227:TRP:CD1	2.35	0.61
1:A:297:HIS:CE1	1:E:145:THR:HG21	2.35	0.61
1:B:164:VAL:HG12	1:B:165:PHE:N	2.15	0.61
1:B:177:LEU:HD22	1:B:208:LEU:N	2.16	0.61
1:C:269:VAL:HG12	1:C:270:GLY:O	2.01	0.61
1:E:320:PRO:HG2	1:E:323:SER:HB3	1.82	0.61
1:A:104:GLN:HE22	1:A:276:GLU:HB2	1.65	0.61
1:C:105:LEU:HB3	1:C:120:TRP:NE1	2.16	0.61
1:C:335:GLN:HA	1:C:335:GLN:OE1	2.01	0.61
1:F:192:THR:H	1:F:195:THR:CB	2.12	0.61
1:A:238:ARG:NH2	1:A:265:ASP:HB3	2.15	0.61
1:B:100:MET:SD	1:B:101:ALA:N	2.73	0.61
1:C:82:ALA:HB2	1:C:88:ASP:OD1	2.00	0.61
1:E:166:ALA:HB2	1:E:239:TYR:HB3	1.82	0.61
1:A:370:VAL:HG13	1:A:374:GLY:O	2.00	0.61
1:D:288:TRP:HB3	1:D:299:TRP:HA	1.82	0.61
1:D:342:GLU:HG2	1:D:343:GLY:N	2.15	0.61
1:E:112:LEU:HB3	1:E:116:THR:CG2	2.31	0.61
1:E:253:LEU:HD23	1:E:254:GLN:N	2.12	0.61
1:F:104:GLN:NE2	1:F:105:LEU:N	2.49	0.61
1:F:243:TYR:CZ	1:F:245:GLY:CA	2.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:285:ILE:N	1:F:285:ILE:HD12	2.15	0.61
1:D:161:GLN:OE1	1:D:251:PRO:HA	2.01	0.61
1:D:192:THR:H	1:D:195:THR:HB	1.65	0.61
1:E:246:GLY:HA3	1:E:249:THR:OG1	2.01	0.61
1:E:25:VAL:HG12	1:E:26:PRO:HD2	1.83	0.61
1:E:84:SER:O	1:E:86:THR:N	2.34	0.61
1:A:352:ARG:HG3	1:A:354:TYR:HE1	1.66	0.60
1:B:122:ALA:HA	1:B:310:LEU:HB3	1.83	0.60
1:C:233:LYS:HD3	1:C:234:ASN:CB	2.31	0.60
1:C:28:LEU:HD23	1:C:30:ILE:N	2.15	0.60
1:D:191:VAL:HA	1:D:195:THR:HG21	1.83	0.60
1:E:177:LEU:CD2	1:E:178:VAL:N	2.64	0.60
1:E:66:LEU:HD23	1:E:66:LEU:N	2.16	0.60
1:E:79:ILE:O	1:E:79:ILE:HG22	2.01	0.60
1:F:177:LEU:CD2	1:F:205:ASP:O	2.49	0.60
1:B:193:ILE:HD11	1:B:201:MET:SD	2.41	0.60
1:C:153:ILE:HG22	1:C:154:SER:N	2.15	0.60
1:D:239:TYR:C	1:D:240:PHE:CD1	2.75	0.60
1:E:308:ILE:HD12	1:E:308:ILE:N	2.16	0.60
1:A:300:ARG:HH11	1:A:300:ARG:HG3	1.66	0.60
1:A:308:ILE:CG2	1:A:310:LEU:HD12	2.28	0.60
1:D:104:GLN:HE21	1:D:105:LEU:N	1.99	0.60
1:E:346:THR:HG22	1:E:348:VAL:HG23	1.82	0.60
1:F:125:VAL:HG12	1:F:263:LEU:HD21	1.82	0.60
1:B:103:LEU:CD2	1:F:341:MET:HG3	2.31	0.60
1:B:125:VAL:CG1	1:B:263:LEU:HD21	2.31	0.60
1:B:341:MET:CE	1:B:348:VAL:HB	2.31	0.60
1:D:342:GLU:HG2	1:D:343:GLY:H	1.66	0.60
1:D:55:PRO:HD3	1:D:303:PRO:HA	1.82	0.60
1:A:71:GLN:HA	1:A:71:GLN:OE1	2.02	0.60
1:B:198:LYS:H	1:B:198:LYS:HE3	1.66	0.60
1:B:258:THR:HB	1:B:259:LEU:CD2	2.31	0.60
1:C:232:ALA:C	1:C:234:ASN:N	2.55	0.60
1:F:211:ILE:N	1:F:211:ILE:HD12	2.16	0.60
1:A:25:VAL:HG13	1:A:26:PRO:HD2	1.83	0.60
1:B:50:GLU:CD	1:C:233:LYS:HB2	2.22	0.60
1:C:50:GLU:HG3	1:C:307:LYS:HG3	1.82	0.60
1:C:53:LEU:CD2	1:C:306:PHE:HE1	2.15	0.60
1:F:193:ILE:HG12	1:F:201:MET:CE	2.31	0.60
1:F:233:LYS:HE2	1:F:234:ASN:CG	2.21	0.60
1:B:111:ASP:OD2	1:B:114:CYS:SG	2.60	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:262:VAL:HG12	1:B:264:LEU:N	2.13	0.60
1:B:323:SER:O	1:B:327:SER:N	2.33	0.60
1:C:62:THR:HG1	1:C:63:PRO:HD3	1.65	0.60
1:C:82:ALA:CB	1:C:88:ASP:HA	2.31	0.60
1:F:150:THR:HG21	1:F:292:ARG:HH21	1.65	0.60
1:A:192:THR:CB	1:A:194:LYS:HE2	2.30	0.60
1:B:192:THR:O	1:B:196:ILE:HG22	2.02	0.60
1:C:174:LEU:HA	1:C:228:HIS:O	2.02	0.60
1:D:192:THR:CB	1:D:194:LYS:HD3	2.29	0.60
1:D:278:LEU:HD12	1:D:310:LEU:HD21	1.82	0.60
1:A:174:LEU:HA	1:A:230:ASP:H	1.65	0.60
1:A:228:HIS:HB3	1:A:229:PRO:HD2	1.84	0.60
1:A:339:GLN:HG3	1:A:340:PRO:HD2	1.84	0.60
1:B:25:VAL:HG12	1:B:26:PRO:HD2	1.83	0.60
1:C:313:ARG:HG2	1:C:314:TRP:H	1.65	0.60
1:C:76:SER:OG	1:C:299:TRP:HE3	1.84	0.60
1:A:328:LEU:HD21	1:A:333:LEU:HD11	1.84	0.60
1:B:121:GLU:HG2	1:B:271:PRO:O	2.01	0.60
1:B:339:GLN:NE2	1:B:347:GLN:NE2	2.50	0.60
1:C:67:THR:OG1	1:C:68:GLU:HG3	2.01	0.60
1:C:69:GLY:O	1:C:71:GLN:N	2.35	0.60
1:E:136:LEU:O	1:E:138:VAL:HG22	2.02	0.60
1:E:192:THR:HG22	1:E:193:ILE:CD1	2.32	0.60
1:E:217:ASP:C	1:E:218:LYS:HD2	2.22	0.60
1:E:298:HIS:N	1:E:298:HIS:CD2	2.70	0.60
1:A:75:TRP:NE1	1:A:300:ARG:HB2	2.17	0.59
1:C:285:ILE:N	1:C:285:ILE:HD12	2.16	0.59
1:D:265:ASP:CG	1:D:269:VAL:HB	2.22	0.59
1:D:308:ILE:N	1:D:308:ILE:HD12	2.17	0.59
1:D:317:ASN:HD22	1:D:318:PRO:HD2	1.67	0.59
1:A:192:THR:HB	1:A:194:LYS:HD3	1.83	0.59
1:A:233:LYS:HA	1:E:50:GLU:CG	2.32	0.59
1:C:175:GLN:HG2	1:C:213:LYS:HG2	1.83	0.59
1:D:30:ILE:HG21	1:D:39:LEU:HD23	1.84	0.59
1:F:259:LEU:HD22	1:F:259:LEU:N	2.16	0.59
1:A:175:GLN:HB2	1:A:213:LYS:HD3	1.83	0.59
1:A:164:VAL:HG13	1:A:241:GLY:HA3	1.84	0.59
1:A:285:ILE:N	1:A:285:ILE:HD12	2.17	0.59
1:C:304:ARG:HG2	1:C:306:PHE:CE1	2.37	0.59
1:C:233:LYS:CE	1:F:350:GLU:HG2	2.32	0.59
1:B:175:GLN:HE21	1:B:176:GLY:N	2.00	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:236:ASN:OD1	1:C:272:LEU:HD12	2.02	0.59
1:C:286:MET:CE	1:C:286:MET:HA	2.32	0.59
1:C:77:ARG:HB2	1:C:93:ASN:HB2	1.84	0.59
1:D:232:ALA:HB3	1:D:235:GLU:OE1	2.02	0.59
1:E:333:LEU:HD22	1:E:333:LEU:H	1.67	0.59
1:A:86:THR:HG23	1:A:87:GLU:H	1.67	0.59
1:B:145:THR:HB	1:B:152:GLY:HA3	1.85	0.59
1:C:186:LYS:H	1:C:186:LYS:CD	2.15	0.59
1:C:341:MET:HE2	1:C:347:GLN:HB2	1.83	0.59
1:F:19:CYS:CB	1:F:20:PRO:HD2	2.32	0.59
1:F:293:ASN:OD1	1:F:294:TYR:HB2	2.02	0.59
1:A:176:GLY:C	1:A:177:LEU:HD23	2.23	0.59
1:E:342:GLU:H	1:E:346:THR:HG23	1.66	0.59
1:A:164:VAL:HA	1:A:241:GLY:HA3	1.84	0.59
1:B:233:LYS:HG2	1:B:234:ASN:H	1.65	0.59
1:B:370:VAL:HA	1:B:375:LYS:HA	1.84	0.59
1:C:233:LYS:HG2	1:F:350:GLU:HB2	1.84	0.59
1:B:175:GLN:CB	1:B:230:ASP:HB2	2.22	0.59
1:B:288:TRP:CZ3	1:B:299:TRP:CD1	2.90	0.59
1:D:142:ASN:ND2	1:D:289:ARG:HG3	2.17	0.59
1:D:144:PRO:HA	1:D:153:ILE:O	2.03	0.59
1:D:179:THR:O	1:D:206:GLN:HG3	2.03	0.59
1:E:264:LEU:HD12	1:E:270:GLY:HA3	1.83	0.59
1:F:263:LEU:O	1:F:270:GLY:HA2	2.02	0.59
1:F:71:GLN:HA	1:F:71:GLN:NE2	2.09	0.59
1:B:207:VAL:HG23	1:B:208:LEU:N	2.18	0.59
1:B:25:VAL:HG21	1:F:360:VAL:HA	1.84	0.59
1:D:191:VAL:HG21	1:D:222:TYR:CE1	2.37	0.59
1:E:177:LEU:HD23	1:E:205:ASP:O	2.02	0.59
1:E:122:ALA:HA	1:E:310:LEU:HB3	1.85	0.59
1:B:75:TRP:CZ2	1:B:300:ARG:HD2	2.38	0.59
1:B:313:ARG:HG2	1:B:314:TRP:N	2.17	0.59
1:B:328:LEU:O	1:B:330:ASN:N	2.36	0.59
1:C:123:VAL:HG13	1:C:264:LEU:HD13	1.84	0.59
1:D:141:PHE:CD1	1:D:292:ARG:HG3	2.38	0.59
1:F:181:ALA:HB1	1:F:201:MET:HB3	1.84	0.59
1:A:272:LEU:N	1:A:272:LEU:HD12	2.18	0.58
1:D:72:TYR:O	1:D:75:TRP:HB2	2.02	0.58
1:E:335:GLN:OE1	1:E:336:VAL:HG22	2.03	0.58
1:E:366:MET:HG2	1:E:367:THR:N	2.18	0.58
1:A:192:THR:HB	1:A:194:LYS:CD	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:198:LYS:H	1:A:198:LYS:HE2	1.66	0.58
1:A:265:ASP:CG	1:A:269:VAL:HB	2.23	0.58
1:B:166:ALA:HB2	1:B:239:TYR:HB3	1.86	0.58
1:C:117:LEU:HD13	1:C:118:GLN:N	2.18	0.58
1:C:300:ARG:HH11	1:C:300:ARG:HG3	1.66	0.58
1:E:54:ASN:HD22	1:E:303:PRO:HB3	1.68	0.58
1:B:360:VAL:HG12	1:B:361:PRO:HD2	1.85	0.58
1:C:142:ASN:ND2	1:C:289:ARG:HG3	2.16	0.58
1:D:72:TYR:CE2	1:D:77:ARG:NH2	2.71	0.58
1:F:196:ILE:O	1:F:196:ILE:HD12	2.03	0.58
1:B:211:ILE:O	1:B:213:LYS:N	2.37	0.58
1:F:218:LYS:O	1:F:219:ASP:HB2	2.03	0.58
1:F:97:THR:HG22	1:F:222:TYR:C	2.24	0.58
1:A:271:PRO:C	1:A:272:LEU:HD12	2.24	0.58
1:C:265:ASP:CG	1:C:269:VAL:HB	2.23	0.58
1:D:203:ASN:O	1:D:206:GLN:HB3	2.03	0.58
1:D:133:GLY:CA	1:E:228:HIS:HE1	2.17	0.58
1:F:184:LYS:N	1:F:184:LYS:HD2	2.18	0.58
1:B:379:VAL:HG12	1:B:380:PHE:O	2.03	0.58
1:D:83:THR:HB	1:D:87:GLU:HB3	1.86	0.58
1:F:108:LEU:HB3	1:F:118:GLN:NE2	2.18	0.58
1:A:246:GLY:HA3	1:A:249:THR:OG1	2.03	0.58
1:B:170:GLU:HB2	1:B:171:PRO:HD2	1.85	0.58
1:B:205:ASP:HA	1:B:209:ASN:HB2	1.86	0.58
1:B:165:PHE:CE1	1:B:240:PHE:HE1	2.22	0.58
1:C:30:ILE:HD13	1:C:36:VAL:HG13	1.85	0.58
1:D:178:VAL:CG2	1:D:179:THR:N	2.66	0.58
1:D:90:PRO:HB3	1:D:95:LEU:HD11	1.86	0.58
1:E:113:THR:C	1:E:115:ASP:H	2.07	0.58
1:A:87:GLU:HA	1:A:184:LYS:HZ1	1.65	0.58
1:B:62:THR:OG1	1:B:63:PRO:HD3	2.03	0.58
1:C:116:THR:HG23	1:C:314:TRP:CE3	2.38	0.58
1:D:175:GLN:CG	1:D:213:LYS:HG2	2.33	0.58
1:D:337:GLN:HA	1:D:337:GLN:OE1	2.02	0.58
1:E:135:LEU:H	1:E:135:LEU:HD22	1.68	0.58
1:E:181:ALA:H	1:E:206:GLN:NE2	2.02	0.58
1:E:354:TYR:N	1:E:354:TYR:CD1	2.70	0.58
1:A:192:THR:HB	1:A:194:LYS:CE	2.34	0.58
1:F:186:LYS:H	1:F:186:LYS:HE2	1.68	0.58
1:F:192:THR:H	1:F:195:THR:HB	1.68	0.58
1:F:265:ASP:H	1:F:270:GLY:H	1.49	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:100:MET:SD	1:A:219:ASP:HB2	2.44	0.58
1:A:114:CYS:C	1:A:116:THR:H	2.08	0.58
1:A:185:TYR:CZ	1:A:226:ILE:HD11	2.39	0.58
1:B:97:THR:HG22	1:B:222:TYR:O	2.03	0.58
1:E:170:GLU:HB2	1:E:171:PRO:HD2	1.86	0.58
1:A:181:ALA:H	1:A:206:GLN:NE2	2.02	0.57
1:A:69:GLY:O	1:A:71:GLN:N	2.37	0.57
1:B:52:PHE:CE2	1:C:208:LEU:HD23	2.39	0.57
1:C:34:MET:O	1:C:37:LEU:HB2	2.04	0.57
1:D:71:GLN:HE21	1:D:73:TYR:H	1.50	0.57
1:E:109:ASN:OD1	1:E:118:GLN:N	2.37	0.57
1:F:192:THR:HG22	1:F:193:ILE:CD1	2.34	0.57
1:F:50:GLU:HA	1:F:306:PHE:O	2.04	0.57
1:A:138:VAL:O	1:A:153:ILE:HG23	2.03	0.57
1:B:46:VAL:HG12	1:B:47:THR:H	1.67	0.57
1:B:76:SER:OG	1:B:299:TRP:HE3	1.85	0.57
1:C:192:THR:HB	1:C:194:LYS:CD	2.32	0.57
1:C:232:ALA:C	1:C:234:ASN:H	2.07	0.57
1:C:321:MET:HA	1:C:324:LEU:HD12	1.85	0.57
1:D:349:GLU:C	1:D:350:GLU:HG2	2.24	0.57
1:E:90:PRO:HG2	1:E:185:TYR:HA	1.86	0.57
1:E:193:ILE:H	1:E:193:ILE:HD12	1.69	0.57
1:D:257:ASN:CB	1:E:239:TYR:CE2	2.86	0.57
1:F:125:VAL:HB	1:F:263:LEU:HD11	1.86	0.57
1:A:161:GLN:OE1	1:A:251:PRO:HA	2.03	0.57
1:A:129:VAL:HB	1:A:253:LEU:HD21	1.86	0.57
1:C:153:ILE:HD11	1:D:297:HIS:CB	2.35	0.57
1:D:98:TRP:HH2	1:D:164:VAL:CG1	2.16	0.57
1:F:30:ILE:CD1	1:F:36:VAL:HG22	2.35	0.57
1:F:336:VAL:C	1:F:337:GLN:HA	2.25	0.57
1:A:124:SER:CA	1:A:263:LEU:HG	2.35	0.57
1:A:46:VAL:HG12	1:A:47:THR:N	2.19	0.57
1:B:342:GLU:HG2	1:B:343:GLY:H	1.69	0.57
1:C:152:GLY:O	1:C:153:ILE:HD13	2.04	0.57
1:C:310:LEU:N	1:C:310:LEU:HD12	2.19	0.57
1:D:254:GLN:HA	1:D:254:GLN:OE1	2.00	0.57
1:A:298:HIS:HD2	1:A:298:HIS:H	1.53	0.57
1:B:193:ILE:CG2	1:B:212:SER:HB3	2.35	0.57
1:B:77:ARG:CB	1:B:93:ASN:HB2	2.33	0.57
1:C:111:ASP:OD2	1:C:114:CYS:HB3	2.04	0.57
1:C:142:ASN:N	1:C:154:SER:OG	2.36	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:362:GLY:O	1:C:364:PRO:HD3	2.05	0.57
1:D:313:ARG:HG2	1:D:314:TRP:N	2.20	0.57
1:E:135:LEU:N	1:E:135:LEU:HD13	2.19	0.57
1:E:233:LYS:CD	1:E:234:ASN:N	2.66	0.57
1:A:288:TRP:CZ3	1:A:299:TRP:CD1	2.93	0.57
1:C:178:VAL:HG22	1:C:179:THR:N	2.20	0.57
1:D:76:SER:HG	1:D:299:TRP:HB2	1.69	0.57
1:A:35:GLU:HG2	1:A:36:VAL:H	1.68	0.57
1:D:172:LEU:HD22	1:D:173:ASP:O	2.05	0.57
1:E:125:VAL:HG11	1:E:263:LEU:HD21	1.87	0.57
1:A:295:ASP:O	1:E:152:GLY:HA2	2.05	0.57
1:A:366:MET:HA	1:A:380:PHE:CE1	2.40	0.57
1:B:228:HIS:HB3	1:B:229:PRO:HD2	1.86	0.57
1:C:109:ASN:HB3	1:C:117:LEU:HD21	1.87	0.57
1:C:125:VAL:HA	1:C:307:LYS:O	2.05	0.57
1:F:367:THR:HG22	1:F:368:ARG:H	1.69	0.57
1:F:94:THR:O	1:F:95:LEU:HD23	2.03	0.57
1:C:75:TRP:NE1	1:C:300:ARG:HB2	2.19	0.57
1:E:122:ALA:O	1:E:271:PRO:HD2	2.05	0.57
1:F:28:LEU:HD23	1:F:29:LEU:N	2.20	0.57
1:A:105:LEU:HB3	1:A:106:PRO:HD2	1.86	0.56
1:A:192:THR:HG23	1:A:226:ILE:HD13	1.87	0.56
1:B:141:PHE:CE1	1:B:144:PRO:HG3	2.31	0.56
1:B:166:ALA:HB2	1:B:239:TYR:CB	2.34	0.56
1:B:360:VAL:CG1	1:B:361:PRO:HD2	2.34	0.56
1:C:186:LYS:N	1:C:186:LYS:HE2	2.19	0.56
1:E:124:SER:HA	1:E:261:THR:O	2.05	0.56
1:E:130:VAL:O	1:E:302:LEU:HD22	2.05	0.56
1:E:265:ASP:OD1	1:E:269:VAL:HB	2.05	0.56
1:E:313:ARG:HH11	1:E:313:ARG:HG3	1.67	0.56
1:E:367:THR:CG2	1:E:368:ARG:N	2.68	0.56
1:F:259:LEU:HD13	1:F:259:LEU:H	1.67	0.56
1:F:66:LEU:HD23	1:F:66:LEU:H	1.69	0.56
1:B:55:PRO:HB3	1:B:302:LEU:O	2.05	0.56
1:D:304:ARG:HG2	1:D:306:PHE:CE1	2.40	0.56
1:D:60:PRO:CB	1:D:61:PRO:HD2	2.35	0.56
1:F:287:GLY:C	1:F:299:TRP:HB2	2.25	0.56
1:A:263:LEU:HD23	1:A:263:LEU:N	2.20	0.56
1:B:185:TYR:CD2	1:B:192:THR:HG21	2.40	0.56
1:D:265:ASP:OD1	1:D:269:VAL:HB	2.04	0.56
1:F:121:GLU:HG2	1:F:271:PRO:O	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:380:PHE:CD1	1:A:381:PRO:HD2	2.41	0.56
1:D:190:VAL:HA	1:D:221:MET:HG3	1.86	0.56
1:D:278:LEU:C	1:D:278:LEU:HD23	2.25	0.56
1:F:177:LEU:HD21	1:F:209:ASN:H	1.68	0.56
1:F:269:VAL:CG1	1:F:272:LEU:HD11	2.35	0.56
1:F:55:PRO:HD3	1:F:303:PRO:CA	2.36	0.56
1:A:286:MET:HA	1:A:286:MET:CE	2.35	0.56
1:A:326:SER:O	1:A:327:SER:O	2.22	0.56
1:C:132:SER:O	1:C:135:LEU:HD23	2.06	0.56
1:D:211:ILE:CD1	1:D:211:ILE:N	2.67	0.56
1:E:71:GLN:HE21	1:E:73:TYR:HB2	1.71	0.56
1:A:174:LEU:HD11	1:A:227:TRP:CE3	2.41	0.56
1:A:28:LEU:HD12	1:A:29:LEU:H	1.70	0.56
1:B:105:LEU:HD23	1:B:120:TRP:CD1	2.39	0.56
1:B:269:VAL:HG12	1:B:270:GLY:O	2.05	0.56
1:C:190:VAL:HG22	1:C:191:VAL:O	2.06	0.56
1:D:91:GLY:H	1:D:186:LYS:CE	2.17	0.56
1:A:28:LEU:HD21	1:A:31:LYS:HB3	1.87	0.56
1:A:305:TYR:HE1	1:A:307:LYS:HB2	1.71	0.56
1:C:211:ILE:O	1:C:213:LYS:N	2.39	0.56
1:D:25:VAL:HG23	1:D:26:PRO:CD	2.36	0.56
1:E:207:VAL:HG23	1:E:208:LEU:N	2.20	0.56
1:A:197:THR:O	1:A:197:THR:HG23	2.06	0.56
1:A:372:ARG:O	1:A:373:PHE:CD1	2.58	0.56
1:C:346:THR:HG22	1:C:348:VAL:HG23	1.87	0.56
1:E:197:THR:HG23	1:E:197:THR:O	2.06	0.56
1:F:263:LEU:HB3	1:F:271:PRO:HD3	1.88	0.56
1:F:65:SER:HB3	1:F:68:GLU:CG	2.33	0.56
1:A:275:GLY:O	1:A:277:GLY:N	2.39	0.56
1:B:278:LEU:HD23	1:B:279:TYR:H	1.71	0.56
1:B:78:GLY:O	1:B:79:ILE:HD13	2.05	0.56
1:C:43:PRO:HD2	1:C:44:ASP:H	1.71	0.56
1:D:112:LEU:HD12	1:D:112:LEU:N	2.20	0.56
1:E:141:PHE:CZ	1:E:292:ARG:HG3	2.41	0.56
1:E:223:PRO:HG3	1:E:226:ILE:HD12	1.88	0.56
1:E:243:TYR:CZ	1:E:245:GLY:CA	2.89	0.56
1:E:75:TRP:NE1	1:E:300:ARG:HB2	2.20	0.56
1:F:313:ARG:HG2	1:F:314:TRP:N	2.21	0.56
1:F:66:LEU:HD23	1:F:66:LEU:N	2.21	0.56
2:H:2:GAL:H3	2:H:3:SIA:O1B	2.05	0.56
1:A:208:LEU:HD23	1:A:208:LEU:C	2.27	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:94:THR:O	1:B:95:LEU:HG	2.05	0.56
1:C:28:LEU:CD2	1:C:30:ILE:N	2.68	0.56
1:C:352:ARG:HG3	1:C:354:TYR:CE1	2.41	0.56
1:D:186:LYS:HD2	1:D:186:LYS:N	2.17	0.56
1:D:57:MET:HB2	1:D:96:PRO:HB3	1.88	0.56
1:E:94:THR:C	1:E:95:LEU:HD23	2.26	0.56
1:A:130:VAL:O	1:A:302:LEU:HD22	2.05	0.56
1:B:135:LEU:HD13	1:B:135:LEU:N	2.21	0.56
1:B:69:GLY:HA3	1:B:71:GLN:OE1	2.06	0.56
1:D:243:TYR:CZ	1:D:245:GLY:CA	2.89	0.56
1:D:71:GLN:NE2	1:D:73:TYR:H	2.04	0.56
1:F:192:THR:HG22	1:F:193:ILE:HD12	1.87	0.56
1:F:305:TYR:C	1:F:306:PHE:CD1	2.80	0.56
1:B:142:ASN:O	1:B:292:ARG:HB2	2.05	0.55
1:B:172:LEU:HD22	1:B:173:ASP:O	2.06	0.55
1:D:342:GLU:CA	1:D:346:THR:HG23	2.36	0.55
1:E:75:TRP:CH2	1:E:300:ARG:HD2	2.40	0.55
1:E:318:PRO:HG2	1:E:319:TYR:CG	2.41	0.55
1:F:86:THR:HG23	1:F:87:GLU:N	2.21	0.55
1:A:224:VAL:HG11	1:A:283:VAL:HG11	1.88	0.55
1:C:76:SER:OG	1:C:299:TRP:HB2	2.06	0.55
1:F:59:GLN:HE21	1:F:71:GLN:HE22	1.54	0.55
1:A:238:ARG:HH21	1:A:265:ASP:HB3	1.71	0.55
1:A:305:TYR:CE1	1:A:307:LYS:HB2	2.41	0.55
1:A:50:GLU:HG2	1:A:305:TYR:OH	2.06	0.55
1:C:193:ILE:HG12	1:C:201:MET:HE1	1.89	0.55
1:C:316:LYS:HE3	1:F:359:PRO:HB2	1.88	0.55
1:D:145:THR:HG21	1:E:297:HIS:HE1	1.70	0.55
1:E:62:THR:O	1:E:64:GLU:N	2.39	0.55
1:B:219:ASP:HB3	1:F:338:GLY:H	1.71	0.55
1:B:264:LEU:HD12	1:B:270:GLY:HA3	1.88	0.55
1:B:48:GLU:HG2	1:B:309:THR:HG23	1.87	0.55
1:B:336:VAL:C	1:B:337:GLN:HA	2.25	0.55
1:D:91:GLY:N	1:D:186:LYS:HZ2	2.04	0.55
1:E:175:GLN:NE2	1:E:176:GLY:O	2.39	0.55
1:E:82:ALA:HB2	1:E:88:ASP:OD1	2.05	0.55
1:A:138:VAL:HB	1:A:153:ILE:CG2	2.34	0.55
1:B:111:ASP:OD2	1:B:113:THR:HB	2.07	0.55
1:B:177:LEU:CD2	1:B:208:LEU:CA	2.84	0.55
1:C:232:ALA:O	1:C:234:ASN:N	2.39	0.55
1:E:193:ILE:O	1:E:196:ILE:HG23	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:288:TRP:HE3	1:E:299:TRP:CG	2.24	0.55
1:F:232:ALA:HB3	1:F:235:GLU:OE1	2.06	0.55
1:F:72:TYR:HE2	1:F:77:ARG:NH2	2.04	0.55
1:A:278:LEU:HD22	1:A:280:LEU:HD22	1.87	0.55
1:C:164:VAL:HG22	1:C:241:GLY:HA3	1.88	0.55
1:E:368:ARG:HA	1:E:376:THR:O	2.06	0.55
1:B:193:ILE:HG12	1:B:201:MET:CE	2.36	0.55
1:B:265:ASP:N	1:B:270:GLY:H	2.04	0.55
1:B:265:ASP:OD1	1:B:269:VAL:HB	2.06	0.55
1:B:43:PRO:HA	1:B:312:LYS:HD2	1.89	0.55
1:E:139:HIS:O	1:E:154:SER:HB2	2.06	0.55
1:E:354:TYR:N	1:E:354:TYR:HD1	2.03	0.55
1:B:110:GLU:CD	1:F:322:ALA:H	2.10	0.55
1:A:106:PRO:HD2	1:A:120:TRP:HE1	1.71	0.55
1:B:177:LEU:CD2	1:B:205:ASP:O	2.55	0.55
1:B:75:TRP:HE1	1:B:300:ARG:HB2	1.72	0.55
1:D:135:LEU:HD22	1:D:135:LEU:H	1.72	0.55
1:E:186:LYS:HE2	1:E:186:LYS:H	1.71	0.55
1:E:192:THR:HB	1:E:194:LYS:CD	2.36	0.55
1:E:76:SER:OG	1:E:299:TRP:CE3	2.56	0.55
1:E:54:ASN:ND2	1:E:303:PRO:HB3	2.21	0.55
1:E:342:GLU:HG2	1:E:343:GLY:N	2.21	0.55
1:F:42:GLY:O	1:F:312:LYS:NZ	2.31	0.55
1:A:178:VAL:HG22	1:A:180:ASP:N	2.22	0.55
1:A:211:ILE:O	1:A:213:LYS:N	2.39	0.55
1:A:372:ARG:O	1:A:373:PHE:HD1	1.90	0.55
1:B:104:GLN:HE21	1:B:105:LEU:N	2.04	0.55
1:B:114:CYS:HB2	1:B:116:THR:HG22	1.88	0.55
1:B:165:PHE:CZ	1:B:240:PHE:HE1	2.23	0.55
1:A:251:PRO:CG	1:B:245:GLY:HA3	2.32	0.55
1:B:66:LEU:O	1:B:70:GLY:HA2	2.05	0.55
1:C:82:ALA:HB1	1:C:87:GLU:O	2.07	0.55
1:E:33:GLY:O	1:E:36:VAL:HG23	2.07	0.55
1:F:90:PRO:HB2	1:F:186:LYS:HE3	1.89	0.55
1:B:193:ILE:HD12	1:B:193:ILE:N	2.21	0.55
1:C:164:VAL:HG12	1:C:165:PHE:N	2.21	0.55
1:D:193:ILE:H	1:D:193:ILE:HD12	1.71	0.55
1:D:290:VAL:HG22	1:D:297:HIS:CD2	2.41	0.55
1:E:179:THR:O	1:E:206:GLN:HG3	2.07	0.55
1:E:192:THR:H	1:E:195:THR:CB	2.19	0.55
1:E:117:LEU:O	1:E:314:TRP:HE3	1.90	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:193:ILE:CD1	1:F:201:MET:SD	2.95	0.55
1:A:130:VAL:CG2	1:A:303:PRO:HG2	2.38	0.54
1:A:241:GLY:O	1:E:255:PHE:HB2	2.07	0.54
1:B:103:LEU:HB2	1:B:278:LEU:HB3	1.89	0.54
1:C:145:THR:HG21	1:D:297:HIS:HE1	1.72	0.54
1:C:193:ILE:O	1:C:197:THR:N	2.40	0.54
1:C:53:LEU:HD21	1:C:306:PHE:HE1	1.69	0.54
1:D:272:LEU:HD12	1:D:272:LEU:N	2.21	0.54
1:D:32:GLY:CA	1:D:36:VAL:HG21	2.37	0.54
1:D:346:THR:C	1:D:348:VAL:H	2.10	0.54
1:E:208:LEU:O	1:E:210:PRO:HD3	2.07	0.54
1:F:104:GLN:NE2	1:F:105:LEU:O	2.39	0.54
1:F:209:ASN:OD1	1:F:211:ILE:HD13	2.06	0.54
1:F:174:LEU:HD23	1:F:227:TRP:HB3	1.89	0.54
1:A:106:PRO:HD2	1:A:120:TRP:NE1	2.22	0.54
1:A:82:ALA:CB	1:A:88:ASP:HA	2.37	0.54
1:B:152:GLY:O	1:B:153:ILE:HD13	2.06	0.54
1:D:98:TRP:HH2	1:D:164:VAL:HG11	1.72	0.54
1:E:291:THR:HB	1:E:293:ASN:HB3	1.88	0.54
1:E:320:PRO:HG2	1:E:323:SER:HB2	1.89	0.54
1:E:321:MET:O	1:E:324:LEU:HB2	2.07	0.54
1:F:185:TYR:HB2	1:F:194:LYS:CE	2.38	0.54
1:D:125:VAL:HG12	1:D:263:LEU:HD21	1.89	0.54
1:F:186:LYS:N	1:F:186:LYS:HE2	2.21	0.54
1:B:72:TYR:O	1:B:75:TRP:HB2	2.07	0.54
1:F:124:SER:HA	1:F:261:THR:O	2.08	0.54
1:A:174:LEU:HD12	1:A:175:GLN:N	2.21	0.54
1:B:161:GLN:CD	1:B:251:PRO:HA	2.28	0.54
1:A:54:ASN:ND2	1:B:207:VAL:HB	2.22	0.54
1:B:290:VAL:HG22	1:B:297:HIS:CD2	2.43	0.54
1:B:346:THR:HG22	1:B:348:VAL:H	1.73	0.54
1:C:271:PRO:C	1:C:272:LEU:HG	2.28	0.54
1:C:39:LEU:HD12	1:C:40:VAL:N	2.21	0.54
1:D:269:VAL:HA	1:D:313:ARG:HH21	1.73	0.54
1:A:231:PRO:HG2	1:E:305:TYR:HD2	1.71	0.54
1:E:321:MET:O	1:E:325:ILE:HD12	2.07	0.54
1:F:288:TRP:CE3	1:F:299:TRP:HB3	2.41	0.54
1:C:233:LYS:HZ2	1:F:350:GLU:HG2	1.71	0.54
1:A:166:ALA:HB1	1:A:237:THR:HG22	1.88	0.54
1:A:243:TYR:CZ	1:A:245:GLY:CA	2.91	0.54
1:A:74:GLY:O	1:A:300:ARG:NH1	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:83:THR:O	1:A:84:SER:HB2	2.06	0.54
1:C:111:ASP:CG	1:C:114:CYS:HB3	2.28	0.54
1:C:131:GLY:H	1:C:255:PHE:HZ	1.56	0.54
1:E:193:ILE:N	1:E:193:ILE:HD12	2.23	0.54
1:F:197:THR:HG23	1:F:197:THR:O	2.07	0.54
1:A:336:VAL:HG23	1:A:337:GLN:H	1.50	0.54
1:A:80:ASN:HB3	1:A:90:PRO:O	2.07	0.54
1:C:253:LEU:O	1:D:242:ASN:HB2	2.08	0.54
1:E:115:ASP:OD1	1:E:317:ASN:HB3	2.08	0.54
1:F:39:LEU:O	1:F:41:THR:N	2.40	0.54
1:A:108:LEU:HD11	1:A:120:TRP:CZ2	2.43	0.54
1:A:76:SER:OG	1:A:299:TRP:CE3	2.61	0.54
1:E:164:VAL:HA	1:E:241:GLY:CA	2.38	0.54
1:E:288:TRP:CE3	1:E:299:TRP:CG	2.96	0.54
1:E:306:PHE:HB3	1:E:308:ILE:CD1	2.38	0.54
1:F:201:MET:HA	1:F:201:MET:CE	2.38	0.54
1:F:175:GLN:HG3	1:F:213:LYS:NZ	2.23	0.54
1:B:378:THR:HG22	1:B:379:VAL:N	2.22	0.54
1:C:72:TYR:O	1:C:75:TRP:HB2	2.08	0.54
1:D:28:LEU:HD11	1:D:30:ILE:O	2.07	0.54
1:E:320:PRO:C	1:E:324:LEU:HD12	2.27	0.54
1:F:304:ARG:HG2	1:F:305:TYR:N	2.23	0.54
1:A:139:HIS:O	1:A:154:SER:HB2	2.08	0.54
1:B:175:GLN:NE2	1:B:176:GLY:O	2.40	0.54
1:C:25:VAL:HG13	1:C:26:PRO:HD2	1.89	0.54
1:C:360:VAL:CG1	1:C:361:PRO:HD2	2.37	0.54
1:D:135:LEU:HD22	1:D:135:LEU:N	2.22	0.54
1:D:57:MET:HE3	1:D:96:PRO:HB3	1.90	0.54
1:E:370:VAL:HG22	1:E:375:LYS:CB	2.37	0.54
1:C:76:SER:CB	1:C:299:TRP:HE3	2.22	0.53
1:D:139:HIS:HD2	1:E:88:ASP:OD1	1.91	0.53
1:D:288:TRP:CE3	1:D:299:TRP:CD1	2.95	0.53
1:E:166:ALA:HB2	1:E:239:TYR:CB	2.38	0.53
1:E:190:VAL:HG23	1:E:223:PRO:HD3	1.90	0.53
1:E:161:GLN:NE2	1:E:251:PRO:HA	2.23	0.53
1:E:50:GLU:HG3	1:E:307:LYS:HG3	1.90	0.53
1:E:317:ASN:ND2	1:E:319:TYR:H	2.06	0.53
1:E:328:LEU:HG	1:E:329:PHE:N	2.23	0.53
1:E:370:VAL:HA	1:E:375:LYS:HA	1.90	0.53
1:F:40:VAL:HG23	1:F:40:VAL:O	2.08	0.53
1:B:251:PRO:HD2	1:C:245:GLY:CA	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:261:THR:CG2	1:B:262:VAL:N	2.71	0.53
1:B:78:GLY:HA2	1:B:298:HIS:CD2	2.43	0.53
1:C:190:VAL:HG23	1:C:221:MET:O	2.08	0.53
1:C:352:ARG:HD2	1:F:234:ASN:HD21	1.72	0.53
1:E:222:TYR:CD1	1:E:222:TYR:N	2.75	0.53
1:F:194:LYS:HA	1:F:197:THR:O	2.08	0.53
1:A:54:ASN:OD1	1:B:208:LEU:HB3	2.08	0.53
1:B:233:LYS:C	1:B:234:ASN:HD22	2.11	0.53
1:C:76:SER:O	1:C:298:HIS:HB2	2.08	0.53
1:C:53:LEU:HD22	1:C:53:LEU:N	2.24	0.53
1:C:69:GLY:C	1:C:71:GLN:N	2.60	0.53
1:D:192:THR:HB	1:D:194:LYS:CD	2.33	0.53
1:D:180:ASP:HA	1:D:206:GLN:HE21	1.74	0.53
1:D:62:THR:O	1:D:64:GLU:N	2.41	0.53
1:F:239:TYR:C	1:F:240:PHE:CD1	2.81	0.53
1:A:280:LEU:HD12	1:A:306:PHE:CD2	2.42	0.53
1:A:328:LEU:CD1	1:A:332:MET:HE3	2.24	0.53
1:B:341:MET:HA	1:B:346:THR:HG23	1.91	0.53
1:C:162:TYR:HB3	1:C:285:ILE:HD13	1.89	0.53
1:C:97:THR:HG22	1:C:223:PRO:N	2.23	0.53
1:F:286:MET:CE	1:F:286:MET:HA	2.37	0.53
1:A:121:GLU:O	1:A:310:LEU:HB2	2.08	0.53
1:A:238:ARG:HA	1:E:257:ASN:HD22	1.74	0.53
1:A:90:PRO:HG2	1:A:185:TYR:CA	2.38	0.53
1:B:166:ALA:HA	1:B:238:ARG:O	2.08	0.53
1:C:152:GLY:HA2	1:D:295:ASP:CB	2.38	0.53
1:E:177:LEU:HG	1:E:207:VAL:O	2.08	0.53
1:A:278:LEU:HD22	1:A:280:LEU:HD21	1.89	0.53
1:B:122:ALA:HB3	1:B:271:PRO:HD2	1.90	0.53
1:B:202:VAL:HG12	1:B:203:ASN:H	1.73	0.53
1:B:293:ASN:OD1	1:B:294:TYR:HB2	2.09	0.53
1:B:341:MET:CA	1:B:346:THR:HG23	2.39	0.53
1:C:131:GLY:HA2	1:D:228:HIS:CE1	2.43	0.53
1:D:229:PRO:HB2	1:D:239:TYR:CE2	2.43	0.53
1:D:268:GLY:O	1:D:313:ARG:NH2	2.41	0.53
1:D:76:SER:O	1:D:298:HIS:HB2	2.07	0.53
1:E:145:THR:OG1	1:E:153:ILE:HB	2.08	0.53
1:E:94:THR:O	1:E:94:THR:HG22	2.08	0.53
1:F:28:LEU:HD23	1:F:30:ILE:N	2.23	0.53
1:C:316:LYS:HZ2	1:F:359:PRO:HD2	1.72	0.53
1:A:165:PHE:HB2	1:A:281:SER:O	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:62:THR:O	1:A:64:GLU:N	2.41	0.53
1:B:176:GLY:O	1:B:177:LEU:HD23	2.09	0.53
1:B:192:THR:H	1:B:195:THR:CB	2.21	0.53
1:C:123:VAL:HG13	1:C:264:LEU:CD1	2.39	0.53
1:D:305:TYR:CE2	1:E:231:PRO:HB2	2.44	0.53
1:A:122:ALA:HB3	1:A:271:PRO:HD2	1.90	0.53
1:A:178:VAL:HG22	1:A:180:ASP:H	1.73	0.53
1:B:317:ASN:OD1	1:B:318:PRO:HD2	2.08	0.53
1:D:207:VAL:O	1:D:208:LEU:HB2	2.09	0.53
1:C:139:HIS:HD2	1:D:88:ASP:OD2	1.92	0.53
1:E:115:ASP:HB3	1:E:317:ASN:H	1.73	0.53
1:A:131:GLY:O	1:A:134:SER:HB3	2.09	0.53
1:A:372:ARG:NH1	1:A:372:ARG:HB2	2.14	0.53
1:B:165:PHE:CD1	1:B:165:PHE:C	2.81	0.53
1:B:285:ILE:HD12	1:B:285:ILE:H	1.73	0.53
1:B:286:MET:HA	1:B:286:MET:CE	2.38	0.53
1:B:325:ILE:O	1:B:328:LEU:HB2	2.09	0.53
1:C:104:GLN:NE2	1:C:276:GLU:HB2	2.22	0.53
1:C:288:TRP:HB2	1:C:297:HIS:HB3	1.90	0.53
1:C:321:MET:O	1:C:324:LEU:HB2	2.08	0.53
1:D:218:LYS:O	1:D:219:ASP:CB	2.52	0.53
1:D:325:ILE:O	1:D:328:LEU:HB3	2.08	0.53
1:D:54:ASN:HD22	1:D:303:PRO:HB3	1.73	0.53
1:E:150:THR:HG21	1:E:292:ARG:HH21	1.73	0.53
1:C:318:PRO:HB3	1:F:363:ASP:H	1.74	0.53
1:C:54:ASN:ND2	1:D:207:VAL:HG23	2.24	0.53
1:D:125:VAL:HA	1:D:307:LYS:O	2.09	0.53
1:A:88:ASP:OD1	1:E:139:HIS:HD2	1.91	0.53
1:E:233:LYS:C	1:E:234:ASN:HD22	2.13	0.53
1:E:307:LYS:C	1:E:308:ILE:HD12	2.29	0.53
1:F:145:THR:HB	1:F:152:GLY:HA3	1.91	0.53
1:F:324:LEU:O	1:F:327:SER:HB2	2.08	0.53
1:B:46:VAL:HG12	1:B:47:THR:N	2.24	0.52
1:B:50:GLU:CD	1:C:233:LYS:CB	2.77	0.52
1:C:339:GLN:NE2	1:C:347:GLN:HE22	2.07	0.52
1:D:144:PRO:HD3	1:D:292:ARG:HG2	1.90	0.52
1:D:185:TYR:HB2	1:D:194:LYS:CE	2.39	0.52
1:D:41:THR:HB	1:D:45:SER:OG	2.09	0.52
1:F:178:VAL:CG2	1:F:179:THR:H	2.21	0.52
1:A:104:GLN:NE2	1:A:105:LEU:N	2.56	0.52
1:A:181:ALA:O	1:A:201:MET:HB2	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:305:TYR:CG	1:A:306:PHE:N	2.76	0.52
1:C:341:MET:C	1:C:346:THR:HG23	2.30	0.52
1:D:175:GLN:HG2	1:D:213:LYS:HG2	1.90	0.52
1:E:258:THR:HB	1:E:259:LEU:CD2	2.35	0.52
1:E:77:ARG:O	1:E:298:HIS:CG	2.61	0.52
1:F:161:GLN:OE1	1:F:251:PRO:HA	2.09	0.52
1:F:142:ASN:C	1:F:292:ARG:HB2	2.29	0.52
1:A:166:ALA:HA	1:A:238:ARG:O	2.09	0.52
1:A:76:SER:OG	1:A:299:TRP:HE3	1.93	0.52
1:A:88:ASP:OD2	1:A:183:THR:HG23	2.08	0.52
1:B:239:TYR:C	1:B:240:PHE:CG	2.83	0.52
1:B:308:ILE:N	1:B:308:ILE:CD1	2.67	0.52
1:D:165:PHE:HB2	1:D:282:CYS:HB3	1.91	0.52
1:D:54:ASN:HD22	1:D:55:PRO:HD2	1.72	0.52
1:F:164:VAL:HA	1:F:240:PHE:O	2.09	0.52
1:F:176:GLY:O	1:F:177:LEU:HD23	2.09	0.52
1:F:84:SER:O	1:F:87:GLU:N	2.42	0.52
1:B:193:ILE:CD1	1:B:201:MET:SD	2.98	0.52
1:B:177:LEU:HD22	1:B:205:ASP:O	2.10	0.52
1:C:234:ASN:OD1	1:F:352:ARG:NH2	2.42	0.52
1:D:43:PRO:O	1:D:312:LYS:HB2	2.09	0.52
1:E:256:THR:OG1	1:E:257:ASN:N	2.43	0.52
1:A:231:PRO:HG2	1:E:305:TYR:CD2	2.44	0.52
1:E:368:ARG:CZ	1:E:377:LYS:HE3	2.40	0.52
1:F:166:ALA:HB2	1:F:239:TYR:CB	2.40	0.52
1:F:182:ARG:HG3	1:F:183:THR:N	2.20	0.52
1:F:256:THR:OG1	1:F:257:ASN:N	2.41	0.52
1:A:150:THR:HG22	1:A:150:THR:O	2.09	0.52
1:A:196:ILE:HD12	1:A:196:ILE:O	2.10	0.52
1:A:234:ASN:HD22	1:A:234:ASN:N	2.08	0.52
1:A:75:TRP:CE2	1:A:300:ARG:HD2	2.45	0.52
1:A:133:GLY:HA3	1:B:228:HIS:HE1	1.74	0.52
1:C:43:PRO:CD	1:C:44:ASP:H	2.22	0.52
1:D:175:GLN:NE2	1:D:176:GLY:O	2.43	0.52
1:D:255:PHE:O	1:E:240:PHE:HA	2.10	0.52
1:F:103:LEU:HD22	1:F:103:LEU:N	2.25	0.52
1:F:350:GLU:HG3	1:F:351:VAL:H	1.74	0.52
1:A:30:ILE:CG1	1:A:36:VAL:HG13	2.40	0.52
1:B:339:GLN:HG2	1:B:340:PRO:HD2	1.91	0.52
1:B:69:GLY:C	1:B:71:GLN:N	2.61	0.52
1:A:141:PHE:HD2	1:B:84:SER:HA	1.71	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:193:ILE:N	1:C:193:ILE:HD12	2.24	0.52
1:D:124:SER:HA	1:D:261:THR:O	2.09	0.52
1:D:255:PHE:HB2	1:E:241:GLY:O	2.10	0.52
1:E:265:ASP:H	1:E:270:GLY:N	2.03	0.52
1:E:304:ARG:HD3	1:E:306:PHE:CE1	2.45	0.52
1:A:104:GLN:HE21	1:A:105:LEU:N	2.07	0.52
1:A:172:LEU:HD22	1:A:173:ASP:O	2.10	0.52
1:B:135:LEU:CD1	1:B:135:LEU:N	2.72	0.52
1:B:71:GLN:NE2	1:B:73:TYR:HB2	2.19	0.52
1:C:145:THR:OG1	1:C:153:ILE:N	2.43	0.52
1:C:366:MET:SD	1:F:319:TYR:CE1	3.03	0.52
1:C:71:GLN:NE2	1:C:73:TYR:H	2.07	0.52
1:C:94:THR:O	1:C:94:THR:HG22	2.09	0.52
1:D:306:PHE:HB3	1:D:308:ILE:HD11	1.92	0.52
1:E:114:CYS:C	1:E:116:THR:N	2.61	0.52
1:A:54:ASN:HD22	1:A:55:PRO:HD2	1.74	0.52
1:B:211:ILE:N	1:B:211:ILE:CD1	2.73	0.52
1:D:105:LEU:HB3	1:D:120:TRP:CD1	2.45	0.52
1:E:165:PHE:HB2	1:E:281:SER:O	2.10	0.52
1:E:329:PHE:O	1:E:332:MET:HB2	2.09	0.52
1:E:350:GLU:CG	1:E:351:VAL:N	2.72	0.52
1:A:138:VAL:CB	1:A:153:ILE:HG23	2.38	0.52
1:B:108:LEU:HB3	1:B:118:GLN:HG3	1.90	0.52
1:B:258:THR:C	1:B:259:LEU:HD22	2.30	0.52
1:F:125:VAL:HG13	1:F:125:VAL:O	2.09	0.52
1:F:172:LEU:HD22	1:F:173:ASP:H	1.69	0.52
1:F:57:MET:CB	1:F:96:PRO:HB3	2.35	0.52
1:A:63:PRO:HB2	1:A:69:GLY:HA3	1.91	0.52
1:B:107:MET:C	1:B:108:LEU:HD12	2.30	0.52
1:D:300:ARG:NH2	1:E:206:GLN:O	2.42	0.52
1:D:30:ILE:CG1	1:D:36:VAL:HG13	2.40	0.52
1:F:39:LEU:HG	1:F:40:VAL:N	2.25	0.52
1:D:77:ARG:NH2	2:J:3:SIA:O1B	2.43	0.52
1:A:185:TYR:CE2	1:A:226:ILE:HD11	2.45	0.51
1:C:54:ASN:HD21	1:D:208:LEU:CB	2.23	0.51
1:C:89:SER:OG	1:C:186:LYS:NZ	2.43	0.51
1:A:162:TYR:HE1	1:E:255:PHE:HE2	1.58	0.51
1:E:284:ASP:OD1	1:E:304:ARG:NH1	2.43	0.51
1:F:232:ALA:HB3	1:F:234:ASN:O	2.09	0.51
1:A:135:LEU:CD1	1:A:135:LEU:H	2.21	0.51
1:B:107:MET:CG	1:C:370:VAL:HG22	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:30:ILE:HG23	1:F:353:VAL:CG2	2.39	0.51
1:B:342:GLU:N	1:B:346:THR:HG23	2.24	0.51
1:C:168:GLY:CA	1:C:237:THR:HG23	2.27	0.51
1:D:50:GLU:HG2	1:D:305:TYR:OH	2.11	0.51
1:E:288:TRP:CB	1:E:299:TRP:HB3	2.32	0.51
1:F:279:TYR:C	1:F:280:LEU:HD23	2.30	0.51
1:A:177:LEU:HD22	1:A:207:VAL:O	2.11	0.51
1:A:239:TYR:C	1:A:240:PHE:CD1	2.84	0.51
1:A:378:THR:HG22	1:A:379:VAL:O	2.11	0.51
1:A:365:ASP:HB3	1:A:380:PHE:CE2	2.45	0.51
1:C:363:ASP:HB3	1:C:366:MET:CE	2.40	0.51
1:D:130:VAL:O	1:D:302:LEU:HD22	2.10	0.51
1:D:300:ARG:HG3	1:D:301:GLY:N	2.25	0.51
1:D:71:GLN:NE2	1:D:71:GLN:HA	2.08	0.51
1:E:115:ASP:HB2	1:E:316:LYS:NZ	2.25	0.51
1:E:203:ASN:O	1:E:206:GLN:HB3	2.11	0.51
1:E:232:ALA:C	1:E:234:ASN:H	2.12	0.51
1:A:130:VAL:O	1:A:130:VAL:HG23	2.11	0.51
1:A:134:SER:HB3	1:A:135:LEU:HD12	1.93	0.51
1:A:257:ASN:HD22	1:B:238:ARG:HA	1.74	0.51
1:B:41:THR:HB	1:B:45:SER:OG	2.10	0.51
1:C:308:ILE:CD1	1:C:308:ILE:H	2.18	0.51
1:C:354:TYR:N	1:C:354:TYR:CD1	2.77	0.51
1:D:257:ASN:HD21	1:E:238:ARG:HA	1.76	0.51
1:E:50:GLU:HG2	1:E:305:TYR:OH	2.10	0.51
1:E:313:ARG:CG	1:E:313:ARG:NH1	2.72	0.51
1:E:321:MET:HG2	1:E:325:ILE:CD1	2.41	0.51
1:A:208:LEU:HD22	1:A:210:PRO:HG3	1.93	0.51
1:B:37:LEU:HD11	1:B:47:THR:HG21	1.93	0.51
1:C:192:THR:O	1:C:193:ILE:C	2.48	0.51
1:C:75:TRP:HD1	1:C:299:TRP:O	1.93	0.51
1:C:67:THR:OG1	1:C:68:GLU:N	2.43	0.51
1:D:98:TRP:N	1:D:222:TYR:O	2.39	0.51
1:E:193:ILE:H	1:E:193:ILE:CD1	2.23	0.51
1:E:180:ASP:HA	1:E:206:GLN:NE2	2.26	0.51
1:F:191:VAL:HA	1:F:195:THR:HG21	1.92	0.51
2:K:2:GAL:H3	2:K:3:SIA:O1B	2.08	0.51
1:B:100:MET:C	1:B:100:MET:SD	2.89	0.51
1:D:97:THR:HG22	1:D:223:PRO:N	2.26	0.51
1:E:285:ILE:N	1:E:285:ILE:CD1	2.73	0.51
1:E:97:THR:HG22	1:E:222:TYR:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:190:VAL:HA	1:F:221:MET:HG3	1.93	0.51
1:F:100:MET:HG2	1:F:216:LEU:HD13	1.93	0.51
1:A:372:ARG:C	1:A:373:PHE:CD1	2.84	0.51
1:C:165:PHE:O	1:C:239:TYR:HA	2.10	0.51
1:D:192:THR:O	1:D:195:THR:HB	2.11	0.51
1:D:219:ASP:C	1:D:221:MET:N	2.64	0.51
1:D:257:ASN:HB3	1:E:239:TYR:CZ	2.45	0.51
1:E:259:LEU:N	1:E:259:LEU:CD2	2.73	0.51
1:E:293:ASN:OD1	1:E:294:TYR:N	2.43	0.51
1:F:342:GLU:HG2	1:F:343:GLY:N	2.26	0.51
1:A:180:ASP:OD1	1:A:182:ARG:HD2	2.11	0.51
1:A:256:THR:OG1	1:A:257:ASN:N	2.44	0.51
1:A:169:GLY:HA2	1:A:273:CYS:HA	1.93	0.51
1:B:181:ALA:H	1:B:206:GLN:HE21	1.58	0.51
1:B:222:TYR:CD1	1:B:222:TYR:N	2.78	0.51
1:B:288:TRP:CZ3	1:B:299:TRP:NE1	2.78	0.51
1:D:52:PHE:HB2	1:D:304:ARG:O	2.11	0.51
1:E:83:THR:HG22	1:E:84:SER:N	2.26	0.51
1:F:141:PHE:CD1	1:F:292:ARG:HG3	2.46	0.51
1:F:37:LEU:HD11	1:F:47:THR:HG21	1.92	0.51
1:A:164:VAL:HG23	1:A:283:VAL:CG2	2.40	0.51
1:A:63:PRO:O	1:A:71:GLN:NE2	2.44	0.51
1:B:373:PHE:N	1:B:373:PHE:CD1	2.77	0.51
1:C:162:TYR:CE2	1:C:224:VAL:HG11	2.46	0.51
1:D:145:THR:HG21	1:E:297:HIS:CE1	2.46	0.51
1:D:246:GLY:HA3	1:D:249:THR:OG1	2.11	0.51
1:E:223:PRO:CG	1:E:226:ILE:HD12	2.40	0.51
1:F:239:TYR:C	1:F:240:PHE:CG	2.84	0.51
1:B:265:ASP:H	1:B:270:GLY:N	2.07	0.51
1:C:173:ASP:C	1:C:174:LEU:HD12	2.32	0.51
1:C:239:TYR:CD1	1:C:239:TYR:C	2.83	0.51
1:D:142:ASN:HA	1:D:290:VAL:O	2.11	0.51
1:E:308:ILE:CD1	1:E:308:ILE:N	2.74	0.51
1:A:177:LEU:HD12	1:E:131:GLY:HA3	1.92	0.50
1:A:280:LEU:CD2	1:A:280:LEU:N	2.74	0.50
1:A:340:PRO:CG	1:A:347:GLN:HE22	2.21	0.50
1:A:40:VAL:HG12	1:A:42:GLY:H	1.75	0.50
1:B:109:ASN:H	1:B:118:GLN:HE21	1.58	0.50
1:C:243:TYR:CZ	1:C:245:GLY:HA2	2.45	0.50
1:D:106:PRO:HD2	1:D:120:TRP:NE1	2.25	0.50
1:D:91:GLY:H	1:D:186:LYS:HE3	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:300:ARG:CG	1:F:301:GLY:N	2.74	0.50
1:A:211:ILE:HD12	1:A:211:ILE:N	2.25	0.50
1:A:87:GLU:HA	1:A:184:LYS:HZ2	1.75	0.50
1:B:105:LEU:HD23	1:B:120:TRP:CG	2.46	0.50
1:B:143:LYS:HA	1:B:292:ARG:HA	1.92	0.50
1:B:364:PRO:HG2	1:B:365:ASP:N	2.26	0.50
1:B:76:SER:O	1:B:298:HIS:HB2	2.10	0.50
1:B:82:ALA:HB1	1:B:88:ASP:HA	1.93	0.50
1:C:105:LEU:CB	1:C:120:TRP:CD1	2.94	0.50
1:E:174:LEU:HD13	1:E:227:TRP:CE3	2.46	0.50
1:E:261:THR:HG22	1:E:262:VAL:N	2.26	0.50
1:F:170:GLU:HB2	1:F:171:PRO:HD2	1.92	0.50
1:F:205:ASP:CA	1:F:209:ASN:HB2	2.32	0.50
1:F:306:PHE:N	1:F:306:PHE:HD1	2.07	0.50
1:A:178:VAL:CG2	1:A:179:THR:N	2.74	0.50
1:A:233:LYS:HE2	1:A:234:ASN:HD21	1.76	0.50
1:A:305:TYR:CD1	1:A:306:PHE:N	2.79	0.50
1:A:306:PHE:HB3	1:A:308:ILE:CD1	2.40	0.50
1:A:367:THR:HB	1:A:378:THR:OG1	2.11	0.50
1:B:328:LEU:C	1:B:332:MET:SD	2.90	0.50
1:C:174:LEU:CD1	1:C:174:LEU:N	2.72	0.50
1:C:172:LEU:HB3	1:C:216:LEU:HD12	1.93	0.50
1:C:239:TYR:C	1:C:240:PHE:CD1	2.85	0.50
1:D:288:TRP:CD1	1:D:288:TRP:N	2.75	0.50
1:E:207:VAL:HG23	1:E:208:LEU:H	1.76	0.50
1:E:291:THR:OG1	1:E:296:VAL:HB	2.11	0.50
1:E:351:VAL:HG12	1:E:352:ARG:N	2.27	0.50
1:E:35:GLU:HG2	1:E:36:VAL:N	2.26	0.50
1:A:194:LYS:O	1:A:198:LYS:N	2.45	0.50
1:A:350:GLU:CG	1:A:351:VAL:H	2.25	0.50
1:B:318:PRO:HB2	1:B:319:TYR:CZ	2.46	0.50
1:B:139:HIS:HD2	1:C:88:ASP:OD2	1.94	0.50
1:D:181:ALA:HA	1:D:201:MET:CE	2.41	0.50
1:D:28:LEU:CG	1:D:29:LEU:N	2.73	0.50
1:D:54:ASN:HD21	1:E:208:LEU:HB2	1.76	0.50
1:E:178:VAL:CG2	1:E:179:THR:N	2.75	0.50
1:E:349:GLU:O	1:E:350:GLU:HB2	2.11	0.50
1:F:135:LEU:N	1:F:135:LEU:HD22	2.24	0.50
1:F:136:LEU:O	1:F:138:VAL:HG22	2.11	0.50
1:B:150:THR:HG22	1:B:150:THR:O	2.11	0.50
1:B:193:ILE:HD13	1:B:201:MET:HG2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:288:TRP:HA	1:B:299:TRP:HA	1.93	0.50
1:B:367:THR:HG22	1:B:368:ARG:H	1.77	0.50
1:C:288:TRP:CE3	1:C:299:TRP:CD1	3.00	0.50
1:D:263:LEU:O	1:D:270:GLY:HA2	2.12	0.50
1:D:289:ARG:O	1:D:297:HIS:O	2.30	0.50
1:D:305:TYR:CG	1:D:306:PHE:N	2.79	0.50
1:E:105:LEU:HD12	1:E:105:LEU:H	1.73	0.50
1:E:181:ALA:H	1:E:206:GLN:HE21	1.57	0.50
1:F:180:ASP:HB3	1:F:182:ARG:HG2	1.94	0.50
1:F:90:PRO:HG2	1:F:185:TYR:CD1	2.47	0.50
1:A:194:LYS:HB2	1:A:198:LYS:O	2.12	0.50
1:A:245:GLY:O	1:A:249:THR:HG21	2.12	0.50
1:A:265:ASP:H	1:A:270:GLY:N	2.09	0.50
1:B:123:VAL:HG13	1:B:264:LEU:HD13	1.92	0.50
1:B:69:GLY:O	1:B:71:GLN:N	2.44	0.50
1:C:186:LYS:CE	1:C:186:LYS:H	2.25	0.50
1:E:138:VAL:O	1:E:153:ILE:HG23	2.12	0.50
1:E:346:THR:HG22	1:E:348:VAL:H	1.76	0.50
1:E:65:SER:HB3	1:E:68:GLU:OE2	2.12	0.50
1:C:233:LYS:HE3	1:F:350:GLU:HB3	1.94	0.50
1:A:265:ASP:OD1	1:A:269:VAL:N	2.44	0.50
1:A:94:THR:O	1:A:94:THR:HG22	2.12	0.50
1:B:108:LEU:HD11	1:B:120:TRP:CE2	2.47	0.50
1:B:305:TYR:C	1:B:306:PHE:CD1	2.85	0.50
1:B:350:GLU:HG2	1:B:352:ARG:HH21	1.76	0.50
1:C:69:GLY:HA3	1:C:71:GLN:OE1	2.11	0.50
1:D:56:ARG:NH2	1:D:219:ASP:OD2	2.45	0.50
1:D:83:THR:HG22	1:D:84:SER:N	2.26	0.50
1:A:84:SER:C	1:A:86:THR:N	2.63	0.50
1:B:76:SER:CB	1:B:299:TRP:HE3	2.24	0.50
1:C:186:LYS:H	1:C:186:LYS:HE2	1.77	0.50
1:C:71:GLN:HG3	1:D:203:ASN:CB	2.23	0.50
1:E:329:PHE:O	1:E:332:MET:N	2.43	0.50
1:F:19:CYS:CB	1:F:20:PRO:CD	2.89	0.50
1:A:272:LEU:O	1:A:274:LYS:N	2.45	0.50
1:A:61:PRO:HG2	1:A:62:THR:H	1.76	0.50
1:B:104:GLN:NE2	1:B:105:LEU:N	2.59	0.50
1:B:165:PHE:HA	1:B:282:CYS:HA	1.94	0.50
1:C:109:ASN:HB3	1:C:117:LEU:CD2	2.42	0.50
1:C:91:GLY:H	1:C:186:LYS:HE3	1.77	0.50
1:C:233:LYS:CD	1:C:234:ASN:N	2.73	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:123:VAL:O	1:D:263:LEU:N	2.44	0.50
1:E:69:GLY:O	1:E:71:GLN:N	2.45	0.50
1:F:243:TYR:CZ	1:F:245:GLY:HA2	2.47	0.50
1:A:207:VAL:HB	1:E:54:ASN:ND2	2.26	0.49
1:B:185:TYR:HD2	1:B:192:THR:HG21	1.76	0.49
1:C:103:LEU:N	1:C:103:LEU:HD22	2.26	0.49
1:C:129:VAL:HB	1:C:253:LEU:HD21	1.93	0.49
1:E:90:PRO:HD2	1:E:186:LYS:HZ1	1.74	0.49
1:E:368:ARG:HG3	1:E:376:THR:O	2.12	0.49
1:A:79:ILE:HD11	1:A:298:HIS:N	2.27	0.49
1:B:265:ASP:HB3	1:B:270:GLY:N	2.26	0.49
1:B:103:LEU:O	1:B:277:GLY:HA2	2.10	0.49
1:B:75:TRP:CE2	1:B:300:ARG:HD2	2.47	0.49
1:C:288:TRP:CZ3	1:C:299:TRP:NE1	2.80	0.49
1:D:103:LEU:CD2	1:D:103:LEU:N	2.76	0.49
1:D:145:THR:OG1	1:D:153:ILE:N	2.44	0.49
1:D:217:ASP:OD1	1:D:218:LYS:N	2.44	0.49
1:B:101:ALA:HB2	1:F:339:GLN:HB2	1.94	0.49
1:A:116:THR:HA	1:A:315:VAL:O	2.12	0.49
1:A:147:THR:OG1	1:A:148:VAL:N	2.45	0.49
1:A:190:VAL:HG23	1:A:223:PRO:HD3	1.94	0.49
1:A:298:HIS:HD2	1:A:298:HIS:N	2.07	0.49
1:B:35:GLU:O	1:B:38:ASP:HB2	2.11	0.49
1:C:54:ASN:ND2	1:D:207:VAL:O	2.45	0.49
1:E:194:LYS:H	1:E:194:LYS:CD	2.25	0.49
1:A:339:GLN:HG2	1:A:347:GLN:NE2	2.27	0.49
1:A:75:TRP:CZ2	1:A:300:ARG:HD2	2.47	0.49
1:C:25:VAL:CG1	1:C:26:PRO:HD2	2.43	0.49
1:D:30:ILE:HG12	1:D:36:VAL:HG13	1.93	0.49
1:E:125:VAL:CG1	1:E:263:LEU:HD21	2.43	0.49
1:A:238:ARG:HA	1:E:257:ASN:ND2	2.26	0.49
1:E:124:SER:HB2	1:E:260:THR:HG22	1.93	0.49
1:E:126:LYS:HG2	1:E:260:THR:HG23	1.93	0.49
1:E:72:TYR:O	1:E:75:TRP:HB2	2.12	0.49
1:F:150:THR:O	1:F:150:THR:CG2	2.55	0.49
1:F:194:LYS:C	1:F:196:ILE:H	2.14	0.49
1:F:201:MET:HE3	1:F:201:MET:HA	1.93	0.49
1:F:25:VAL:HG12	1:F:26:PRO:HD2	1.94	0.49
1:A:105:LEU:N	1:A:105:LEU:HD12	2.26	0.49
1:A:253:LEU:O	1:B:242:ASN:HB2	2.13	0.49
1:A:58:GLY:HA3	1:A:76:SER:HA	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:287:GLY:O	1:C:299:TRP:HA	2.13	0.49
1:E:143:LYS:NZ	1:E:295:ASP:OD2	2.45	0.49
1:E:175:GLN:HA	1:E:213:LYS:HA	1.94	0.49
1:F:79:ILE:HG21	1:F:297:HIS:H	1.76	0.49
1:A:193:ILE:HG12	1:A:201:MET:CE	2.43	0.49
1:A:52:PHE:HA	1:A:304:ARG:O	2.12	0.49
1:B:178:VAL:CG2	1:B:179:THR:N	2.75	0.49
1:B:54:ASN:HD22	1:B:55:PRO:HD3	1.76	0.49
1:B:60:PRO:HB2	1:B:61:PRO:HD2	1.94	0.49
1:C:211:ILE:CD1	1:C:211:ILE:N	2.76	0.49
1:D:150:THR:HG22	1:D:150:THR:O	2.13	0.49
1:E:178:VAL:HG22	1:E:179:THR:H	1.75	0.49
1:E:258:THR:CB	1:E:259:LEU:HD22	2.36	0.49
1:E:333:LEU:HD22	1:E:333:LEU:N	2.27	0.49
1:E:370:VAL:HG22	1:E:375:LYS:CA	2.42	0.49
1:F:100:MET:C	1:F:100:MET:SD	2.91	0.49
1:F:166:ALA:HB2	1:F:239:TYR:HB3	1.94	0.49
1:F:97:THR:HG22	1:F:222:TYR:O	2.13	0.49
1:F:164:VAL:HG22	1:F:241:GLY:HA3	1.95	0.49
1:B:104:GLN:NE2	1:B:105:LEU:H	2.11	0.49
1:B:177:LEU:HD21	1:B:209:ASN:H	1.76	0.49
1:C:264:LEU:HD23	1:C:268:GLY:HA2	1.95	0.49
1:C:76:SER:HB2	1:C:298:HIS:HB2	1.95	0.49
1:C:41:THR:HB	1:C:312:LYS:HE3	1.95	0.49
1:D:145:THR:OG1	1:D:153:ILE:HB	2.12	0.49
1:D:69:GLY:HA3	1:D:71:GLN:OE1	2.13	0.49
1:E:125:VAL:HB	1:E:263:LEU:HD11	1.95	0.49
1:E:141:PHE:CD1	1:E:292:ARG:HG3	2.47	0.49
1:D:152:GLY:HA2	1:E:295:ASP:O	2.12	0.49
1:E:94:THR:O	1:E:95:LEU:HD23	2.13	0.49
1:F:69:GLY:O	1:F:71:GLN:N	2.45	0.49
1:B:30:ILE:O	1:F:353:VAL:HG22	2.13	0.49
1:C:132:SER:HA	1:C:135:LEU:HD23	1.94	0.49
1:D:168:GLY:N	1:D:237:THR:HG23	2.26	0.49
1:F:104:GLN:NE2	1:F:276:GLU:HB2	2.16	0.49
1:F:28:LEU:C	1:F:28:LEU:HD23	2.33	0.49
1:B:97:THR:HG22	1:B:222:TYR:C	2.33	0.49
1:C:180:ASP:HA	1:C:206:GLN:NE2	2.28	0.49
1:C:208:LEU:HD12	1:C:208:LEU:HA	1.35	0.49
1:C:276:GLU:OE1	1:C:276:GLU:HA	2.11	0.49
1:D:169:GLY:HA3	1:D:272:LEU:O	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:34:MET:O	1:E:37:LEU:HD22	2.13	0.49
1:E:61:PRO:HG2	1:E:62:THR:H	1.78	0.49
1:F:66:LEU:HB3	1:F:71:GLN:HB2	1.95	0.49
1:A:144:PRO:HB2	1:A:146:ASP:O	2.13	0.49
1:A:224:VAL:CG1	1:A:283:VAL:HG11	2.42	0.49
1:A:84:SER:O	1:A:87:GLU:N	2.45	0.49
1:B:219:ASP:C	1:B:221:MET:N	2.66	0.49
1:C:236:ASN:OD1	1:C:271:PRO:HA	2.12	0.49
1:C:97:THR:HG22	1:C:222:TYR:C	2.33	0.49
1:D:161:GLN:HE22	1:D:251:PRO:HA	1.77	0.49
1:D:57:MET:O	1:D:57:MET:HG3	2.13	0.49
1:E:319:TYR:HB3	1:E:320:PRO:HD2	1.94	0.49
1:E:62:THR:OG1	1:E:63:PRO:CD	2.56	0.49
1:F:285:ILE:H	1:F:285:ILE:HD12	1.78	0.49
1:F:75:TRP:CZ2	1:F:300:ARG:HD2	2.48	0.49
1:F:93:ASN:OD1	1:F:93:ASN:N	2.45	0.49
1:A:172:LEU:C	1:A:172:LEU:HD22	2.33	0.48
1:A:83:THR:HB	1:A:87:GLU:CB	2.37	0.48
1:B:105:LEU:HB3	1:B:120:TRP:NE1	2.29	0.48
1:C:205:ASP:OD1	1:C:209:ASN:ND2	2.46	0.48
1:D:103:LEU:HB2	1:D:278:LEU:HB3	1.94	0.48
1:C:54:ASN:ND2	1:D:208:LEU:HB3	2.25	0.48
1:E:123:VAL:HG13	1:E:264:LEU:HD13	1.95	0.48
1:E:57:MET:HA	1:E:96:PRO:HA	1.94	0.48
1:F:209:ASN:HB3	1:F:212:SER:OG	2.13	0.48
1:F:252:VAL:O	1:F:253:LEU:HD12	2.13	0.48
1:F:69:GLY:C	1:F:71:GLN:N	2.66	0.48
1:A:233:LYS:CE	1:A:234:ASN:ND2	2.75	0.48
1:A:141:PHE:CZ	1:A:292:ARG:HG3	2.48	0.48
1:B:350:GLU:HG3	1:B:351:VAL:N	2.27	0.48
1:B:378:THR:CG2	1:B:379:VAL:N	2.76	0.48
1:B:50:GLU:OE2	1:C:233:LYS:HB2	2.12	0.48
1:C:56:ARG:HH22	1:C:219:ASP:CG	2.16	0.48
1:C:83:THR:HB	1:C:87:GLU:HB3	1.95	0.48
1:E:168:GLY:HA3	1:E:237:THR:CG2	2.38	0.48
1:E:171:PRO:HG2	1:E:215:LYS:HD2	1.95	0.48
1:E:320:PRO:O	1:E:324:LEU:HD12	2.13	0.48
1:E:342:GLU:HG2	1:E:343:GLY:H	1.77	0.48
1:F:192:THR:HG21	1:F:194:LYS:HE2	1.96	0.48
1:F:141:PHE:CE1	1:F:292:ARG:HG3	2.46	0.48
1:F:43:PRO:HA	1:F:312:LYS:HD3	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:52:PHE:CD2	1:C:208:LEU:HD23	2.48	0.48
1:C:166:ALA:HB2	1:C:239:TYR:CB	2.44	0.48
1:C:166:ALA:HA	1:C:238:ARG:O	2.13	0.48
1:C:329:PHE:HA	1:C:332:MET:HG2	1.95	0.48
1:D:142:ASN:N	1:D:154:SER:OG	2.41	0.48
1:D:264:LEU:HG	1:D:268:GLY:HA2	1.96	0.48
1:E:75:TRP:CE2	1:E:300:ARG:HB2	2.49	0.48
1:F:172:LEU:HD13	1:F:174:LEU:HG	1.95	0.48
1:F:254:GLN:HA	1:F:254:GLN:OE1	2.14	0.48
1:F:269:VAL:HA	1:F:313:ARG:NH2	2.29	0.48
1:A:105:LEU:HB3	1:A:120:TRP:CD1	2.49	0.48
1:A:293:ASN:CG	1:A:294:TYR:H	2.15	0.48
1:A:69:GLY:C	1:A:71:GLN:N	2.66	0.48
1:B:165:PHE:CD1	1:B:166:ALA:N	2.81	0.48
1:C:170:GLU:HB2	1:C:171:PRO:HD2	1.95	0.48
1:D:327:SER:O	1:D:330:ASN:N	2.46	0.48
1:E:192:THR:O	1:E:196:ILE:HG22	2.14	0.48
1:F:164:VAL:CG1	1:F:165:PHE:N	2.76	0.48
1:F:216:LEU:HA	1:F:216:LEU:HD23	1.71	0.48
1:A:229:PRO:O	1:A:229:PRO:HG2	2.13	0.48
1:A:280:LEU:HD11	1:A:308:ILE:HD11	1.96	0.48
1:A:269:VAL:HG22	1:A:313:ARG:HH12	1.79	0.48
1:A:56:ARG:CB	1:A:56:ARG:HH11	2.26	0.48
1:C:194:LYS:O	1:C:196:ILE:N	2.47	0.48
1:C:354:TYR:HD1	1:C:354:TYR:N	2.12	0.48
1:D:236:ASN:OD1	1:D:271:PRO:HA	2.13	0.48
1:D:320:PRO:O	1:D:321:MET:C	2.51	0.48
1:D:348:VAL:HG12	1:D:348:VAL:O	2.13	0.48
1:E:208:LEU:C	1:E:208:LEU:HD23	2.34	0.48
1:F:193:ILE:HD11	1:F:201:MET:SD	2.54	0.48
1:F:175:GLN:CB	1:F:230:ASP:HB2	2.24	0.48
1:A:208:LEU:O	1:A:210:PRO:HD3	2.13	0.48
1:A:174:LEU:HB2	1:A:228:HIS:O	2.12	0.48
1:A:303:PRO:HG3	1:B:207:VAL:O	2.13	0.48
1:B:164:VAL:HG22	1:B:241:GLY:HA3	1.94	0.48
1:B:243:TYR:CZ	1:B:245:GLY:CA	2.96	0.48
1:D:175:GLN:HG3	1:D:213:LYS:HG2	1.95	0.48
1:E:104:GLN:HA	1:E:104:GLN:NE2	2.28	0.48
1:E:286:MET:HA	1:E:286:MET:CE	2.40	0.48
1:F:236:ASN:ND2	1:F:272:LEU:O	2.46	0.48
1:F:55:PRO:HD3	1:F:303:PRO:HA	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:290:VAL:HG22	1:B:297:HIS:HD2	1.77	0.48
1:B:50:GLU:HG2	1:C:233:LYS:CA	2.42	0.48
1:B:60:PRO:CB	1:B:61:PRO:HD2	2.44	0.48
1:C:346:THR:HG22	1:C:348:VAL:CG2	2.43	0.48
1:C:52:PHE:C	1:C:53:LEU:HD13	2.33	0.48
1:D:19:CYS:SG	1:E:112:LEU:CD2	2.96	0.48
1:D:207:VAL:O	1:D:208:LEU:CB	2.61	0.48
1:D:228:HIS:HB3	1:D:229:PRO:HD2	1.95	0.48
1:D:25:VAL:HG23	1:D:26:PRO:N	2.29	0.48
1:E:109:ASN:OD1	1:E:117:LEU:HD22	2.13	0.48
1:E:175:GLN:CB	1:E:230:ASP:HB2	2.44	0.48
1:F:41:THR:HB	1:F:45:SER:OG	2.13	0.48
1:A:92:ASN:HD21	1:A:190:VAL:HG12	1.79	0.48
1:A:285:ILE:N	1:A:285:ILE:CD1	2.77	0.48
1:B:194:LYS:CG	1:B:195:THR:H	2.20	0.48
1:B:311:ARG:HH21	1:B:313:ARG:NH2	2.12	0.48
1:E:108:LEU:N	1:E:108:LEU:HD12	2.28	0.48
1:F:25:VAL:CG1	1:F:26:PRO:HD2	2.44	0.48
1:A:142:ASN:ND2	1:A:289:ARG:HG3	2.29	0.48
1:A:239:TYR:CE1	1:E:257:ASN:CB	2.97	0.48
1:A:261:THR:HG22	1:A:262:VAL:N	2.27	0.48
1:B:134:SER:OG	1:C:179:THR:HG23	2.13	0.48
1:C:341:MET:HE1	1:C:347:GLN:HB2	1.94	0.48
1:D:79:ILE:HG12	1:D:298:HIS:N	2.28	0.48
1:E:300:ARG:CG	1:E:301:GLY:N	2.76	0.48
1:F:194:LYS:C	1:F:196:ILE:N	2.65	0.48
1:A:193:ILE:HG12	1:A:201:MET:HE3	1.96	0.48
1:A:194:LYS:HD3	1:A:194:LYS:H	1.79	0.48
1:A:84:SER:O	1:A:86:THR:N	2.47	0.48
1:D:257:ASN:ND2	1:E:239:TYR:N	2.58	0.48
1:D:54:ASN:HD22	1:D:54:ASN:HA	1.64	0.48
1:E:160:SER:HA	1:E:244:THR:O	2.13	0.48
1:D:133:GLY:HA3	1:E:228:HIS:CE1	2.49	0.48
1:E:259:LEU:HA	1:E:259:LEU:HD13	1.49	0.48
1:F:164:VAL:HA	1:F:241:GLY:HA3	1.94	0.48
1:B:108:LEU:CD1	1:B:108:LEU:N	2.77	0.47
1:B:164:VAL:CG1	1:B:165:PHE:N	2.77	0.47
1:B:305:TYR:CG	1:B:306:PHE:N	2.82	0.47
1:C:194:LYS:H	1:C:194:LYS:HD3	1.79	0.47
1:C:194:LYS:HA	1:C:197:THR:HG22	1.96	0.47
1:C:300:ARG:NH2	1:D:206:GLN:O	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:258:THR:O	1:D:259:LEU:HD22	2.13	0.47
1:F:109:ASN:OD1	1:F:109:ASN:N	2.47	0.47
1:F:185:TYR:CD2	1:F:192:THR:HG21	2.49	0.47
1:F:30:ILE:HD11	1:F:36:VAL:HG22	1.94	0.47
1:B:250:PRO:HA	1:B:251:PRO:HD3	1.62	0.47
1:B:288:TRP:HZ3	1:B:299:TRP:NE1	2.11	0.47
1:B:84:SER:O	1:B:87:GLU:N	2.45	0.47
1:C:186:LYS:H	1:C:186:LYS:HD2	1.79	0.47
1:C:194:LYS:HG2	1:C:195:THR:N	2.29	0.47
1:E:115:ASP:HB3	1:E:316:LYS:HD3	1.95	0.47
1:E:204:LYS:O	1:E:208:LEU:N	2.47	0.47
1:A:181:ALA:H	1:A:206:GLN:HE21	1.61	0.47
1:A:175:GLN:HB2	1:A:230:ASP:HB2	1.92	0.47
1:A:268:GLY:O	1:A:313:ARG:NH2	2.46	0.47
1:A:96:PRO:HD2	1:A:299:TRP:CH2	2.48	0.47
1:A:69:GLY:CA	1:A:71:GLN:NE2	2.74	0.47
1:A:257:ASN:HB2	1:B:239:TYR:CD2	2.49	0.47
1:B:35:GLU:HG2	1:B:36:VAL:N	2.29	0.47
1:D:105:LEU:HD23	1:D:120:TRP:CD1	2.49	0.47
1:E:100:MET:HG2	1:E:216:LEU:HD13	1.96	0.47
1:E:287:GLY:O	1:E:299:TRP:HB2	2.14	0.47
1:F:233:LYS:HE3	1:F:233:LYS:HB2	1.60	0.47
1:F:293:ASN:OD1	1:F:294:TYR:N	2.47	0.47
1:A:105:LEU:HB3	1:A:106:PRO:CD	2.45	0.47
1:A:135:LEU:HD12	1:A:135:LEU:H	1.78	0.47
1:A:72:TYR:O	1:A:75:TRP:N	2.47	0.47
1:B:22:PRO:HG2	1:F:359:PRO:CB	2.40	0.47
1:B:275:GLY:C	1:B:277:GLY:N	2.66	0.47
1:B:305:TYR:CE1	1:B:307:LYS:HB2	2.49	0.47
1:C:238:ARG:HH21	1:C:270:GLY:HA2	1.80	0.47
1:C:30:ILE:HD11	1:C:36:VAL:HG22	1.95	0.47
1:E:232:ALA:C	1:E:234:ASN:N	2.68	0.47
1:E:46:VAL:CG1	1:E:47:THR:N	2.77	0.47
1:F:193:ILE:C	1:F:197:THR:HG22	2.35	0.47
1:F:321:MET:C	1:F:323:SER:H	2.18	0.47
1:F:341:MET:HE2	1:F:347:GLN:HG3	1.95	0.47
1:F:35:GLU:O	1:F:36:VAL:C	2.53	0.47
1:F:78:GLY:HA3	2:L:2:GAL:H4	1.97	0.47
1:A:245:GLY:HA3	1:E:251:PRO:HD2	1.97	0.47
1:A:308:ILE:N	1:A:308:ILE:CD1	2.73	0.47
1:A:35:GLU:O	1:A:36:VAL:C	2.52	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:93:ASN:OD1	1:A:93:ASN:N	2.46	0.47
1:B:358:GLU:HG3	1:B:359:PRO:O	2.14	0.47
1:B:371:ASP:C	1:B:373:PHE:N	2.68	0.47
1:B:52:PHE:CZ	1:F:347:GLN:HB3	2.50	0.47
1:C:133:GLY:O	1:C:135:LEU:N	2.47	0.47
1:C:132:SER:C	1:C:135:LEU:HD23	2.35	0.47
1:C:210:PRO:HA	1:C:213:LYS:HE2	1.96	0.47
1:C:302:LEU:HB3	1:C:303:PRO:HD2	1.96	0.47
1:D:175:GLN:HG3	1:D:213:LYS:NZ	2.30	0.47
1:D:161:GLN:NE2	1:D:251:PRO:HA	2.29	0.47
1:D:321:MET:O	1:D:322:ALA:C	2.53	0.47
1:E:239:TYR:CD1	1:E:239:TYR:C	2.85	0.47
1:F:339:GLN:CB	1:F:340:PRO:HD2	2.43	0.47
1:A:100:MET:HB3	1:A:216:LEU:HD13	1.96	0.47
1:A:56:ARG:NH1	1:A:219:ASP:OD1	2.48	0.47
1:A:292:ARG:O	1:A:293:ASN:HB2	2.15	0.47
1:A:90:PRO:HD2	1:A:186:LYS:HE3	1.97	0.47
1:B:54:ASN:HD22	1:B:55:PRO:CD	2.27	0.47
1:C:112:LEU:N	1:C:112:LEU:HD22	2.27	0.47
1:C:28:LEU:C	1:C:28:LEU:HD23	2.35	0.47
1:C:350:GLU:OE1	1:C:352:ARG:NH1	2.48	0.47
1:C:367:THR:HB	1:C:372:ARG:HB2	1.95	0.47
1:D:133:GLY:CA	1:E:228:HIS:CE1	2.98	0.47
1:D:54:ASN:HD21	1:E:208:LEU:HB3	1.79	0.47
1:E:141:PHE:C	1:E:292:ARG:HB2	2.35	0.47
1:F:100:MET:SD	1:F:101:ALA:N	2.87	0.47
1:F:211:ILE:N	1:F:211:ILE:CD1	2.78	0.47
1:F:265:ASP:CG	1:F:269:VAL:HB	2.34	0.47
1:A:145:THR:HB	1:A:152:GLY:HA3	1.97	0.47
1:A:209:ASN:ND2	1:A:212:SER:OG	2.47	0.47
1:C:52:PHE:CD2	1:C:52:PHE:C	2.88	0.47
1:D:100:MET:HG2	1:D:216:LEU:HD13	1.96	0.47
1:D:193:ILE:H	1:D:193:ILE:CD1	2.26	0.47
1:C:71:GLN:CG	1:D:203:ASN:HB3	2.24	0.47
1:E:211:ILE:N	1:E:211:ILE:HD12	2.30	0.47
1:F:265:ASP:OD1	1:F:269:VAL:N	2.48	0.47
1:C:360:VAL:O	1:F:316:LYS:N	2.45	0.47
1:A:233:LYS:HE2	1:E:31:LYS:HD2	1.97	0.47
1:B:63:PRO:HB2	1:B:69:GLY:HA3	1.97	0.47
1:C:105:LEU:HB3	1:C:106:PRO:HD2	1.97	0.47
1:C:77:ARG:O	1:C:298:HIS:CD2	2.68	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:279:TYR:CD1	1:D:279:TYR:N	2.82	0.47
1:F:30:ILE:CG2	1:F:36:VAL:HG13	2.44	0.47
1:A:313:ARG:HG2	1:A:314:TRP:N	2.30	0.47
1:B:262:VAL:HG12	1:B:264:LEU:CB	2.44	0.47
1:C:243:TYR:CZ	1:C:245:GLY:CA	2.98	0.47
1:D:120:TRP:O	1:D:272:LEU:HA	2.15	0.47
1:D:308:ILE:HG22	1:D:310:LEU:HG	1.97	0.47
1:F:161:GLN:CD	1:F:251:PRO:HA	2.35	0.47
1:B:294:TYR:HA	1:B:294:TYR:HD1	1.61	0.47
1:C:161:GLN:HE22	1:C:251:PRO:HA	1.78	0.47
1:C:265:ASP:OD1	1:C:269:VAL:HB	2.14	0.47
1:C:28:LEU:HD21	1:C:30:ILE:C	2.36	0.47
1:C:75:TRP:CE2	1:C:300:ARG:HD2	2.50	0.47
1:E:165:PHE:CD2	1:E:166:ALA:N	2.83	0.47
1:E:194:LYS:C	1:E:196:ILE:N	2.68	0.47
1:F:142:ASN:HB2	1:F:154:SER:HB3	1.97	0.47
2:G:2:GAL:H3	2:G:3:SIA:O1B	2.15	0.47
1:A:125:VAL:O	1:A:125:VAL:HG13	2.14	0.47
1:A:243:TYR:CZ	1:A:245:GLY:HA2	2.50	0.47
1:A:292:ARG:HD2	1:A:292:ARG:C	2.34	0.47
1:A:57:MET:HA	1:A:96:PRO:HA	1.96	0.47
1:A:83:THR:CB	1:A:87:GLU:HB3	2.35	0.47
1:B:25:VAL:HG21	1:F:360:VAL:CG1	2.40	0.47
1:C:172:LEU:O	1:C:174:LEU:CD1	2.62	0.47
1:E:197:THR:O	1:E:197:THR:CG2	2.63	0.47
1:E:76:SER:O	1:E:298:HIS:CB	2.63	0.47
1:E:66:LEU:HB3	1:E:71:GLN:HB2	1.96	0.47
1:F:141:PHE:HD1	1:F:141:PHE:HA	1.54	0.47
1:A:149:ASN:O	1:A:150:THR:HB	2.14	0.46
1:A:33:GLY:O	1:A:36:VAL:HG23	2.14	0.46
1:B:306:PHE:HB3	1:B:308:ILE:HD11	1.97	0.46
1:C:53:LEU:CD2	1:C:306:PHE:CE1	2.93	0.46
1:C:66:LEU:HD23	1:C:66:LEU:N	2.30	0.46
1:D:203:ASN:N	1:D:203:ASN:OD1	2.46	0.46
1:C:305:TYR:CZ	1:D:231:PRO:HB2	2.50	0.46
1:D:254:GLN:HE22	1:E:242:ASN:HB2	1.80	0.46
1:D:316:LYS:HG3	1:D:317:ASN:O	2.14	0.46
1:D:76:SER:OG	1:D:299:TRP:N	2.48	0.46
1:E:57:MET:CB	1:E:96:PRO:HA	2.44	0.46
1:A:300:ARG:NH1	1:A:300:ARG:HG3	2.28	0.46
1:B:339:GLN:HE21	1:B:347:GLN:CD	2.19	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:380:PHE:HA	1:B:381:PRO:HD2	1.46	0.46
1:C:192:THR:H	1:C:195:THR:HG1	1.62	0.46
1:C:175:GLN:CB	1:C:230:ASP:HB2	2.41	0.46
1:D:109:ASN:H	1:D:118:GLN:HE21	1.63	0.46
1:D:327:SER:O	1:D:328:LEU:C	2.52	0.46
1:E:31:LYS:HG3	1:E:32:GLY:N	2.30	0.46
1:F:127:THR:OG1	1:F:304:ARG:HD3	2.15	0.46
1:B:287:GLY:O	1:B:299:TRP:HB2	2.15	0.46
1:B:300:ARG:CG	1:B:301:GLY:N	2.78	0.46
1:C:177:LEU:C	1:C:177:LEU:HD23	2.36	0.46
1:C:257:ASN:ND2	1:C:257:ASN:H	2.06	0.46
1:E:209:ASN:HA	1:E:210:PRO:HD3	1.60	0.46
1:E:77:ARG:O	1:E:298:HIS:CB	2.62	0.46
1:F:256:THR:OG1	1:F:258:THR:OG1	2.30	0.46
1:F:78:GLY:HA3	2:L:2:GAL:C4	2.46	0.46
1:A:204:LYS:C	1:A:209:ASN:HB2	2.36	0.46
1:A:294:TYR:HA	1:A:294:TYR:HD1	1.64	0.46
1:A:332:MET:HE3	1:A:333:LEU:HD23	1.98	0.46
1:A:336:VAL:HB	1:A:338:GLY:H	1.79	0.46
1:A:77:ARG:O	1:A:298:HIS:CG	2.69	0.46
1:A:94:THR:O	1:A:95:LEU:HG	2.16	0.46
1:B:198:LYS:CE	1:B:198:LYS:N	2.74	0.46
1:B:276:GLU:OE2	1:B:276:GLU:N	2.49	0.46
1:B:354:TYR:N	1:B:354:TYR:CD1	2.84	0.46
1:C:153:ILE:HG22	1:C:154:SER:O	2.15	0.46
1:D:211:ILE:H	1:D:211:ILE:HD12	1.80	0.46
1:D:60:PRO:HB2	1:D:61:PRO:HD2	1.98	0.46
1:E:112:LEU:O	1:E:114:CYS:N	2.49	0.46
1:E:300:ARG:HG3	1:E:300:ARG:HH11	1.81	0.46
1:E:369:TYR:CD1	1:E:371:ASP:HA	2.50	0.46
1:E:60:PRO:HB2	1:E:61:PRO:HD2	1.97	0.46
1:F:273:CYS:HB3	1:F:277:GLY:O	2.16	0.46
1:F:283:VAL:HG23	1:F:283:VAL:O	2.15	0.46
1:A:328:LEU:CD2	1:A:328:LEU:C	2.80	0.46
1:A:43:PRO:HA	1:A:312:LYS:HD2	1.97	0.46
1:C:207:VAL:HG23	1:C:208:LEU:N	2.31	0.46
1:C:285:ILE:H	1:C:285:ILE:HD12	1.80	0.46
1:F:139:HIS:O	1:F:154:SER:HB2	2.16	0.46
1:F:34:MET:SD	1:F:37:LEU:CD2	3.03	0.46
1:A:362:GLY:O	1:A:363:ASP:C	2.52	0.46
1:B:125:VAL:HA	1:B:307:LYS:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:271:PRO:C	1:B:272:LEU:HD12	2.35	0.46
1:D:100:MET:C	1:D:100:MET:SD	2.94	0.46
1:D:249:THR:HA	1:D:250:PRO:HD3	1.68	0.46
1:D:317:ASN:ND2	1:D:318:PRO:HD2	2.31	0.46
1:E:165:PHE:O	1:E:239:TYR:HA	2.16	0.46
1:E:79:ILE:HA	1:E:79:ILE:HD13	1.79	0.46
1:E:92:ASN:C	1:E:94:THR:H	2.19	0.46
1:F:218:LYS:HB2	1:F:222:TYR:HE1	1.79	0.46
1:F:30:ILE:HG23	1:F:36:VAL:CG1	2.45	0.46
1:F:94:THR:HG22	1:F:94:THR:O	2.15	0.46
1:E:78:GLY:HA3	2:K:2:GAL:C4	2.45	0.46
1:A:263:LEU:O	1:A:270:GLY:HA2	2.15	0.46
1:A:335:GLN:NE2	1:A:336:VAL:HG13	2.31	0.46
1:B:76:SER:CB	1:B:299:TRP:CE3	2.98	0.46
1:B:372:ARG:C	1:B:373:PHE:CD1	2.89	0.46
1:C:284:ASP:O	1:C:301:GLY:HA2	2.15	0.46
1:C:46:VAL:HG12	1:C:47:THR:N	2.30	0.46
1:D:198:LYS:HA	1:D:198:LYS:HD3	1.47	0.46
1:E:192:THR:CB	1:E:194:LYS:HE2	2.45	0.46
1:E:82:ALA:HB1	1:E:87:GLU:O	2.16	0.46
1:F:105:LEU:HD12	1:F:105:LEU:N	2.31	0.46
1:A:257:ASN:HB2	1:B:239:TYR:CZ	2.51	0.46
1:A:163:HIS:HB3	1:A:284:ASP:OD1	2.16	0.46
1:A:293:ASN:CG	1:A:294:TYR:N	2.69	0.46
1:A:352:ARG:HG3	1:A:354:TYR:CE1	2.48	0.46
1:B:172:LEU:CD2	1:B:173:ASP:N	2.78	0.46
1:B:163:HIS:O	1:B:241:GLY:HA3	2.15	0.46
1:B:341:MET:HE3	1:B:346:THR:CG2	2.46	0.46
1:C:133:GLY:O	1:C:136:LEU:HG	2.16	0.46
1:C:192:THR:HB	1:C:193:ILE:HD12	1.98	0.46
1:D:164:VAL:CG1	1:D:165:PHE:N	2.77	0.46
1:D:316:LYS:HE3	1:D:316:LYS:HA	1.96	0.46
1:D:69:GLY:O	1:D:71:GLN:N	2.49	0.46
1:E:175:GLN:CG	1:E:213:LYS:HG2	2.38	0.46
1:E:340:PRO:O	1:E:346:THR:HA	2.16	0.46
1:F:177:LEU:HD21	1:F:208:LEU:CA	2.40	0.46
1:F:180:ASP:HB3	1:F:182:ARG:HG3	1.96	0.46
1:F:208:LEU:CD2	1:F:210:PRO:HG3	2.46	0.46
1:F:351:VAL:CG1	1:F:352:ARG:N	2.79	0.46
1:B:253:LEU:O	1:C:242:ASN:HB2	2.16	0.46
1:B:311:ARG:NH2	1:B:313:ARG:NH2	2.63	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:233:LYS:HD3	1:C:234:ASN:CA	2.46	0.46
1:C:142:ASN:O	1:C:292:ARG:HB2	2.16	0.46
1:D:46:VAL:HG12	1:D:47:THR:N	2.31	0.46
1:D:76:SER:OG	1:D:299:TRP:HE3	1.99	0.46
1:E:192:THR:H	1:E:195:THR:HB	1.80	0.46
1:E:93:ASN:OD1	1:E:93:ASN:N	2.47	0.46
1:F:192:THR:O	1:F:195:THR:HB	2.15	0.46
1:F:97:THR:HG22	1:F:223:PRO:N	2.31	0.46
1:F:243:TYR:CZ	1:F:245:GLY:HA3	2.50	0.46
1:F:162:TYR:CE1	1:F:283:VAL:HG21	2.51	0.46
1:F:302:LEU:HB3	1:F:303:PRO:HD2	1.98	0.46
1:A:118:GLN:HB2	1:A:314:TRP:CE3	2.51	0.46
1:A:302:LEU:HD23	1:A:302:LEU:HA	1.75	0.46
1:A:319:TYR:N	1:A:320:PRO:CD	2.79	0.46
1:A:72:TYR:O	1:A:75:TRP:HB2	2.15	0.46
1:B:177:LEU:HA	1:B:205:ASP:O	2.16	0.46
1:B:72:TYR:CD2	1:B:77:ARG:NE	2.84	0.46
1:C:28:LEU:HD23	1:C:29:LEU:C	2.37	0.46
1:E:123:VAL:O	1:E:263:LEU:N	2.49	0.46
1:E:289:ARG:O	1:E:297:HIS:O	2.34	0.46
1:E:291:THR:O	1:E:293:ASN:N	2.49	0.46
1:C:233:LYS:HZ1	1:F:350:GLU:HG2	1.80	0.46
1:A:46:VAL:HG12	1:A:47:THR:H	1.80	0.45
1:B:192:THR:CG2	1:B:193:ILE:HD12	2.45	0.45
1:B:58:GLY:HA2	1:B:93:ASN:HA	1.97	0.45
1:D:115:ASP:O	1:D:316:LYS:HE2	2.16	0.45
1:D:278:LEU:HD12	1:D:310:LEU:CD2	2.45	0.45
1:E:59:GLN:HG3	1:E:60:PRO:N	2.29	0.45
1:F:175:GLN:HG3	1:F:213:LYS:HZ3	1.81	0.45
1:A:269:VAL:HG22	1:A:313:ARG:NH1	2.31	0.45
1:B:131:GLY:O	1:B:134:SER:HB3	2.15	0.45
1:B:328:LEU:HD13	1:B:328:LEU:HA	1.53	0.45
1:C:192:THR:O	1:C:195:THR:N	2.48	0.45
1:B:256:THR:HA	1:C:239:TYR:CE1	2.51	0.45
1:C:79:ILE:CG2	1:C:79:ILE:O	2.64	0.45
1:E:194:LYS:O	1:E:196:ILE:N	2.49	0.45
1:E:150:THR:HG23	1:E:292:ARG:HH21	1.82	0.45
1:F:255:PHE:O	1:F:256:THR:HB	2.16	0.45
1:A:145:THR:OG1	1:A:153:ILE:N	2.49	0.45
1:A:207:VAL:O	1:A:209:ASN:N	2.50	0.45
1:A:288:TRP:HZ3	1:A:299:TRP:CE2	2.35	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:125:VAL:HG22	1:B:126:LYS:O	2.16	0.45
1:B:138:VAL:CB	1:B:153:ILE:HG23	2.40	0.45
1:B:255:PHE:O	1:C:240:PHE:HA	2.15	0.45
1:B:257:ASN:HB3	1:C:239:TYR:CE2	2.51	0.45
1:B:320:PRO:O	1:B:324:LEU:HD22	2.16	0.45
1:C:108:LEU:HD12	1:C:108:LEU:N	2.32	0.45
1:C:117:LEU:HD13	1:C:118:GLN:H	1.80	0.45
1:C:164:VAL:HA	1:C:240:PHE:O	2.16	0.45
1:D:194:LYS:HG2	1:D:195:THR:N	2.32	0.45
1:D:97:THR:HG22	1:D:222:TYR:O	2.16	0.45
1:D:50:GLU:HA	1:D:306:PHE:O	2.16	0.45
1:E:112:LEU:HD23	1:E:112:LEU:HA	1.57	0.45
1:E:136:LEU:HD23	1:E:136:LEU:HA	1.75	0.45
1:E:60:PRO:CB	1:E:61:PRO:HD2	2.46	0.45
1:F:52:PHE:HB2	1:F:304:ARG:O	2.15	0.45
1:A:167:VAL:C	1:A:237:THR:HG23	2.36	0.45
1:B:117:LEU:CD1	1:B:117:LEU:N	2.71	0.45
1:B:174:LEU:HA	1:B:230:ASP:H	1.82	0.45
1:C:192:THR:CG2	1:C:194:LYS:HE2	2.44	0.45
1:C:118:GLN:HB3	1:C:314:TRP:CE3	2.51	0.45
1:D:105:LEU:HB3	1:D:120:TRP:NE1	2.32	0.45
1:D:132:SER:O	1:D:135:LEU:CD2	2.63	0.45
1:D:165:PHE:HA	1:D:282:CYS:HA	1.99	0.45
1:D:285:ILE:N	1:D:285:ILE:CD1	2.76	0.45
1:D:342:GLU:HA	1:D:346:THR:HG23	1.97	0.45
1:D:59:GLN:OE1	1:D:77:ARG:HD2	2.17	0.45
1:D:59:GLN:HA	1:D:60:PRO:HD2	1.81	0.45
1:D:79:ILE:HA	1:D:94:THR:HG23	1.97	0.45
1:E:120:TRP:O	1:E:272:LEU:HA	2.15	0.45
1:E:95:LEU:HA	1:E:96:PRO:HD3	1.80	0.45
1:F:178:VAL:CG2	1:F:179:THR:N	2.76	0.45
1:F:332:MET:O	1:F:334:PRO:HD3	2.17	0.45
1:B:45:SER:HA	1:F:354:TYR:O	2.17	0.45
1:A:288:TRP:CZ3	1:A:299:TRP:NE1	2.85	0.45
1:A:305:TYR:C	1:A:306:PHE:CD1	2.90	0.45
1:B:108:LEU:HD12	1:B:108:LEU:N	2.32	0.45
1:B:121:GLU:OE2	1:B:313:ARG:NH2	2.48	0.45
1:B:316:LYS:HD3	1:B:317:ASN:N	2.32	0.45
1:B:30:ILE:CG1	1:B:31:LYS:N	2.79	0.45
1:C:192:THR:CB	1:C:194:LYS:HE2	2.46	0.45
1:B:139:HIS:CD2	1:C:90:PRO:HG3	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:116:THR:OG1	1:D:314:TRP:CE3	2.69	0.45
1:D:180:ASP:CG	1:D:182:ARG:HD3	2.37	0.45
1:D:209:ASN:HA	1:D:210:PRO:HD3	1.72	0.45
1:D:69:GLY:C	1:D:71:GLN:N	2.69	0.45
1:E:90:PRO:HD2	1:E:186:LYS:HZ2	1.80	0.45
1:F:335:GLN:NE2	1:F:335:GLN:HA	2.30	0.45
1:B:319:TYR:HA	1:B:320:PRO:HD3	1.50	0.45
1:C:165:PHE:CZ	1:C:240:PHE:CD1	3.04	0.45
1:E:279:TYR:N	1:E:279:TYR:CD1	2.85	0.45
1:E:329:PHE:O	1:E:331:ASN:N	2.50	0.45
1:F:192:THR:HG22	1:F:193:ILE:H	1.80	0.45
1:F:28:LEU:HD21	1:F:30:ILE:C	2.37	0.45
1:A:299:TRP:HE3	1:A:299:TRP:H	1.65	0.45
1:A:328:LEU:CD2	1:A:333:LEU:HD11	2.46	0.45
1:B:66:LEU:HD23	1:B:66:LEU:N	2.32	0.45
1:C:233:LYS:HD2	1:F:350:GLU:OE2	2.16	0.45
1:B:153:ILE:HG12	1:C:297:HIS:CE1	2.51	0.45
1:D:153:ILE:HD13	1:D:153:ILE:HA	1.66	0.45
1:E:325:ILE:O	1:E:326:SER:C	2.55	0.45
1:F:218:LYS:O	1:F:219:ASP:CB	2.65	0.45
1:F:118:GLN:HB2	1:F:314:TRP:CZ3	2.51	0.45
1:A:175:GLN:HA	1:A:213:LYS:HA	1.99	0.45
1:A:194:LYS:CD	1:A:194:LYS:H	2.29	0.45
1:A:194:LYS:C	1:A:196:ILE:N	2.69	0.45
1:A:231:PRO:O	1:E:305:TYR:HE2	1.99	0.45
1:A:233:LYS:CG	1:A:234:ASN:N	2.75	0.45
1:A:142:ASN:HD21	1:A:289:ARG:HG3	1.81	0.45
1:A:308:ILE:HD12	1:A:308:ILE:H	1.81	0.45
1:B:236:ASN:OD1	1:B:271:PRO:HA	2.17	0.45
1:B:243:TYR:OH	1:B:245:GLY:HA2	2.17	0.45
1:B:276:GLU:CD	1:B:276:GLU:N	2.69	0.45
1:C:308:ILE:HG22	1:C:310:LEU:HG	1.99	0.45
1:D:243:TYR:CZ	1:D:245:GLY:HA3	2.51	0.45
1:D:29:LEU:HB3	1:D:30:ILE:HG22	1.98	0.45
1:E:138:VAL:CB	1:E:153:ILE:HG23	2.45	0.45
1:E:234:ASN:N	1:E:234:ASN:HD22	2.15	0.45
1:E:288:TRP:HZ3	1:E:299:TRP:CE2	2.35	0.45
1:F:79:ILE:O	1:F:79:ILE:HG23	2.17	0.45
1:A:162:TYR:HD2	1:A:285:ILE:HD13	1.82	0.45
1:B:336:VAL:O	1:B:337:GLN:CA	2.54	0.45
1:B:83:THR:O	1:B:84:SER:HB2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:135:LEU:HD12	1:C:157:VAL:HG21	1.99	0.45
1:C:209:ASN:HA	1:C:210:PRO:HD3	1.76	0.45
1:C:256:THR:OG1	1:C:257:ASN:N	2.50	0.45
1:D:236:ASN:ND2	1:D:272:LEU:O	2.49	0.45
1:D:285:ILE:HD12	1:D:285:ILE:H	1.80	0.45
1:D:33:GLY:H	1:D:36:VAL:HG23	1.81	0.45
1:E:117:LEU:HD22	1:E:117:LEU:HA	1.50	0.45
1:E:194:LYS:N	1:E:194:LYS:CD	2.80	0.45
1:E:43:PRO:O	1:E:312:LYS:HB2	2.17	0.45
1:F:127:THR:HA	1:F:305:TYR:O	2.17	0.45
1:A:206:GLN:O	1:E:300:ARG:NH2	2.48	0.45
1:B:111:ASP:C	1:B:113:THR:N	2.69	0.45
1:B:341:MET:HE3	1:B:348:VAL:HB	1.98	0.45
1:C:139:HIS:HD2	1:D:88:ASP:OD1	2.00	0.45
1:C:198:LYS:HD3	1:C:198:LYS:N	2.32	0.45
1:D:274:LYS:C	1:D:275:GLY:O	2.51	0.45
1:E:109:ASN:HD22	1:E:110:GLU:N	2.12	0.45
1:E:117:LEU:O	1:E:314:TRP:CE3	2.70	0.45
1:F:194:LYS:O	1:F:196:ILE:N	2.50	0.45
1:A:108:LEU:HD21	1:A:120:TRP:CD2	2.52	0.44
1:A:191:VAL:HG21	1:A:222:TYR:CZ	2.52	0.44
1:A:79:ILE:HG13	1:A:297:HIS:CB	2.47	0.44
1:B:141:PHE:HE1	1:B:144:PRO:CG	2.22	0.44
1:B:177:LEU:CD2	1:B:209:ASN:H	2.30	0.44
1:B:259:LEU:HA	1:B:259:LEU:HD13	1.54	0.44
1:C:120:TRP:CE3	1:C:120:TRP:HA	2.52	0.44
1:C:150:THR:O	1:C:150:THR:HG22	2.17	0.44
1:C:181:ALA:H	1:C:206:GLN:HE21	1.61	0.44
1:D:208:LEU:O	1:D:210:PRO:HD3	2.16	0.44
1:D:288:TRP:CZ3	1:D:299:TRP:NE1	2.85	0.44
1:D:305:TYR:C	1:D:306:PHE:CD1	2.91	0.44
1:D:340:PRO:HG2	1:D:347:GLN:CG	2.46	0.44
1:E:192:THR:CG2	1:E:193:ILE:HD12	2.46	0.44
1:E:144:PRO:CD	1:E:292:ARG:HD3	2.43	0.44
1:F:308:ILE:HG21	1:F:310:LEU:HD23	1.98	0.44
1:C:269:VAL:HA	1:C:313:ARG:NH2	2.32	0.44
1:D:109:ASN:H	1:D:118:GLN:NE2	2.14	0.44
1:D:164:VAL:HA	1:D:241:GLY:HA3	1.99	0.44
1:E:125:VAL:HG13	1:E:125:VAL:O	2.17	0.44
1:E:250:PRO:HA	1:E:251:PRO:HD3	1.48	0.44
1:B:359:PRO:O	1:B:360:VAL:C	2.56	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:193:ILE:N	1:D:193:ILE:CD1	2.74	0.44
1:F:268:GLY:O	1:F:313:ARG:NH2	2.50	0.44
1:A:339:GLN:HA	1:A:340:PRO:HD2	1.68	0.44
1:B:232:ALA:HB3	1:B:235:GLU:OE1	2.17	0.44
1:B:161:GLN:HE22	1:B:251:PRO:N	2.16	0.44
1:C:111:ASP:O	1:C:114:CYS:O	2.34	0.44
1:D:193:ILE:CG2	1:D:212:SER:HB3	2.47	0.44
1:D:19:CYS:SG	1:E:116:THR:HG21	2.58	0.44
1:E:264:LEU:HD12	1:E:264:LEU:HA	1.58	0.44
1:E:293:ASN:OD1	1:E:294:TYR:HB2	2.18	0.44
1:E:50:GLU:CG	1:E:305:TYR:OH	2.65	0.44
1:E:339:GLN:HA	1:E:340:PRO:HD3	1.59	0.44
1:F:285:ILE:HG23	1:F:299:TRP:CD1	2.53	0.44
1:B:48:GLU:HB2	1:F:352:ARG:HG3	2.00	0.44
1:A:112:LEU:HG	1:A:112:LEU:O	2.16	0.44
1:A:176:GLY:HA3	1:A:226:ILE:O	2.17	0.44
1:A:180:ASP:CG	1:A:182:ARG:HD2	2.37	0.44
1:A:233:LYS:HG3	1:A:234:ASN:ND2	2.32	0.44
1:A:336:VAL:HB	1:A:338:GLY:N	2.33	0.44
1:A:61:PRO:HA	1:A:73:TYR:CD1	2.52	0.44
1:B:179:THR:O	1:B:206:GLN:HG3	2.18	0.44
1:B:23:ALA:HA	1:B:24:PRO:HD3	1.71	0.44
1:B:259:LEU:CD2	1:B:259:LEU:N	2.75	0.44
1:B:57:MET:SD	1:B:301:GLY:HA3	2.57	0.44
1:C:340:PRO:HG2	1:C:347:GLN:HG3	1.98	0.44
1:E:164:VAL:HG12	1:E:165:PHE:N	2.33	0.44
1:E:184:LYS:N	1:E:184:LYS:HD2	2.33	0.44
1:E:305:TYR:C	1:E:306:PHE:CD1	2.91	0.44
1:F:177:LEU:HD23	1:F:177:LEU:HA	1.74	0.44
1:F:90:PRO:HD2	1:F:186:LYS:NZ	2.33	0.44
1:F:285:ILE:CD1	1:F:285:ILE:N	2.78	0.44
1:F:74:GLY:O	1:F:300:ARG:NH1	2.50	0.44
1:A:222:TYR:N	1:A:222:TYR:CD1	2.86	0.44
1:A:233:LYS:CE	1:A:234:ASN:HD21	2.31	0.44
1:A:304:ARG:HD3	1:A:306:PHE:CE1	2.52	0.44
1:B:274:LYS:C	1:B:275:GLY:O	2.55	0.44
1:B:285:ILE:HG22	1:B:287:GLY:N	2.32	0.44
1:C:37:LEU:HG	1:C:106:PRO:HD3	1.99	0.44
1:C:178:VAL:HG22	1:C:179:THR:H	1.82	0.44
1:D:125:VAL:CG1	1:D:263:LEU:HD21	2.47	0.44
1:D:205:ASP:CA	1:D:209:ASN:HB2	2.46	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:252:VAL:HA	1:E:243:TYR:O	2.18	0.44
1:E:180:ASP:CG	1:E:182:ARG:HG2	2.38	0.44
1:E:59:GLN:HG3	1:E:60:PRO:O	2.18	0.44
1:E:80:ASN:HB3	1:E:90:PRO:O	2.17	0.44
1:B:54:ASN:H	1:F:339:GLN:HE22	1.64	0.44
1:F:30:ILE:HD13	1:F:36:VAL:HG22	1.98	0.44
1:B:170:GLU:HA	1:B:279:TYR:CE1	2.52	0.44
1:A:255:PHE:O	1:B:240:PHE:HA	2.17	0.44
1:C:105:LEU:N	1:C:105:LEU:CD1	2.76	0.44
1:C:337:GLN:HE21	1:C:337:GLN:HB2	1.56	0.44
1:D:23:ALA:HA	1:D:24:PRO:HD3	1.66	0.44
1:E:57:MET:HB2	1:E:96:PRO:HB3	1.99	0.44
1:A:193:ILE:O	1:A:197:THR:HG22	2.17	0.44
1:A:285:ILE:H	1:A:285:ILE:CD1	2.31	0.44
1:B:323:SER:O	1:B:327:SER:HB3	2.18	0.44
1:C:249:THR:HA	1:C:250:PRO:HD3	1.55	0.44
1:D:202:VAL:HG23	1:D:205:ASP:OD1	2.18	0.44
1:D:52:PHE:CZ	1:E:208:LEU:HD22	2.53	0.44
1:E:165:PHE:CZ	1:E:240:PHE:CE1	3.05	0.44
1:E:121:GLU:O	1:E:310:LEU:CB	2.66	0.44
1:E:380:PHE:O	1:E:382:GLY:N	2.51	0.44
1:F:162:TYR:CD1	1:F:283:VAL:HG21	2.53	0.44
1:A:25:VAL:CG1	1:A:26:PRO:HD2	2.47	0.44
1:B:364:PRO:HG2	1:B:365:ASP:H	1.83	0.44
1:B:86:THR:HG23	1:B:87:GLU:N	2.33	0.44
1:C:153:ILE:CG2	1:C:154:SER:N	2.81	0.44
1:D:161:GLN:HE22	1:D:251:PRO:CA	2.30	0.44
1:E:104:GLN:HE21	1:E:105:LEU:N	2.16	0.44
1:A:162:TYR:CE1	1:E:255:PHE:HE2	2.35	0.44
1:F:139:HIS:HB2	1:F:140:GLY:H	1.56	0.44
1:F:59:GLN:NE2	1:F:69:GLY:HA3	2.33	0.44
1:F:93:ASN:ND2	2:L:2:GAL:H62	2.32	0.44
1:A:136:LEU:HA	1:A:136:LEU:HD23	1.55	0.43
1:A:28:LEU:HD12	1:A:29:LEU:N	2.31	0.43
1:A:81:LEU:HG	1:A:82:ALA:H	1.83	0.43
1:C:293:ASN:OD1	1:C:294:TYR:N	2.51	0.43
1:C:300:ARG:NH1	1:C:300:ARG:HG3	2.32	0.43
1:C:320:PRO:C	1:C:322:ALA:N	2.69	0.43
1:C:320:PRO:HD3	1:F:366:MET:CE	2.47	0.43
1:D:193:ILE:HD13	1:D:201:MET:SD	2.58	0.43
1:E:105:LEU:CD1	1:E:105:LEU:N	2.77	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:122:ALA:O	1:E:271:PRO:CD	2.65	0.43
1:F:164:VAL:HG12	1:F:165:PHE:N	2.33	0.43
1:F:168:GLY:HA2	1:F:237:THR:HA	2.00	0.43
1:A:142:ASN:ND2	1:A:289:ARG:CG	2.81	0.43
1:A:165:PHE:CD2	1:A:166:ALA:N	2.86	0.43
1:A:172:LEU:HB3	1:A:216:LEU:HB2	1.98	0.43
1:A:88:ASP:C	1:A:184:LYS:HD3	2.38	0.43
1:A:192:THR:HG22	1:A:193:ILE:HD11	1.96	0.43
1:A:89:SER:HA	1:A:184:LYS:HB2	2.00	0.43
1:B:194:LYS:CG	1:B:195:THR:N	2.78	0.43
1:B:35:GLU:O	1:B:36:VAL:C	2.55	0.43
1:B:88:ASP:O	1:B:184:LYS:HB2	2.18	0.43
1:C:322:ALA:O	1:C:326:SER:N	2.47	0.43
1:D:131:GLY:O	1:D:134:SER:HB3	2.18	0.43
1:D:182:ARG:O	1:D:183:THR:C	2.57	0.43
1:D:193:ILE:HD12	1:D:194:LYS:HD3	2.00	0.43
1:D:29:LEU:CB	1:D:30:ILE:HG22	2.48	0.43
1:E:211:ILE:O	1:E:213:LYS:N	2.52	0.43
1:E:229:PRO:O	1:E:229:PRO:HG2	2.18	0.43
1:E:326:SER:O	1:E:330:ASN:N	2.41	0.43
1:F:138:VAL:CB	1:F:153:ILE:HG23	2.38	0.43
1:F:219:ASP:C	1:F:221:MET:N	2.68	0.43
1:F:262:VAL:CG1	1:F:264:LEU:HB2	2.47	0.43
1:F:290:VAL:HG13	1:F:297:HIS:HA	2.00	0.43
1:F:308:ILE:CD1	1:F:308:ILE:N	2.70	0.43
1:F:322:ALA:C	1:F:324:LEU:N	2.70	0.43
1:F:60:PRO:HB2	1:F:61:PRO:HD2	2.00	0.43
1:A:209:ASN:OD1	1:A:211:ILE:HD13	2.17	0.43
1:A:169:GLY:HA3	1:A:236:ASN:ND2	2.33	0.43
1:B:181:ALA:H	1:B:206:GLN:NE2	2.15	0.43
1:B:239:TYR:CD1	1:B:239:TYR:C	2.92	0.43
1:B:50:GLU:HA	1:B:306:PHE:O	2.18	0.43
1:D:47:THR:O	1:D:310:LEU:HD12	2.19	0.43
1:D:117:LEU:O	1:D:314:TRP:HE3	2.01	0.43
1:D:328:LEU:HA	1:D:331:ASN:HD22	1.83	0.43
1:D:37:LEU:HD23	1:D:106:PRO:HD3	2.00	0.43
1:E:205:ASP:HA	1:E:209:ASN:HB2	1.99	0.43
1:E:269:VAL:HG12	1:E:270:GLY:O	2.17	0.43
1:E:162:TYR:CE1	1:E:283:VAL:HG21	2.53	0.43
1:E:91:GLY:H	1:E:186:LYS:CE	2.23	0.43
1:F:184:LYS:N	1:F:184:LYS:CD	2.81	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:124:SER:HB2	1:F:260:THR:HG22	2.01	0.43
1:B:56:ARG:HE	1:F:339:GLN:NE2	2.14	0.43
1:A:168:GLY:N	1:A:237:THR:HG23	2.33	0.43
1:A:297:HIS:O	1:A:298:HIS:C	2.57	0.43
1:B:136:LEU:O	1:B:138:VAL:HG22	2.18	0.43
1:B:178:VAL:HG22	1:B:179:THR:H	1.81	0.43
1:B:304:ARG:HG2	1:B:305:TYR:N	2.33	0.43
1:C:131:GLY:C	1:C:133:GLY:N	2.70	0.43
1:C:164:VAL:HA	1:C:241:GLY:HA3	2.01	0.43
1:C:43:PRO:HA	1:C:312:LYS:HD2	1.99	0.43
1:D:138:VAL:HG12	1:D:153:ILE:HG23	2.00	0.43
1:D:174:LEU:HD12	1:D:174:LEU:O	2.18	0.43
1:D:197:THR:O	1:D:197:THR:HG23	2.18	0.43
1:D:228:HIS:CD2	1:D:228:HIS:N	2.87	0.43
1:D:275:GLY:C	1:D:277:GLY:H	2.21	0.43
1:D:288:TRP:HB2	1:D:297:HIS:O	2.18	0.43
1:E:145:THR:OG1	1:E:153:ILE:N	2.49	0.43
1:E:286:MET:SD	1:E:302:LEU:HD12	2.58	0.43
1:F:149:ASN:O	1:F:150:THR:HB	2.18	0.43
1:F:254:GLN:O	1:F:256:THR:N	2.51	0.43
1:F:291:THR:HB	1:F:293:ASN:HB3	1.99	0.43
1:F:305:TYR:C	1:F:305:TYR:CD1	2.90	0.43
1:F:39:LEU:HA	1:F:39:LEU:HD12	1.77	0.43
1:A:125:VAL:HA	1:A:307:LYS:O	2.18	0.43
1:B:164:VAL:HB	1:B:283:VAL:CG2	2.48	0.43
1:C:129:VAL:HG12	1:C:130:VAL:N	2.34	0.43
1:C:155:THR:HA	1:C:156:PRO:HD2	1.80	0.43
1:C:170:GLU:HA	1:C:279:TYR:CE1	2.53	0.43
1:C:177:LEU:HD23	1:C:178:VAL:N	2.33	0.43
1:C:254:GLN:O	1:C:256:THR:N	2.51	0.43
1:C:75:TRP:CZ2	1:C:300:ARG:HD2	2.53	0.43
1:E:149:ASN:O	1:E:150:THR:HB	2.18	0.43
1:E:205:ASP:N	1:E:205:ASP:OD1	2.52	0.43
1:E:239:TYR:C	1:E:240:PHE:CG	2.91	0.43
1:E:268:GLY:O	1:E:313:ARG:NH2	2.47	0.43
1:E:306:PHE:HB3	1:E:308:ILE:HD11	2.01	0.43
1:F:103:LEU:HA	1:F:103:LEU:HD13	1.76	0.43
1:F:105:LEU:HB2	1:F:276:GLU:O	2.18	0.43
1:F:123:VAL:O	1:F:263:LEU:N	2.50	0.43
1:C:350:GLU:CG	1:F:233:LYS:HG2	2.31	0.43
1:F:285:ILE:CD1	1:F:285:ILE:H	2.31	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:262:VAL:C	1:B:264:LEU:N	2.72	0.43
1:C:181:ALA:N	1:C:206:GLN:HE21	2.16	0.43
1:C:124:SER:HA	1:C:261:THR:O	2.19	0.43
1:D:180:ASP:HA	1:D:206:GLN:NE2	2.32	0.43
1:D:28:LEU:HD12	1:D:29:LEU:H	1.83	0.43
1:E:108:LEU:H	1:E:108:LEU:HD12	1.82	0.43
1:E:288:TRP:HB2	1:E:297:HIS:O	2.18	0.43
1:F:113:THR:HB	1:F:114:CYS:H	1.58	0.43
1:F:141:PHE:CZ	1:F:292:ARG:CZ	3.01	0.43
1:F:125:VAL:HA	1:F:307:LYS:O	2.18	0.43
1:A:265:ASP:N	1:A:270:GLY:H	2.12	0.43
1:A:142:ASN:C	1:A:292:ARG:HB2	2.39	0.43
1:B:324:LEU:HA	1:B:327:SER:OG	2.19	0.43
1:C:190:VAL:CG2	1:C:223:PRO:HD3	2.48	0.43
1:D:229:PRO:HG2	1:D:229:PRO:O	2.18	0.43
1:D:233:LYS:HG3	1:D:234:ASN:ND2	2.32	0.43
1:E:216:LEU:HD23	1:E:216:LEU:HA	1.52	0.43
1:E:219:ASP:C	1:E:221:MET:N	2.68	0.43
1:E:322:ALA:O	1:E:323:SER:C	2.56	0.43
1:F:105:LEU:CD1	1:F:105:LEU:N	2.81	0.43
1:F:294:TYR:HB3	1:F:295:ASP:H	1.40	0.43
1:F:46:VAL:HG12	1:F:47:THR:N	2.34	0.43
1:F:82:ALA:HB1	1:F:87:GLU:O	2.19	0.43
1:A:88:ASP:N	1:A:184:LYS:HD3	2.31	0.43
1:A:197:THR:O	1:A:199:LYS:N	2.51	0.43
1:A:217:ASP:OD1	1:A:218:LYS:N	2.51	0.43
1:A:288:TRP:CE3	1:A:299:TRP:CG	3.06	0.43
1:A:375:LYS:HE3	1:A:375:LYS:HB2	1.62	0.43
1:A:376:THR:HG22	1:A:377:LYS:O	2.18	0.43
1:D:278:LEU:CD2	1:D:278:LEU:C	2.87	0.43
1:D:29:LEU:HA	1:D:29:LEU:HD23	1.55	0.43
1:D:318:PRO:HG2	1:D:319:TYR:CE2	2.54	0.43
1:E:150:THR:O	1:E:150:THR:CG2	2.64	0.43
1:E:203:ASN:O	1:E:206:GLN:CB	2.67	0.43
1:E:226:ILE:HG22	1:E:227:TRP:CD1	2.54	0.43
1:E:263:LEU:HD23	1:E:263:LEU:HA	1.65	0.43
1:E:96:PRO:HG2	1:E:299:TRP:CE2	2.53	0.43
1:F:197:THR:O	1:F:197:THR:CG2	2.66	0.43
1:F:242:ASN:HD22	1:F:242:ASN:N	2.17	0.43
1:A:172:LEU:HD22	1:A:173:ASP:N	2.34	0.43
1:A:238:ARG:HH21	1:A:270:GLY:HA2	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:333:LEU:HA	1:A:334:PRO:HD3	1.65	0.43
1:B:185:TYR:HB2	1:B:194:LYS:HE3	2.00	0.43
1:B:201:MET:HE3	1:B:201:MET:HB3	1.73	0.43
1:B:217:ASP:C	1:B:218:LYS:HD2	2.38	0.43
1:C:310:LEU:H	1:C:310:LEU:HD12	1.84	0.43
1:C:71:GLN:HE21	1:C:73:TYR:HB2	1.84	0.43
1:D:84:SER:O	1:D:86:THR:N	2.51	0.43
1:F:254:GLN:OE1	1:F:254:GLN:CA	2.67	0.43
1:F:80:ASN:OD1	1:F:90:PRO:O	2.36	0.43
1:A:192:THR:CG2	1:A:193:ILE:HD12	2.42	0.43
1:A:23:ALA:HA	1:A:24:PRO:HD3	1.71	0.43
1:C:193:ILE:N	1:C:193:ILE:CD1	2.82	0.43
1:D:219:ASP:O	1:D:221:MET:HB2	2.19	0.43
1:D:100:MET:HB2	1:D:280:LEU:O	2.19	0.43
1:D:95:LEU:HA	1:D:96:PRO:HD2	1.85	0.43
1:F:111:ASP:C	1:F:113:THR:N	2.71	0.43
1:F:35:GLU:OE2	1:F:36:VAL:HG23	2.18	0.43
1:F:77:ARG:HB2	1:F:93:ASN:O	2.18	0.43
1:A:261:THR:CG2	1:A:262:VAL:N	2.82	0.42
1:A:288:TRP:HA	1:A:299:TRP:HA	2.00	0.42
1:C:135:LEU:N	1:C:135:LEU:CD2	2.81	0.42
1:C:192:THR:HG22	1:C:193:ILE:CD1	2.48	0.42
1:D:192:THR:HG22	1:D:193:ILE:HD12	2.01	0.42
1:D:164:VAL:HG23	1:D:241:GLY:HA3	2.00	0.42
1:D:256:THR:OG1	1:D:257:ASN:N	2.52	0.42
1:D:94:THR:O	1:D:299:TRP:HZ3	2.02	0.42
1:E:207:VAL:CG2	1:E:208:LEU:N	2.81	0.42
1:E:164:VAL:HG22	1:E:241:GLY:HA3	2.01	0.42
1:F:155:THR:HA	1:F:156:PRO:HD2	1.73	0.42
1:F:285:ILE:HG23	1:F:299:TRP:HD1	1.83	0.42
1:F:117:LEU:O	1:F:315:VAL:HG22	2.19	0.42
1:F:320:PRO:HG2	1:F:323:SER:HB3	2.01	0.42
1:A:184:LYS:N	1:A:184:LYS:CD	2.79	0.42
1:A:338:GLY:O	1:A:339:GLN:O	2.37	0.42
1:A:56:ARG:CB	1:A:56:ARG:NH1	2.79	0.42
1:A:72:TYR:O	1:A:73:TYR:C	2.58	0.42
1:B:217:ASP:O	1:F:336:VAL:CG1	2.64	0.42
1:B:232:ALA:C	1:B:234:ASN:N	2.73	0.42
1:C:100:MET:SD	1:C:101:ALA:HA	2.59	0.42
1:C:77:ARG:CB	1:C:93:ASN:HB2	2.49	0.42
1:D:174:LEU:HA	1:D:230:ASP:H	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:57:MET:HE1	1:D:299:TRP:HB3	2.01	0.42
1:E:364:PRO:C	1:E:366:MET:H	2.21	0.42
1:E:57:MET:CB	1:E:96:PRO:HB3	2.49	0.42
1:E:57:MET:HG3	1:E:57:MET:O	2.19	0.42
1:F:32:GLY:N	1:F:36:VAL:HG21	2.34	0.42
1:A:78:GLY:O	1:A:79:ILE:HD13	2.19	0.42
1:B:234:ASN:HD22	1:B:234:ASN:N	2.17	0.42
1:B:288:TRP:CE3	1:B:299:TRP:CD1	3.06	0.42
1:C:100:MET:SD	1:C:101:ALA:CA	3.07	0.42
1:C:133:GLY:C	1:C:135:LEU:N	2.72	0.42
1:C:48:GLU:HG2	1:C:309:THR:HG23	2.01	0.42
1:D:172:LEU:CD2	1:D:173:ASP:N	2.78	0.42
1:D:265:ASP:HB3	1:D:270:GLY:H	1.83	0.42
1:E:143:LYS:HA	1:E:292:ARG:HA	2.01	0.42
1:E:161:GLN:CD	1:E:251:PRO:HA	2.39	0.42
1:E:248:THR:O	1:E:249:THR:C	2.57	0.42
1:E:89:SER:HA	1:E:90:PRO:HD3	1.61	0.42
1:A:174:LEU:CD1	1:A:227:TRP:CE3	3.02	0.42
1:B:134:SER:C	1:B:136:LEU:H	2.22	0.42
1:B:209:ASN:C	1:B:211:ILE:H	2.21	0.42
1:B:288:TRP:CE3	1:B:299:TRP:CG	3.07	0.42
1:C:165:PHE:HA	1:C:282:CYS:HA	2.01	0.42
1:C:62:THR:CB	1:C:63:PRO:HD3	2.48	0.42
1:C:73:TYR:CE2	1:D:207:VAL:HG21	2.54	0.42
1:D:209:ASN:HB3	1:D:212:SER:OG	2.20	0.42
1:D:96:PRO:CD	1:D:299:TRP:CZ3	2.98	0.42
1:E:69:GLY:C	1:E:71:GLN:N	2.72	0.42
1:F:124:SER:HB2	1:F:260:THR:CG2	2.50	0.42
1:A:203:ASN:N	1:A:203:ASN:OD1	2.52	0.42
1:B:164:VAL:HB	1:B:283:VAL:HG23	2.01	0.42
1:B:173:ASP:N	1:B:173:ASP:OD1	2.52	0.42
1:B:346:THR:HG22	1:B:348:VAL:N	2.35	0.42
1:C:194:LYS:O	1:C:195:THR:C	2.57	0.42
1:C:341:MET:HE2	1:C:347:GLN:CB	2.49	0.42
1:D:229:PRO:HB2	1:D:239:TYR:CD2	2.54	0.42
1:E:321:MET:HG2	1:E:325:ILE:HD11	2.02	0.42
1:E:342:GLU:CA	1:E:346:THR:HG23	2.49	0.42
1:E:97:THR:HA	1:E:223:PRO:HA	2.01	0.42
1:F:111:ASP:OD1	1:F:114:CYS:HB3	2.19	0.42
1:F:117:LEU:C	1:F:314:TRP:CE3	2.93	0.42
1:F:182:ARG:CG	1:F:183:THR:H	2.27	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:192:THR:HG23	1:A:226:ILE:CD1	2.49	0.42
1:B:134:SER:O	1:B:136:LEU:N	2.52	0.42
1:B:193:ILE:HD12	1:B:194:LYS:H	1.83	0.42
1:B:255:PHE:O	1:B:256:THR:CB	2.61	0.42
1:B:379:VAL:O	1:B:381:PRO:N	2.53	0.42
1:C:233:LYS:HE3	1:C:233:LYS:HB2	1.72	0.42
1:C:253:LEU:HD23	1:C:254:GLN:H	1.84	0.42
1:C:72:TYR:O	1:C:73:TYR:C	2.56	0.42
1:C:76:SER:O	1:C:77:ARG:O	2.37	0.42
1:C:303:PRO:HG3	1:D:208:LEU:HB2	2.02	0.42
1:E:368:ARG:HB2	1:E:368:ARG:HE	1.62	0.42
1:A:194:LYS:O	1:A:195:THR:C	2.58	0.42
1:A:203:ASN:O	1:A:206:GLN:HB2	2.19	0.42
1:B:152:GLY:HA2	1:C:295:ASP:O	2.18	0.42
1:B:152:GLY:C	1:B:153:ILE:HD13	2.40	0.42
1:C:168:GLY:HA3	1:C:237:THR:CG2	2.29	0.42
1:C:172:LEU:O	1:C:174:LEU:HD12	2.20	0.42
1:C:314:TRP:CE3	1:C:314:TRP:HA	2.55	0.42
1:D:77:ARG:O	1:D:298:HIS:CG	2.73	0.42
1:D:55:PRO:HD3	1:D:303:PRO:HB3	2.02	0.42
1:E:132:SER:O	1:E:135:LEU:CD2	2.68	0.42
1:E:25:VAL:CG1	1:E:26:PRO:HD2	2.49	0.42
1:E:57:MET:CA	1:E:96:PRO:HA	2.49	0.42
1:F:150:THR:CG2	1:F:292:ARG:NH2	2.75	0.42
1:C:352:ARG:HD3	1:F:233:LYS:NZ	2.34	0.42
1:F:65:SER:C	1:F:67:THR:H	2.23	0.42
1:F:97:THR:HG22	1:F:223:PRO:CA	2.50	0.42
1:A:216:LEU:HD23	1:A:216:LEU:HA	1.85	0.42
1:A:233:LYS:HB2	1:A:233:LYS:HE3	1.39	0.42
1:A:79:ILE:HG12	1:A:297:HIS:H	1.85	0.42
1:A:56:ARG:HB2	1:A:56:ARG:HH11	1.77	0.42
1:A:86:THR:CG2	1:A:87:GLU:N	2.83	0.42
1:A:133:GLY:CA	1:B:228:HIS:HE1	2.33	0.42
1:B:233:LYS:HG3	1:B:234:ASN:ND2	2.35	0.42
1:B:358:GLU:OE2	1:B:368:ARG:NH2	2.53	0.42
1:C:103:LEU:CD2	1:C:103:LEU:N	2.83	0.42
1:C:104:GLN:HE21	1:C:105:LEU:N	2.18	0.42
1:C:194:LYS:C	1:C:196:ILE:N	2.72	0.42
1:C:192:THR:N	1:C:195:THR:OG1	2.51	0.42
1:C:216:LEU:HA	1:C:216:LEU:HD23	1.47	0.42
1:E:153:ILE:HG22	1:E:154:SER:N	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:321:MET:O	1:E:322:ALA:C	2.58	0.42
1:F:197:THR:C	1:F:199:LYS:N	2.72	0.42
1:F:56:ARG:NH1	1:F:219:ASP:OD2	2.52	0.42
1:F:222:TYR:N	1:F:222:TYR:CD1	2.87	0.42
1:F:174:LEU:HA	1:F:228:HIS:O	2.20	0.42
1:F:37:LEU:HA	1:F:37:LEU:HD12	1.73	0.42
1:A:133:GLY:HA3	1:B:228:HIS:CE1	2.53	0.42
1:A:197:THR:O	1:A:199:LYS:HG3	2.20	0.42
1:B:96:PRO:O	1:B:224:VAL:HG23	2.20	0.42
1:B:264:LEU:HA	1:B:264:LEU:HD12	1.47	0.42
1:B:328:LEU:O	1:B:331:ASN:N	2.50	0.42
1:B:333:LEU:CD1	1:B:334:PRO:HD3	2.50	0.42
1:B:372:ARG:C	1:B:373:PHE:CG	2.94	0.42
1:C:285:ILE:N	1:C:285:ILE:CD1	2.83	0.42
1:C:346:THR:CG2	1:C:348:VAL:HB	2.49	0.42
1:D:114:CYS:HB2	1:D:116:THR:HG21	2.00	0.42
1:D:98:TRP:CH2	1:D:164:VAL:CG1	3.01	0.42
1:D:21:ARG:H	1:D:21:ARG:NE	2.17	0.42
1:E:193:ILE:HD13	1:E:201:MET:HG2	2.02	0.42
1:E:347:GLN:H	1:E:347:GLN:HG2	1.58	0.42
1:E:37:LEU:HD13	1:E:37:LEU:H	1.84	0.42
1:F:121:GLU:OE2	1:F:313:ARG:NH2	2.53	0.42
1:F:246:GLY:HA3	1:F:249:THR:OG1	2.20	0.42
1:A:165:PHE:O	1:A:239:TYR:HA	2.20	0.42
1:A:174:LEU:HD11	1:A:227:TRP:HB3	1.99	0.42
1:A:255:PHE:HD1	1:A:255:PHE:HA	1.72	0.42
1:B:177:LEU:CD2	1:B:208:LEU:N	2.82	0.42
1:B:222:TYR:H	1:B:222:TYR:HD1	1.65	0.42
1:C:192:THR:HB	1:C:194:LYS:CE	2.50	0.42
1:C:201:MET:HE2	1:C:201:MET:HB3	1.96	0.42
1:C:209:ASN:HB3	1:C:212:SER:HB2	2.01	0.42
1:C:30:ILE:CD1	1:C:36:VAL:HG22	2.50	0.42
1:C:50:GLU:OE2	1:D:233:LYS:CA	2.65	0.42
1:D:306:PHE:HB3	1:D:308:ILE:CD1	2.49	0.42
1:D:71:GLN:HE21	1:D:73:TYR:N	2.16	0.42
1:E:298:HIS:N	1:E:298:HIS:HD2	2.15	0.42
1:F:75:TRP:HE1	1:F:300:ARG:HB2	1.83	0.42
1:A:97:THR:HB	1:A:222:TYR:O	2.20	0.41
1:A:252:VAL:HG12	1:B:244:THR:HA	2.01	0.41
1:A:142:ASN:HD21	1:A:289:ARG:CG	2.32	0.41
1:B:246:GLY:HA3	1:B:249:THR:OG1	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:254:GLN:HA	1:B:254:GLN:OE1	2.20	0.41
1:B:280:LEU:HD13	1:B:306:PHE:CD2	2.55	0.41
1:C:193:ILE:O	1:C:196:ILE:HG23	2.20	0.41
1:C:218:LYS:HB3	1:C:219:ASP:H	1.78	0.41
1:C:59:GLN:OE1	1:C:60:PRO:HD2	2.20	0.41
1:D:302:LEU:HA	1:D:302:LEU:HD23	1.79	0.41
1:E:142:ASN:O	1:E:292:ARG:CG	2.60	0.41
1:E:204:LYS:NZ	1:E:204:LYS:HB3	2.35	0.41
1:E:175:GLN:HB2	1:E:230:ASP:HB2	2.02	0.41
1:F:210:PRO:HA	1:F:213:LYS:HE2	2.00	0.41
1:A:222:TYR:HD1	1:A:222:TYR:H	1.68	0.41
1:A:96:PRO:CD	1:A:299:TRP:CH2	3.03	0.41
1:A:79:ILE:HA	1:A:94:THR:CG2	2.49	0.41
1:A:252:VAL:CG1	1:B:244:THR:HA	2.51	0.41
1:B:167:VAL:HG11	1:B:263:LEU:HD13	2.02	0.41
1:B:77:ARG:HD2	1:B:77:ARG:HA	1.95	0.41
1:C:325:ILE:O	1:C:328:LEU:HB2	2.20	0.41
1:D:104:GLN:NE2	1:D:105:LEU:N	2.68	0.41
1:D:111:ASP:OD1	1:D:113:THR:HB	2.20	0.41
1:D:157:VAL:HG13	1:D:288:TRP:C	2.41	0.41
1:D:239:TYR:C	1:D:240:PHE:CG	2.94	0.41
1:D:25:VAL:HG23	1:D:26:PRO:HD2	2.01	0.41
1:D:265:ASP:H	1:D:270:GLY:N	2.11	0.41
1:D:341:MET:C	1:D:346:THR:HG23	2.40	0.41
1:E:105:LEU:HB3	1:E:120:TRP:NE1	2.35	0.41
1:E:177:LEU:HD21	1:E:206:GLN:C	2.31	0.41
1:D:54:ASN:CG	1:E:207:VAL:HG23	2.41	0.41
1:E:23:ALA:HA	1:E:24:PRO:HD3	1.75	0.41
1:E:273:CYS:HB3	1:E:277:GLY:O	2.20	0.41
1:E:337:GLN:HB3	1:E:338:GLY:H	1.50	0.41
1:A:233:LYS:HB2	1:E:50:GLU:OE2	2.20	0.41
1:A:203:ASN:HD22	1:E:71:GLN:HE21	1.68	0.41
1:F:194:LYS:CD	1:F:194:LYS:H	2.33	0.41
1:F:218:LYS:H	1:F:222:TYR:HE1	1.66	0.41
1:C:233:LYS:HE3	1:F:350:GLU:HG2	2.01	0.41
1:F:77:ARG:HH21	2:L:3:SIA:C1	2.33	0.41
1:A:218:LYS:HD3	1:A:218:LYS:N	2.35	0.41
1:C:118:GLN:HA	1:C:313:ARG:O	2.19	0.41
1:D:138:VAL:HG12	1:D:153:ILE:CG2	2.51	0.41
1:E:263:LEU:O	1:E:264:LEU:C	2.58	0.41
1:F:291:THR:O	1:F:293:ASN:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:77:ARG:O	1:F:298:HIS:CG	2.73	0.41
1:A:132:SER:O	1:A:135:LEU:HD13	2.20	0.41
1:A:293:ASN:OD1	1:A:294:TYR:HB2	2.21	0.41
1:B:300:ARG:HG3	1:B:301:GLY:N	2.36	0.41
1:B:350:GLU:CG	1:B:351:VAL:N	2.82	0.41
1:C:166:ALA:HB2	1:C:239:TYR:HB3	2.02	0.41
1:C:239:TYR:C	1:C:240:PHE:CG	2.94	0.41
1:C:263:LEU:HA	1:C:263:LEU:HD23	1.84	0.41
1:D:104:GLN:NE2	1:D:105:LEU:O	2.52	0.41
1:D:21:ARG:O	1:D:21:ARG:HG2	2.21	0.41
1:E:192:THR:HG23	1:E:226:ILE:CD1	2.50	0.41
1:E:243:TYR:HH	1:E:245:GLY:HA2	1.83	0.41
1:E:254:GLN:OE1	1:E:254:GLN:HA	2.20	0.41
1:E:36:VAL:O	1:E:39:LEU:HG	2.20	0.41
1:A:182:ARG:HG3	1:E:66:LEU:HD12	2.01	0.41
1:F:92:ASN:HD21	1:F:190:VAL:HG12	1.85	0.41
1:A:158:GLU:HB3	1:A:248:THR:O	2.20	0.41
1:A:364:PRO:HG2	1:A:365:ASP:N	2.34	0.41
1:B:198:LYS:HE2	1:B:198:LYS:CA	2.51	0.41
1:B:141:PHE:CD1	1:B:292:ARG:HB2	2.55	0.41
1:C:132:SER:CA	1:C:135:LEU:HD23	2.50	0.41
1:C:165:PHE:CZ	1:C:240:PHE:CE1	3.08	0.41
1:C:196:ILE:O	1:C:196:ILE:HD12	2.20	0.41
1:D:159:GLY:HA3	1:D:288:TRP:NE1	2.36	0.41
1:D:263:LEU:H	1:D:263:LEU:HG	1.58	0.41
1:D:318:PRO:O	1:D:319:TYR:CD1	2.74	0.41
1:E:224:VAL:C	1:E:226:ILE:N	2.73	0.41
1:E:39:LEU:O	1:E:40:VAL:C	2.57	0.41
1:E:76:SER:O	1:E:298:HIS:HB3	2.21	0.41
1:F:91:GLY:O	1:F:93:ASN:N	2.54	0.41
1:A:98:TRP:HB3	1:A:216:LEU:HD11	2.03	0.41
1:A:328:LEU:HD12	1:A:332:MET:HE1	0.50	0.41
1:B:194:LYS:HA	1:B:197:THR:O	2.21	0.41
1:B:265:ASP:CG	1:B:269:VAL:HB	2.41	0.41
1:B:339:GLN:HE21	1:B:347:GLN:NE2	2.17	0.41
1:C:133:GLY:C	1:C:135:LEU:H	2.23	0.41
1:C:54:ASN:ND2	1:D:207:VAL:CG2	2.84	0.41
1:D:139:HIS:O	1:D:154:SER:CB	2.69	0.41
1:D:208:LEU:HD23	1:D:208:LEU:C	2.41	0.41
1:D:33:GLY:O	1:D:36:VAL:N	2.53	0.41
1:E:360:VAL:HA	1:E:361:PRO:HD2	1.66	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:71:GLN:HA	1:E:71:GLN:OE1	2.17	0.41
1:F:165:PHE:CD2	1:F:166:ALA:N	2.88	0.41
1:F:164:VAL:CG2	1:F:241:GLY:HA3	2.49	0.41
1:F:264:LEU:N	1:F:264:LEU:HD12	2.35	0.41
1:F:79:ILE:HA	1:F:79:ILE:HD13	1.57	0.41
1:A:192:THR:O	1:A:195:THR:N	2.54	0.41
1:A:330:ASN:HB3	1:A:331:ASN:H	1.62	0.41
1:B:218:LYS:HA	1:F:337:GLN:N	2.36	0.41
1:C:111:ASP:C	1:C:113:THR:H	2.23	0.41
1:D:151:LYS:HA	1:D:151:LYS:HD3	1.78	0.41
1:D:55:PRO:HD3	1:D:303:PRO:CB	2.51	0.41
1:D:68:GLU:H	1:D:68:GLU:HG2	1.60	0.41
1:E:351:VAL:CG1	1:E:352:ARG:N	2.83	0.41
1:F:25:VAL:HG12	1:F:26:PRO:CD	2.51	0.41
1:A:125:VAL:CG1	1:A:125:VAL:O	2.69	0.41
1:A:148:VAL:C	1:A:150:THR:N	2.74	0.41
1:A:184:LYS:HD2	1:A:184:LYS:H	1.84	0.41
1:A:69:GLY:C	1:A:71:GLN:NE2	2.74	0.41
1:B:80:ASN:HB3	1:B:91:GLY:H	1.85	0.41
1:D:189:GLY:O	1:D:190:VAL:HB	2.21	0.41
1:D:34:MET:O	1:D:37:LEU:HB2	2.21	0.41
1:A:231:PRO:CG	1:E:305:TYR:CD2	3.04	0.41
1:F:175:GLN:HG2	1:F:213:LYS:CD	2.33	0.41
1:F:192:THR:CG2	1:F:193:ILE:HD12	2.51	0.41
1:A:90:PRO:HD3	1:A:184:LYS:HB2	2.02	0.41
1:A:69:GLY:HA3	1:A:71:GLN:NE2	2.17	0.41
1:B:288:TRP:HZ3	1:B:299:TRP:CE2	2.37	0.41
1:B:141:PHE:CZ	1:B:292:ARG:HG3	2.55	0.41
1:B:341:MET:CE	1:B:341:MET:HA	2.48	0.41
1:C:115:ASP:CG	1:C:116:THR:H	2.23	0.41
1:C:116:THR:HG23	1:C:314:TRP:CZ3	2.56	0.41
1:C:139:HIS:HD2	1:D:88:ASP:CG	2.24	0.41
1:C:132:SER:HB2	1:C:255:PHE:CE2	2.56	0.41
1:C:273:CYS:CB	1:C:277:GLY:O	2.66	0.41
1:D:264:LEU:HA	1:D:264:LEU:HD12	1.43	0.41
1:E:265:ASP:OD1	1:E:269:VAL:N	2.54	0.41
1:B:48:GLU:HB2	1:F:352:ARG:CG	2.50	0.41
1:F:79:ILE:O	1:F:79:ILE:CG2	2.69	0.41
1:A:170:GLU:HB2	1:A:171:PRO:CD	2.46	0.41
1:A:175:GLN:HE22	1:A:177:LEU:HD21	1.86	0.41
1:B:360:VAL:HG12	1:B:361:PRO:CD	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:142:ASN:O	1:C:144:PRO:HG3	2.21	0.41
1:C:164:VAL:O	1:C:282:CYS:HB2	2.20	0.41
1:C:319:TYR:HA	1:C:320:PRO:HD3	1.98	0.41
1:D:302:LEU:HD23	1:D:303:PRO:HD3	2.03	0.41
1:E:207:VAL:CG2	1:E:208:LEU:H	2.34	0.41
1:E:224:VAL:C	1:E:226:ILE:H	2.22	0.41
1:E:251:PRO:O	1:E:252:VAL:HG13	2.21	0.41
1:F:289:ARG:HB3	1:F:298:HIS:O	2.21	0.41
1:F:77:ARG:O	1:F:298:HIS:CB	2.69	0.41
1:F:88:ASP:O	1:F:90:PRO:HD3	2.20	0.41
1:A:20:PRO:HG2	1:B:116:THR:HG21	2.03	0.41
1:A:260:THR:HG22	1:A:261:THR:N	2.36	0.41
1:A:142:ASN:O	1:A:292:ARG:HG2	2.21	0.41
1:B:151:LYS:HD3	1:B:151:LYS:HA	1.86	0.41
1:B:194:LYS:O	1:B:197:THR:N	2.54	0.41
1:B:318:PRO:HB2	1:B:319:TYR:CE1	2.56	0.41
1:B:95:LEU:HA	1:B:96:PRO:HD2	1.76	0.41
1:C:127:THR:HA	1:C:305:TYR:O	2.21	0.41
1:D:264:LEU:HD12	1:D:270:GLY:HA3	2.03	0.41
1:D:275:GLY:O	1:D:277:GLY:N	2.54	0.41
1:E:177:LEU:CD2	1:E:177:LEU:C	2.89	0.41
1:E:194:LYS:HD3	1:E:195:THR:N	2.31	0.41
1:E:29:LEU:C	1:E:30:ILE:HG22	2.41	0.41
1:E:90:PRO:HD2	1:E:186:LYS:CE	2.50	0.41
1:F:180:ASP:CG	1:F:182:ARG:HD2	2.42	0.41
1:F:259:LEU:CD1	1:F:259:LEU:H	2.30	0.41
1:F:142:ASN:CA	1:F:292:ARG:HB2	2.51	0.41
1:F:280:LEU:HD13	1:F:306:PHE:CD2	2.56	0.41
1:F:116:THR:HG23	1:F:314:TRP:CZ3	2.56	0.41
1:B:49:ILE:HG12	1:F:351:VAL:HG22	2.01	0.41
1:F:354:TYR:CD1	1:F:354:TYR:N	2.89	0.41
1:A:231:PRO:HB2	1:E:305:TYR:CD2	2.55	0.40
1:A:263:LEU:CD2	1:A:263:LEU:N	2.82	0.40
1:A:125:VAL:CG1	1:A:263:LEU:HD21	2.40	0.40
1:B:153:ILE:HD11	1:C:297:HIS:CG	2.56	0.40
1:B:176:GLY:HA2	1:B:226:ILE:O	2.21	0.40
1:B:52:PHE:CZ	1:C:208:LEU:HD23	2.56	0.40
1:C:175:GLN:NE2	1:C:176:GLY:N	2.60	0.40
1:D:165:PHE:CB	1:D:282:CYS:HB3	2.51	0.40
1:A:233:LYS:CE	1:E:31:LYS:HD2	2.51	0.40
1:F:280:LEU:N	1:F:280:LEU:HD23	2.35	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:165:PHE:HA	1:F:281:SER:O	2.20	0.40
1:F:302:LEU:HA	1:F:302:LEU:HD23	1.77	0.40
1:A:105:LEU:HD23	1:A:120:TRP:CE2	2.56	0.40
1:A:176:GLY:CA	1:A:226:ILE:O	2.70	0.40
1:A:192:THR:H	1:A:195:THR:HB	1.87	0.40
1:B:263:LEU:HG	1:B:263:LEU:H	1.61	0.40
1:B:306:PHE:N	1:B:306:PHE:CD1	2.89	0.40
1:C:55:PRO:HB3	1:C:302:LEU:O	2.20	0.40
1:C:252:VAL:HG13	1:D:244:THR:HG23	2.01	0.40
1:D:326:SER:O	1:D:327:SER:C	2.57	0.40
1:D:54:ASN:ND2	1:E:207:VAL:HG23	2.35	0.40
1:E:209:ASN:OD1	1:E:210:PRO:HD2	2.21	0.40
1:E:222:TYR:H	1:E:222:TYR:HD1	1.68	0.40
1:E:166:ALA:CA	1:E:238:ARG:O	2.67	0.40
1:E:288:TRP:CE3	1:E:299:TRP:HB3	2.56	0.40
1:E:300:ARG:HG3	1:E:301:GLY:N	2.37	0.40
1:F:175:GLN:HE21	1:F:176:GLY:N	2.19	0.40
1:F:250:PRO:HA	1:F:251:PRO:HD3	1.73	0.40
1:F:308:ILE:CD1	1:F:308:ILE:H	2.29	0.40
1:A:182:ARG:O	1:A:183:THR:O	2.40	0.40
1:A:93:ASN:ND2	2:G:2:GAL:H62	2.36	0.40
1:A:71:GLN:CB	1:B:203:ASN:HB3	2.52	0.40
1:B:209:ASN:HA	1:B:210:PRO:HD3	1.68	0.40
1:B:175:GLN:HG2	1:B:213:LYS:HG2	2.04	0.40
1:C:151:LYS:HD3	1:C:151:LYS:HA	1.83	0.40
1:C:28:LEU:HD21	1:C:30:ILE:CA	2.51	0.40
1:C:320:PRO:HD3	1:F:366:MET:HE1	2.04	0.40
1:D:192:THR:O	1:D:196:ILE:HG22	2.21	0.40
1:D:211:ILE:H	1:D:211:ILE:CD1	2.33	0.40
1:D:59:GLN:NE2	1:D:72:TYR:HB2	2.36	0.40
1:E:109:ASN:ND2	1:E:110:GLU:H	2.15	0.40
1:E:113:THR:C	1:E:115:ASP:N	2.73	0.40
1:E:162:TYR:CE1	1:E:164:VAL:HG23	2.56	0.40
1:D:50:GLU:OE2	1:E:233:LYS:O	2.39	0.40
1:E:285:ILE:CG2	1:E:299:TRP:HD1	2.34	0.40
1:F:103:LEU:CD2	1:F:103:LEU:N	2.84	0.40
1:F:105:LEU:HB3	1:F:120:TRP:NE1	2.36	0.40
1:F:192:THR:HB	1:F:194:LYS:CD	2.36	0.40
1:F:209:ASN:C	1:F:211:ILE:H	2.23	0.40
1:F:23:ALA:HA	1:F:24:PRO:HD3	1.70	0.40
1:A:175:GLN:NE2	1:A:177:LEU:HD21	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:208:LEU:CD2	1:A:210:PRO:HG3	2.51	0.40
1:A:371:ASP:C	1:A:373:PHE:N	2.74	0.40
1:B:209:ASN:O	1:B:211:ILE:N	2.55	0.40
1:B:23:ALA:O	1:F:360:VAL:HG22	2.20	0.40
1:B:262:VAL:C	1:B:264:LEU:H	2.23	0.40
1:C:76:SER:OG	1:C:299:TRP:N	2.54	0.40
1:D:140:GLY:O	1:D:154:SER:OG	2.39	0.40
1:D:250:PRO:HA	1:D:251:PRO:HD3	1.43	0.40
1:D:298:HIS:CD2	1:D:298:HIS:N	2.89	0.40
1:E:191:VAL:HG11	1:E:222:TYR:CE2	2.57	0.40
1:E:165:PHE:HB2	1:E:282:CYS:HB3	2.03	0.40
1:E:302:LEU:HA	1:E:302:LEU:HD23	1.90	0.40
1:E:316:LYS:HE2	1:E:316:LYS:HB2	1.95	0.40
1:E:79:ILE:O	1:E:79:ILE:CG2	2.69	0.40
1:F:174:LEU:CD2	1:F:227:TRP:HB3	2.51	0.40
1:F:35:GLU:CD	1:F:35:GLU:H	2.24	0.40
1:A:79:ILE:CG1	1:A:297:HIS:H	2.34	0.40
1:A:29:LEU:HB2	1:A:30:ILE:HG22	2.03	0.40
1:A:57:MET:O	1:A:57:MET:HG3	2.22	0.40
1:A:79:ILE:HD12	1:A:79:ILE:HG23	1.82	0.40
1:B:139:HIS:HB2	1:B:140:GLY:H	1.80	0.40
1:B:144:PRO:HD3	1:B:292:ARG:CG	2.52	0.40
1:A:134:SER:OG	1:B:179:THR:HG23	2.22	0.40
1:B:180:ASP:O	1:B:182:ARG:N	2.55	0.40
1:B:169:GLY:HA3	1:B:272:LEU:O	2.22	0.40
1:B:324:LEU:N	1:B:324:LEU:HD22	2.32	0.40
1:C:79:ILE:HD13	1:C:94:THR:CG2	2.48	0.40
1:D:164:VAL:HA	1:D:240:PHE:O	2.20	0.40
1:D:283:VAL:O	1:D:283:VAL:HG23	2.20	0.40
1:D:122:ALA:HA	1:D:310:LEU:HB3	2.03	0.40
1:D:108:LEU:HG	1:D:312:LYS:HE2	2.04	0.40
1:E:300:ARG:HG3	1:E:301:GLY:H	1.87	0.40
1:F:192:THR:N	1:F:195:THR:HB	2.36	0.40
1:F:46:VAL:HG12	1:F:47:THR:H	1.87	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:274:LYS:CD	1:A:328:LEU:O[2_555]	1.11	1.09

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	364/383 (95%)	254 (70%)	75 (21%)	35 (10%)	0 8
1	B	363/383 (95%)	278 (77%)	62 (17%)	23 (6%)	1 17
1	C	353/383 (92%)	279 (79%)	55 (16%)	19 (5%)	2 20
1	D	336/383 (88%)	257 (76%)	56 (17%)	23 (7%)	1 15
1	E	365/383 (95%)	264 (72%)	67 (18%)	34 (9%)	0 9
1	F	350/383 (91%)	263 (75%)	57 (16%)	30 (9%)	1 10
All	All	2131/2298 (93%)	1595 (75%)	372 (18%)	164 (8%)	1 12

All (164) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	43	PRO
1	A	148	VAL
1	A	183	THR
1	A	276	GLU
1	A	293	ASN
1	A	323	SER
1	A	327	SER
1	A	334	PRO
1	A	339	GLN
1	A	372	ARG
1	A	381	PRO
1	B	43	PRO
1	B	85	ASP
1	B	148	VAL
1	B	212	SER
1	B	329	PHE
1	C	43	PRO
1	C	62	THR
1	C	77	ARG
1	C	85	ASP

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Mol	Chain	Res	Type
1	C	193	ILE
1	C	233	LYS
1	C	293	ASN
1	C	299	TRP
1	D	43	PRO
1	D	84	SER
1	D	85	ASP
1	D	208	LEU
1	D	217	ASP
1	D	219	ASP
1	D	293	ASN
1	D	298	HIS
1	D	320	PRO
1	D	321	MET
1	E	22	PRO
1	E	43	PRO
1	E	77	ARG
1	E	85	ASP
1	E	113	THR
1	E	212	SER
1	E	233	LYS
1	E	257	ASN
1	E	258	THR
1	E	293	ASN
1	E	337	GLN
1	E	342	GLU
1	E	381	PRO
1	F	19	CYS
1	F	40	VAL
1	F	41	THR
1	F	61	PRO
1	F	62	THR
1	F	77	ARG
1	F	92	ASN
1	F	183	THR
1	F	293	ASN
1	F	320	PRO
1	A	70	GLY
1	A	71	GLN
1	A	92	ASN
1	A	110	GLU
1	A	198	LYS

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Mol	Chain	Res	Type
1	A	212	SER
1	A	273	CYS
1	A	322	ALA
1	A	328	LEU
1	A	336	VAL
1	A	337	GLN
1	A	362	GLY
1	A	366	MET
1	B	62	THR
1	B	198	LYS
1	B	276	GLU
1	B	318	PRO
1	B	373	PHE
1	B	381	PRO
1	C	70	GLY
1	C	71	GLN
1	C	148	VAL
1	C	207	VAL
1	C	298	HIS
1	D	71	GLN
1	D	183	THR
1	D	322	ALA
1	D	342	GLU
1	E	20	PRO
1	E	30	ILE
1	E	71	GLN
1	E	80	ASN
1	E	111	ASP
1	E	148	VAL
1	E	298	HIS
1	F	43	PRO
1	F	179	THR
1	F	212	SER
1	F	219	ASP
1	F	255	PHE
1	F	258	THR
1	F	342	GLU
1	F	368	ARG
1	A	18	ALA
1	A	90	PRO
1	A	249	THR
1	A	342	GLU

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Mol	Chain	Res	Type
1	B	77	ARG
1	C	212	SER
1	D	55	PRO
1	D	92	ASN
1	E	70	GLY
1	E	90	PRO
1	E	371	ASP
1	E	379	VAL
1	F	71	GLN
1	F	90	PRO
1	F	113	THR
1	F	148	VAL
1	A	77	ARG
1	A	156	PRO
1	A	330	ASN
1	B	20	PRO
1	B	111	ASP
1	B	135	LEU
1	B	249	THR
1	B	372	ARG
1	C	61	PRO
1	C	255	PHE
1	C	342	GLU
1	D	144	PRO
1	D	179	THR
1	D	190	VAL
1	E	93	ASN
1	E	144	PRO
1	E	330	ASN
1	F	198	LYS
1	B	71	GLN
1	B	361	PRO
1	D	41	THR
1	D	218	LYS
1	E	62	THR
1	F	135	LEU
1	F	190	VAL
1	A	62	THR
1	B	84	SER
1	B	206	GLN
1	D	70	GLY
1	E	145	THR

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Mol	Chain	Res	Type
1	E	249	THR
1	F	70	GLY
1	F	155	THR
1	A	36	VAL
1	E	79	ILE
1	F	269	VAL
1	A	193	ILE
1	A	207	VAL
1	B	70	GLY
1	C	90	PRO
1	E	320	PRO
1	C	320	PRO
1	F	63	PRO
1	B	61	PRO
1	D	90	PRO
1	E	190	VAL
1	E	360	VAL
1	F	249	THR

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	321/335 (96%)	248 (77%)	73 (23%)	1 6
1	B	322/335 (96%)	242 (75%)	80 (25%)	0 5
1	C	314/335 (94%)	233 (74%)	81 (26%)	0 4
1	D	298/335 (89%)	207 (70%)	91 (30%)	0 2
1	E	322/335 (96%)	228 (71%)	94 (29%)	0 2
1	F	311/335 (93%)	233 (75%)	78 (25%)	0 4
All	All	1888/2010 (94%)	1391 (74%)	497 (26%)	0 4

All (497) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	THR
1	A	43	PRO
1	A	53	LEU
1	A	66	LEU
1	A	75	TRP
1	A	76	SER
1	A	93	ASN
1	A	95	LEU
1	A	97	THR
1	A	103	LEU
1	A	107	MET
1	A	108	LEU
1	A	113	THR
1	A	117	LEU
1	A	124	SER
1	A	127	THR
1	A	132	SER
1	A	138	VAL
1	A	141	PHE
1	A	151	LYS
1	A	154	SER
1	A	167	VAL
1	A	172	LEU
1	A	179	THR
1	A	184	LYS
1	A	186	LYS
1	A	187	GLU
1	A	188	GLU
1	A	190	VAL
1	A	193	ILE
1	A	194	LYS
1	A	195	THR
1	A	196	ILE
1	A	197	THR
1	A	198	LYS
1	A	216	LEU
1	A	219	ASP
1	A	224	VAL
1	A	230	ASP
1	A	233	LYS
1	A	234	ASN
1	A	240	PHE
1	A	244	THR

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Mol	Chain	Res	Type
1	A	252	VAL
1	A	253	LEU
1	A	256	THR
1	A	258	THR
1	A	259	LEU
1	A	264	LEU
1	A	278	LEU
1	A	280	LEU
1	A	281	SER
1	A	283	VAL
1	A	286	MET
1	A	288	TRP
1	A	292	ARG
1	A	294	TYR
1	A	298	HIS
1	A	299	TRP
1	A	309	THR
1	A	310	LEU
1	A	315	VAL
1	A	347	GLN
1	A	352	ARG
1	A	360	VAL
1	A	361	PRO
1	A	364	PRO
1	A	368	ARG
1	A	369	TYR
1	A	372	ARG
1	A	373	PHE
1	A	380	PHE
1	A	381	PRO
1	B	30	ILE
1	B	37	LEU
1	B	41	THR
1	B	45	SER
1	B	46	VAL
1	B	53	LEU
1	B	54	ASN
1	B	60	PRO
1	B	66	LEU
1	B	75	TRP
1	B	81	LEU
1	B	93	ASN

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Mol	Chain	Res	Type
1	B	97	THR
1	B	117	LEU
1	B	121	GLU
1	B	130	VAL
1	B	132	SER
1	B	135	LEU
1	B	138	VAL
1	B	139	HIS
1	B	141	PHE
1	B	147	THR
1	B	151	LYS
1	B	154	SER
1	B	172	LEU
1	B	173	ASP
1	B	174	LEU
1	B	175	GLN
1	B	179	THR
1	B	180	ASP
1	B	184	LYS
1	B	186	LYS
1	B	192	THR
1	B	193	ILE
1	B	196	ILE
1	B	197	THR
1	B	198	LYS
1	B	201	MET
1	B	219	ASP
1	B	230	ASP
1	B	233	LYS
1	B	234	ASN
1	B	237	THR
1	B	240	PHE
1	B	242	ASN
1	B	244	THR
1	B	248	THR
1	B	252	VAL
1	B	253	LEU
1	B	256	THR
1	B	257	ASN
1	B	258	THR
1	B	260	THR
1	B	265	ASP

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Mol	Chain	Res	Type
1	B	272	LEU
1	B	276	GLU
1	B	281	SER
1	B	283	VAL
1	B	288	TRP
1	B	290	VAL
1	B	293	ASN
1	B	294	TYR
1	B	297	HIS
1	B	299	TRP
1	B	304	ARG
1	B	309	THR
1	B	310	LEU
1	B	316	LYS
1	B	332	MET
1	B	342	GLU
1	B	347	GLN
1	B	353	VAL
1	B	354	TYR
1	B	361	PRO
1	B	364	PRO
1	B	369	TYR
1	B	371	ASP
1	B	372	ARG
1	B	373	PHE
1	B	380	PHE
1	C	29	LEU
1	C	31	LYS
1	C	37	LEU
1	C	41	THR
1	C	43	PRO
1	C	45	SER
1	C	53	LEU
1	C	57	MET
1	C	66	LEU
1	C	71	GLN
1	C	75	TRP
1	C	76	SER
1	C	79	ILE
1	C	81	LEU
1	C	93	ASN
1	C	97	THR

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Mol	Chain	Res	Type
1	C	99	SER
1	C	100	MET
1	C	109	ASN
1	C	112	LEU
1	C	116	THR
1	C	117	LEU
1	C	121	GLU
1	C	132	SER
1	C	138	VAL
1	C	139	HIS
1	C	141	PHE
1	C	151	LYS
1	C	154	SER
1	C	172	LEU
1	C	173	ASP
1	C	174	LEU
1	C	175	GLN
1	C	179	THR
1	C	182	ARG
1	C	186	LYS
1	C	192	THR
1	C	193	ILE
1	C	194	LYS
1	C	196	ILE
1	C	197	THR
1	C	199	LYS
1	C	201	MET
1	C	206	GLN
1	C	217	ASP
1	C	218	LYS
1	C	219	ASP
1	C	233	LYS
1	C	237	THR
1	C	240	PHE
1	C	242	ASN
1	C	244	THR
1	C	252	VAL
1	C	253	LEU
1	C	255	PHE
1	C	257	ASN
1	C	258	THR
1	C	260	THR

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Mol	Chain	Res	Type
1	C	262	VAL
1	C	264	LEU
1	C	265	ASP
1	C	272	LEU
1	C	278	LEU
1	C	281	SER
1	C	283	VAL
1	C	286	MET
1	C	288	TRP
1	C	290	VAL
1	C	291	THR
1	C	292	ARG
1	C	294	TYR
1	C	296	VAL
1	C	305	TYR
1	C	309	THR
1	C	310	LEU
1	C	329	PHE
1	C	330	ASN
1	C	336	VAL
1	C	337	GLN
1	C	354	TYR
1	C	360	VAL
1	D	21	ARG
1	D	39	LEU
1	D	41	THR
1	D	45	SER
1	D	53	LEU
1	D	54	ASN
1	D	59	GLN
1	D	66	LEU
1	D	71	GLN
1	D	75	TRP
1	D	76	SER
1	D	80	ASN
1	D	81	LEU
1	D	84	SER
1	D	85	ASP
1	D	93	ASN
1	D	97	THR
1	D	99	SER
1	D	100	MET

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Mol	Chain	Res	Type
1	D	108	LEU
1	D	112	LEU
1	D	113	THR
1	D	116	THR
1	D	117	LEU
1	D	118	GLN
1	D	119	MET
1	D	124	SER
1	D	132	SER
1	D	138	VAL
1	D	139	HIS
1	D	141	PHE
1	D	151	LYS
1	D	153	ILE
1	D	154	SER
1	D	161	GLN
1	D	172	LEU
1	D	174	LEU
1	D	175	GLN
1	D	179	THR
1	D	182	ARG
1	D	184	LYS
1	D	186	LYS
1	D	192	THR
1	D	193	ILE
1	D	194	LYS
1	D	197	THR
1	D	201	MET
1	D	202	VAL
1	D	218	LYS
1	D	219	ASP
1	D	228	HIS
1	D	230	ASP
1	D	234	ASN
1	D	237	THR
1	D	240	PHE
1	D	242	ASN
1	D	244	THR
1	D	252	VAL
1	D	253	LEU
1	D	254	GLN
1	D	255	PHE

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Mol	Chain	Res	Type
1	D	256	THR
1	D	257	ASN
1	D	258	THR
1	D	260	THR
1	D	264	LEU
1	D	265	ASP
1	D	266	GLU
1	D	279	TYR
1	D	281	SER
1	D	286	MET
1	D	288	TRP
1	D	292	ARG
1	D	297	HIS
1	D	298	HIS
1	D	300	ARG
1	D	304	ARG
1	D	309	THR
1	D	310	LEU
1	D	313	ARG
1	D	321	MET
1	D	329	PHE
1	D	333	LEU
1	D	335	GLN
1	D	336	VAL
1	D	342	GLU
1	D	345	ASN
1	D	346	THR
1	D	348	VAL
1	D	349	GLU
1	D	352	ARG
1	E	19	CYS
1	E	21	ARG
1	E	25	VAL
1	E	37	LEU
1	E	39	LEU
1	E	41	THR
1	E	44	ASP
1	E	53	LEU
1	E	54	ASN
1	E	64	GLU
1	E	66	LEU
1	E	67	THR

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Mol	Chain	Res	Type
1	E	68	GLU
1	E	75	TRP
1	E	79	ILE
1	E	97	THR
1	E	99	SER
1	E	103	LEU
1	E	108	LEU
1	E	109	ASN
1	E	111	ASP
1	E	112	LEU
1	E	113	THR
1	E	117	LEU
1	E	121	GLU
1	E	132	SER
1	E	135	LEU
1	E	138	VAL
1	E	141	PHE
1	E	151	LYS
1	E	154	SER
1	E	157	VAL
1	E	174	LEU
1	E	177	LEU
1	E	179	THR
1	E	180	ASP
1	E	184	LYS
1	E	186	LYS
1	E	192	THR
1	E	193	ILE
1	E	194	LYS
1	E	202	VAL
1	E	205	ASP
1	E	216	LEU
1	E	217	ASP
1	E	219	ASP
1	E	222	TYR
1	E	230	ASP
1	E	233	LYS
1	E	235	GLU
1	E	237	THR
1	E	240	PHE
1	E	242	ASN
1	E	252	VAL

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Mol	Chain	Res	Type
1	E	253	LEU
1	E	256	THR
1	E	258	THR
1	E	260	THR
1	E	262	VAL
1	E	265	ASP
1	E	278	LEU
1	E	279	TYR
1	E	281	SER
1	E	283	VAL
1	E	288	TRP
1	E	292	ARG
1	E	294	TYR
1	E	295	ASP
1	E	298	HIS
1	E	299	TRP
1	E	309	THR
1	E	310	LEU
1	E	313	ARG
1	E	315	VAL
1	E	316	LYS
1	E	328	LEU
1	E	329	PHE
1	E	330	ASN
1	E	332	MET
1	E	335	GLN
1	E	337	GLN
1	E	341	MET
1	E	342	GLU
1	E	344	GLU
1	E	347	GLN
1	E	352	ARG
1	E	354	TYR
1	E	357	THR
1	E	359	PRO
1	E	360	VAL
1	E	366	MET
1	E	369	TYR
1	E	375	LYS
1	E	381	PRO
1	F	29	LEU
1	F	30	ILE

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Mol	Chain	Res	Type
1	F	37	LEU
1	F	46	VAL
1	F	53	LEU
1	F	54	ASN
1	F	66	LEU
1	F	71	GLN
1	F	75	TRP
1	F	77	ARG
1	F	79	ILE
1	F	90	PRO
1	F	93	ASN
1	F	97	THR
1	F	100	MET
1	F	104	GLN
1	F	109	ASN
1	F	112	LEU
1	F	113	THR
1	F	117	LEU
1	F	130	VAL
1	F	132	SER
1	F	138	VAL
1	F	139	HIS
1	F	141	PHE
1	F	151	LYS
1	F	154	SER
1	F	172	LEU
1	F	173	ASP
1	F	175	GLN
1	F	179	THR
1	F	184	LYS
1	F	186	LYS
1	F	192	THR
1	F	193	ILE
1	F	194	LYS
1	F	201	MET
1	F	216	LEU
1	F	217	ASP
1	F	224	VAL
1	F	230	ASP
1	F	233	LYS
1	F	237	THR
1	F	240	PHE

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Mol	Chain	Res	Type
1	F	242	ASN
1	F	244	THR
1	F	252	VAL
1	F	253	LEU
1	F	255	PHE
1	F	258	THR
1	F	259	LEU
1	F	262	VAL
1	F	278	LEU
1	F	281	SER
1	F	290	VAL
1	F	294	TYR
1	F	299	TRP
1	F	306	PHE
1	F	309	THR
1	F	310	LEU
1	F	321	MET
1	F	325	ILE
1	F	328	LEU
1	F	330	ASN
1	F	333	LEU
1	F	336	VAL
1	F	337	GLN
1	F	347	GLN
1	F	350	GLU
1	F	351	VAL
1	F	352	ARG
1	F	354	TYR
1	F	357	THR
1	F	359	PRO
1	F	360	VAL
1	F	367	THR
1	F	368	ARG
1	F	371	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (80) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	ASN
1	A	71	GLN
1	A	92	ASN
1	A	104	GLN

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Continued from previous page...

Mol	Chain	Res	Type
1	A	139	HIS
1	A	142	ASN
1	A	175	GLN
1	A	206	GLN
1	A	228	HIS
1	A	234	ASN
1	A	257	ASN
1	A	297	HIS
1	A	335	GLN
1	A	337	GLN
1	A	347	GLN
1	B	54	ASN
1	B	93	ASN
1	B	104	GLN
1	B	118	GLN
1	B	139	HIS
1	B	142	ASN
1	B	175	GLN
1	B	206	GLN
1	B	228	HIS
1	B	257	ASN
1	B	339	GLN
1	B	347	GLN
1	C	54	ASN
1	C	71	GLN
1	C	93	ASN
1	C	104	GLN
1	C	109	ASN
1	C	139	HIS
1	C	142	ASN
1	C	175	GLN
1	C	206	GLN
1	C	228	HIS
1	C	257	ASN
1	C	331	ASN
1	C	337	GLN
1	C	339	GLN
1	D	54	ASN
1	D	71	GLN
1	D	80	ASN
1	D	93	ASN
1	D	104	GLN

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Mol	Chain	Res	Type
1	D	109	ASN
1	D	118	GLN
1	D	139	HIS
1	D	206	GLN
1	D	234	ASN
1	D	257	ASN
1	D	297	HIS
1	D	317	ASN
1	D	331	ASN
1	D	335	GLN
1	D	347	GLN
1	E	54	ASN
1	E	104	GLN
1	E	139	HIS
1	E	206	GLN
1	E	228	HIS
1	E	234	ASN
1	E	297	HIS
1	E	317	ASN
1	E	331	ASN
1	E	339	GLN
1	E	347	GLN
1	F	54	ASN
1	F	59	GLN
1	F	104	GLN
1	F	118	GLN
1	F	142	ASN
1	F	175	GLN
1	F	242	ASN
1	F	297	HIS
1	F	317	ASN
1	F	331	ASN
1	F	335	GLN
1	F	339	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

24 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	NAG	G	1	2	15,15,15	1.35	1 (6%)	21,21,21	1.52	4 (19%)
2	GAL	G	2	2	11,11,12	0.48	0	15,15,17	1.52	2 (13%)
2	SIA	G	3	2	17,20,21	1.12	1 (5%)	21,28,31	0.90	1 (4%)
2	SIA	G	4	2	17,20,21	1.41	3 (17%)	21,28,31	1.27	3 (14%)
2	NAG	H	1	2	15,15,15	1.64	2 (13%)	21,21,21	2.15	5 (23%)
2	GAL	H	2	2	11,11,12	0.48	0	15,15,17	1.74	1 (6%)
2	SIA	H	3	2	17,20,21	0.97	2 (11%)	21,28,31	1.05	2 (9%)
2	SIA	H	4	2	17,20,21	1.60	4 (23%)	21,28,31	1.11	2 (9%)
2	NAG	I	1	2	15,15,15	1.49	1 (6%)	21,21,21	1.90	5 (23%)
2	GAL	I	2	2	11,11,12	0.39	0	15,15,17	1.38	1 (6%)
2	SIA	I	3	2	17,20,21	0.65	0	21,28,31	1.02	2 (9%)
2	SIA	I	4	2	17,20,21	1.40	3 (17%)	21,28,31	1.21	2 (9%)
2	NAG	J	1	2	15,15,15	0.87	1 (6%)	21,21,21	0.90	1 (4%)
2	GAL	J	2	2	11,11,12	0.49	0	15,15,17	1.41	1 (6%)
2	SIA	J	3	2	17,20,21	1.25	2 (11%)	21,28,31	1.34	3 (14%)
2	SIA	J	4	2	17,20,21	1.49	4 (23%)	21,28,31	0.88	1 (4%)
2	NAG	K	1	2	15,15,15	1.77	1 (6%)	21,21,21	2.37	5 (23%)
2	GAL	K	2	2	11,11,12	0.31	0	15,15,17	1.75	2 (13%)
2	SIA	K	3	2	17,20,21	0.64	0	21,28,31	1.26	2 (9%)
2	SIA	K	4	2	17,20,21	1.74	3 (17%)	21,28,31	0.84	1 (4%)
2	NAG	L	1	2	15,15,15	1.52	1 (6%)	21,21,21	1.79	4 (19%)
2	GAL	L	2	2	11,11,12	0.42	0	15,15,17	1.95	1 (6%)
2	SIA	L	3	2	17,20,21	0.91	2 (11%)	21,28,31	1.11	1 (4%)
2	SIA	L	4	2	17,20,21	1.62	3 (17%)	21,28,31	0.95	1 (4%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	G	1	2	-	2/6/26/26	0/1/1/1
2	GAL	G	2	2	-	0/2/19/22	0/1/1/1
2	SIA	G	3	2	-	4/14/34/38	0/1/1/1
2	SIA	G	4	2	-	1/14/34/38	0/1/1/1
2	NAG	H	1	2	-	2/6/26/26	0/1/1/1
2	GAL	H	2	2	-	0/2/19/22	0/1/1/1
2	SIA	H	3	2	-	4/14/34/38	0/1/1/1
2	SIA	H	4	2	-	2/14/34/38	0/1/1/1
2	NAG	I	1	2	-	2/6/26/26	0/1/1/1
2	GAL	I	2	2	-	0/2/19/22	0/1/1/1
2	SIA	I	3	2	-	1/14/34/38	0/1/1/1
2	SIA	I	4	2	-	1/14/34/38	0/1/1/1
2	NAG	J	1	2	-	4/6/26/26	0/1/1/1
2	GAL	J	2	2	-	0/2/19/22	0/1/1/1
2	SIA	J	3	2	-	4/14/34/38	0/1/1/1
2	SIA	J	4	2	-	0/14/34/38	0/1/1/1
2	NAG	K	1	2	-	2/6/26/26	0/1/1/1
2	GAL	K	2	2	-	0/2/19/22	0/1/1/1
2	SIA	K	3	2	-	5/14/34/38	0/1/1/1
2	SIA	K	4	2	-	3/14/34/38	0/1/1/1
2	NAG	L	1	2	-	2/6/26/26	0/1/1/1
2	GAL	L	2	2	-	0/2/19/22	0/1/1/1
2	SIA	L	3	2	-	2/14/34/38	0/1/1/1
2	SIA	L	4	2	-	0/14/34/38	0/1/1/1

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	K	1	NAG	C1-C2	6.03	1.60	1.52
2	H	1	NAG	C1-C2	5.33	1.59	1.52
2	I	1	NAG	C1-C2	5.01	1.58	1.52
2	L	1	NAG	C1-C2	4.97	1.58	1.52
2	G	1	NAG	C1-C2	4.43	1.58	1.52
2	K	4	SIA	C4-C5	3.79	1.56	1.53
2	G	3	SIA	C4-C5	-3.76	1.49	1.53
2	J	3	SIA	C4-C5	-3.76	1.49	1.53
2	H	4	SIA	C7-C6	3.64	1.57	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	K	4	SIA	C7-C6	3.54	1.57	1.53
2	L	4	SIA	C7-C6	3.48	1.57	1.53
2	K	4	SIA	C6-C5	3.47	1.58	1.53
2	J	4	SIA	C7-C6	3.45	1.57	1.53
2	L	4	SIA	C4-C5	3.30	1.56	1.53
2	L	4	SIA	C6-C5	3.29	1.58	1.53
2	G	4	SIA	C3-C2	3.04	1.57	1.52
2	I	4	SIA	C7-C6	2.76	1.56	1.53
2	H	4	SIA	C6-C5	2.67	1.57	1.53
2	J	4	SIA	C4-C5	2.64	1.55	1.53
2	H	4	SIA	C3-C2	2.64	1.56	1.52
2	G	4	SIA	C7-C6	2.57	1.56	1.53
2	I	4	SIA	C4-C5	2.48	1.55	1.53
2	J	4	SIA	C3-C2	2.43	1.56	1.52
2	G	4	SIA	C6-C5	2.41	1.57	1.53
2	J	1	NAG	C1-C2	2.38	1.55	1.52
2	J	4	SIA	C6-C5	2.38	1.57	1.53
2	I	4	SIA	C3-C2	2.35	1.56	1.52
2	H	3	SIA	C7-C6	-2.30	1.50	1.53
2	L	3	SIA	C4-C5	-2.28	1.51	1.53
2	J	3	SIA	C6-C5	-2.22	1.49	1.53
2	H	4	SIA	C8-C7	2.20	1.57	1.53
2	L	3	SIA	C3-C2	2.16	1.55	1.52
2	H	1	NAG	C3-C2	2.07	1.57	1.53
2	H	3	SIA	C4-C5	-2.06	1.51	1.53

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	K	1	NAG	O5-C1-C2	6.79	116.34	109.52
2	L	2	GAL	C1-C2-C3	-6.74	101.38	109.67
2	H	2	GAL	C1-C2-C3	-6.24	102.00	109.67
2	K	2	GAL	C1-C2-C3	-5.96	102.34	109.67
2	H	1	NAG	O5-C1-C2	5.82	115.36	109.52
2	K	1	NAG	C3-C4-C5	-5.67	100.13	110.24
2	I	1	NAG	O5-C1-C2	5.20	114.75	109.52
2	G	2	GAL	C1-C2-C3	-5.15	103.34	109.67
2	J	2	GAL	C1-C2-C3	-5.02	103.50	109.67
2	I	2	GAL	C1-C2-C3	-4.55	104.08	109.67
2	L	1	NAG	O5-C1-C2	4.42	113.95	109.52
2	L	1	NAG	C3-C4-C5	-4.17	102.80	110.24
2	I	1	NAG	C1-C2-C3	4.16	116.22	110.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	1	NAG	C3-C4-C5	-4.02	103.06	110.24
2	J	3	SIA	C3-C4-C5	-4.00	106.63	111.46
2	G	1	NAG	O5-C1-C2	3.84	113.37	109.52
2	G	1	NAG	C3-C4-C5	-3.59	103.84	110.24
2	H	1	NAG	C1-C2-N2	-3.58	106.58	110.73
2	K	3	SIA	C4-C3-C2	3.57	116.20	109.81
2	L	3	SIA	C3-C4-C5	-3.33	107.43	111.46
2	K	1	NAG	C1-C2-C3	3.17	114.86	110.54
2	L	4	SIA	C6-O6-C2	3.14	118.05	111.34
2	H	1	NAG	C1-C2-C3	3.13	114.81	110.54
2	J	3	SIA	C8-C7-C6	-3.08	107.19	113.03
2	I	1	NAG	C3-C4-C5	-3.02	104.85	110.24
2	K	1	NAG	O3-C3-C2	3.00	115.72	109.66
2	I	3	SIA	C3-C4-C5	-3.00	107.84	111.46
2	H	1	NAG	C4-C3-C2	2.97	114.69	110.34
2	K	1	NAG	C1-C2-N2	-2.90	107.37	110.73
2	G	4	SIA	C3-C4-C5	-2.84	108.03	111.46
2	I	4	SIA	C4-C3-C2	2.83	114.88	109.81
2	H	3	SIA	C4-C3-C2	2.79	114.82	109.81
2	G	3	SIA	C3-C4-C5	-2.77	108.11	111.46
2	G	1	NAG	C1-C2-N2	-2.75	107.54	110.73
2	H	3	SIA	C8-C7-C6	-2.74	107.84	113.03
2	L	1	NAG	C1-C2-N2	-2.72	107.58	110.73
2	I	4	SIA	C6-O6-C2	2.70	117.12	111.34
2	L	1	NAG	C1-C2-C3	2.69	114.21	110.54
2	H	4	SIA	C6-O6-C2	2.62	116.96	111.34
2	H	4	SIA	C3-C4-C5	-2.60	108.32	111.46
2	G	4	SIA	C6-O6-C2	2.58	116.85	111.34
2	I	1	NAG	C1-C2-N2	-2.52	107.81	110.73
2	G	4	SIA	C4-C3-C2	2.38	114.07	109.81
2	J	1	NAG	C1-C2-N2	-2.36	108.00	110.73
2	K	4	SIA	C6-O6-C2	2.34	116.35	111.34
2	I	1	NAG	C3-C2-N2	-2.32	106.23	110.62
2	J	4	SIA	C6-O6-C2	2.31	116.28	111.34
2	K	3	SIA	C3-C4-C5	-2.26	108.73	111.46
2	G	1	NAG	O3-C3-C2	2.23	114.16	109.66
2	K	2	GAL	O5-C1-C2	-2.15	107.46	110.77
2	I	3	SIA	C8-C7-C6	-2.04	109.17	113.03
2	G	2	GAL	O2-C2-C1	2.01	113.26	109.15
2	J	3	SIA	C5-N5-C10	-2.00	118.31	123.18

There are no chirality outliers.

All (41) torsion outliers are listed below:

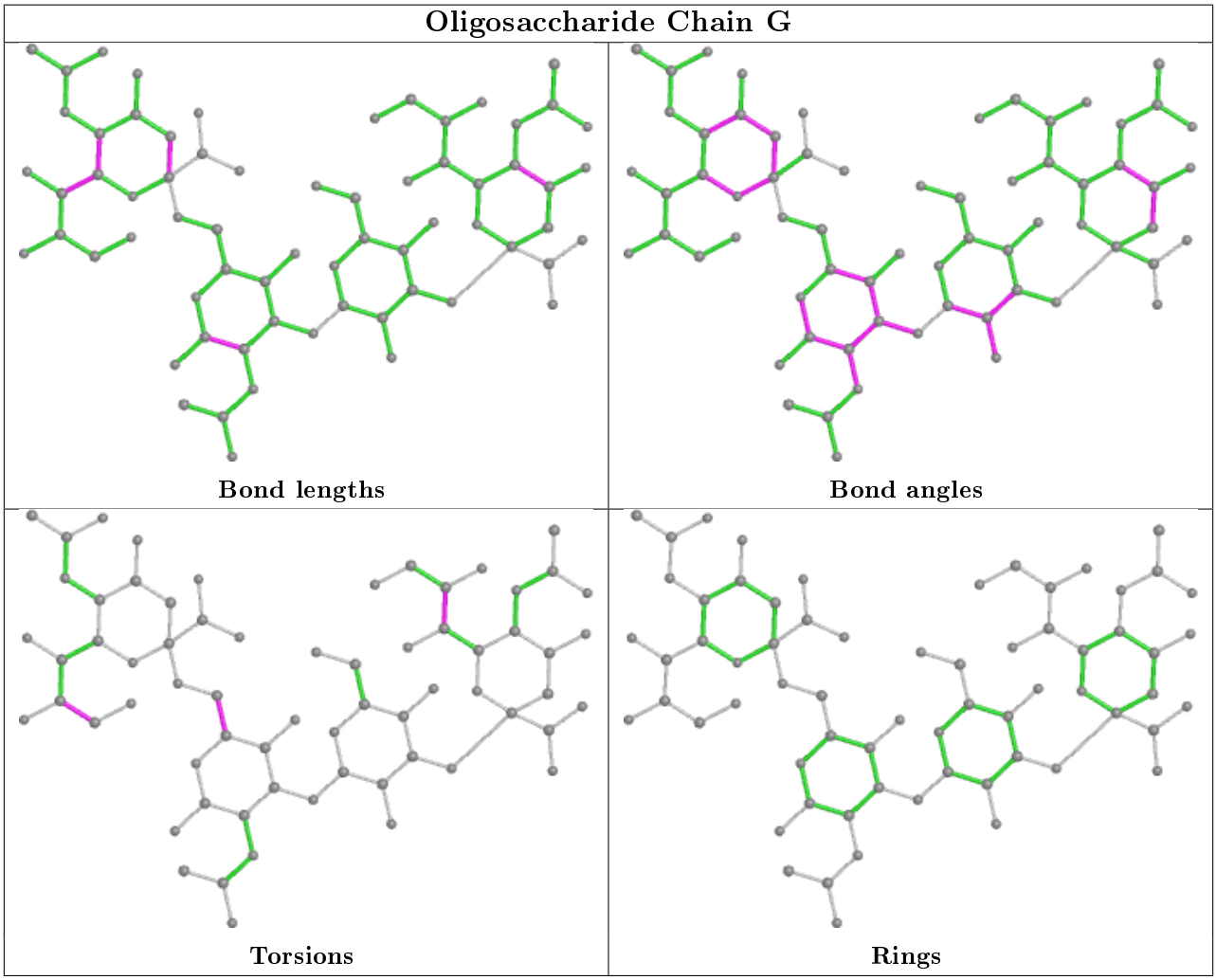
Mol	Chain	Res	Type	Atoms
2	H	4	SIA	C7-C8-C9-O9
2	H	4	SIA	O8-C8-C9-O9
2	K	3	SIA	O7-C7-C8-C9
2	H	3	SIA	C5-C6-C7-O7
2	H	3	SIA	O6-C6-C7-O7
2	L	3	SIA	C5-C6-C7-O7
2	L	3	SIA	O6-C6-C7-O7
2	J	1	NAG	C1-C2-N2-C7
2	J	3	SIA	C5-C6-C7-C8
2	J	3	SIA	C5-C6-C7-O7
2	J	3	SIA	O6-C6-C7-C8
2	J	3	SIA	O6-C6-C7-O7
2	G	3	SIA	O7-C7-C8-C9
2	G	1	NAG	O5-C5-C6-O6
2	K	3	SIA	O7-C7-C8-O8
2	G	3	SIA	O7-C7-C8-O8
2	L	1	NAG	C4-C5-C6-O6
2	K	3	SIA	C6-C7-C8-O8
2	G	3	SIA	C6-C7-C8-O8
2	I	1	NAG	O5-C5-C6-O6
2	J	1	NAG	O5-C5-C6-O6
2	H	1	NAG	C4-C5-C6-O6
2	G	1	NAG	C4-C5-C6-O6
2	K	3	SIA	C6-C7-C8-C9
2	G	3	SIA	C6-C7-C8-C9
2	I	1	NAG	C4-C5-C6-O6
2	L	1	NAG	O5-C5-C6-O6
2	H	1	NAG	O5-C5-C6-O6
2	J	1	NAG	C4-C5-C6-O6
2	K	1	NAG	C4-C5-C6-O6
2	H	3	SIA	C7-C8-C9-O9
2	K	1	NAG	O5-C5-C6-O6
2	H	3	SIA	O8-C8-C9-O9
2	K	4	SIA	O8-C8-C9-O9
2	K	3	SIA	O6-C6-C7-O7
2	G	4	SIA	O8-C8-C9-O9
2	I	4	SIA	O8-C8-C9-O9
2	J	1	NAG	C3-C2-N2-C7
2	K	4	SIA	C7-C8-C9-O9
2	I	3	SIA	C7-C8-C9-O9
2	K	4	SIA	C4-C5-N5-C10

There are no ring outliers.

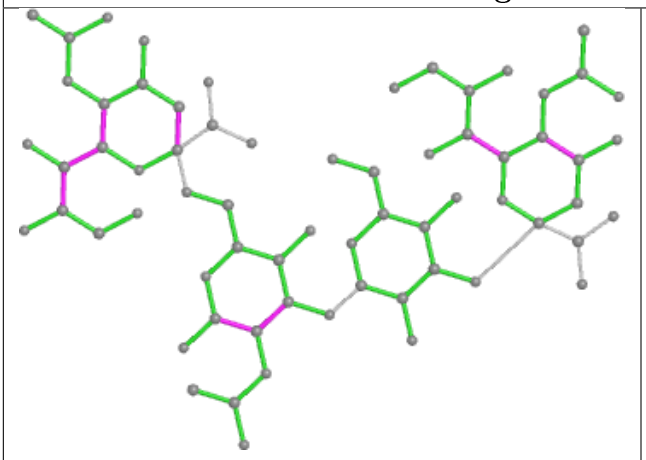
9 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	L	2	GAL	4	0
2	K	3	SIA	1	0
2	G	2	GAL	2	0
2	H	2	GAL	1	0
2	H	3	SIA	2	0
2	L	3	SIA	2	0
2	J	3	SIA	1	0
2	G	3	SIA	1	0
2	K	2	GAL	3	0

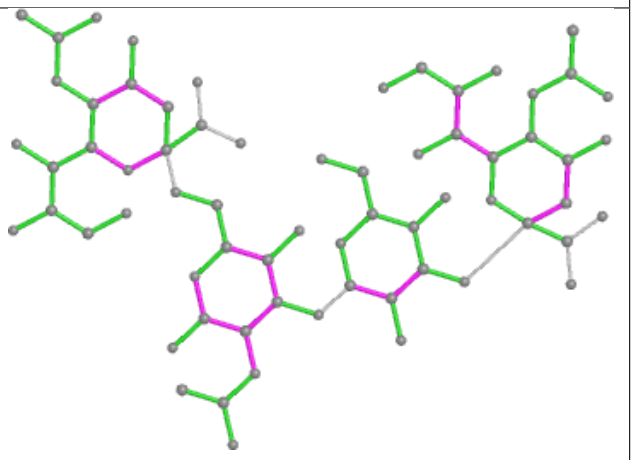
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



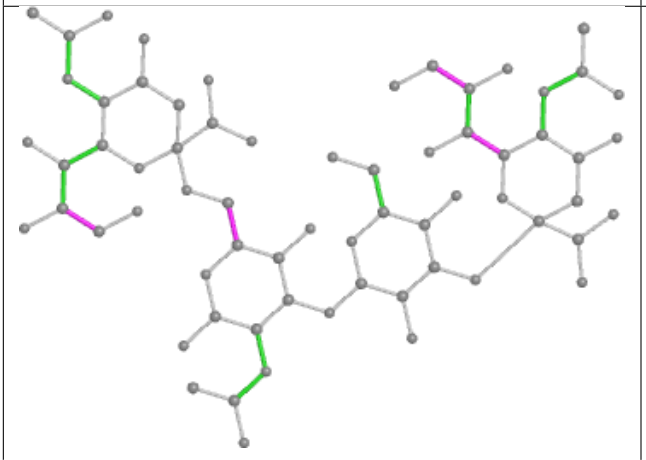
Oligosaccharide Chain H



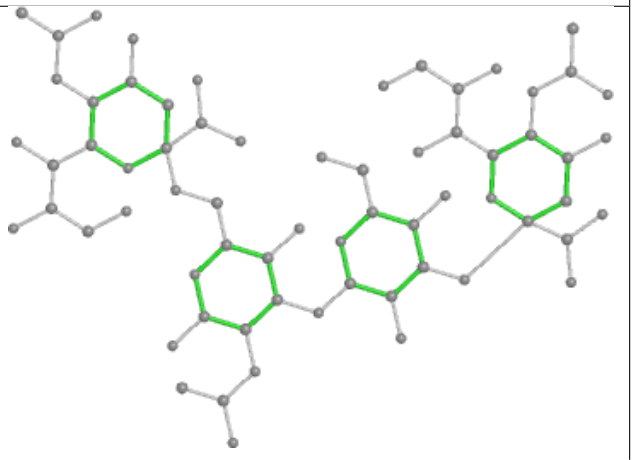
Bond lengths



Bond angles

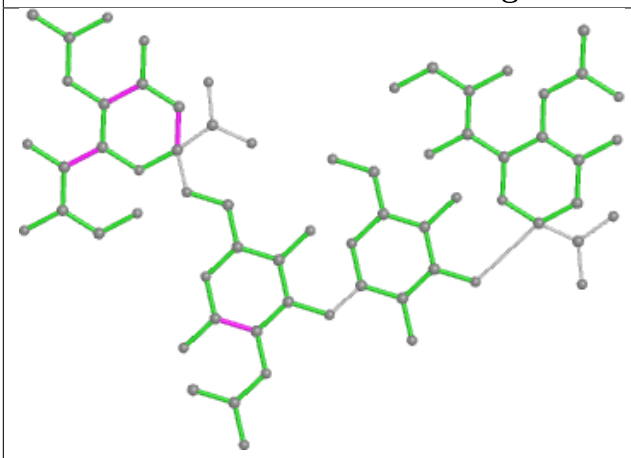


Torsions

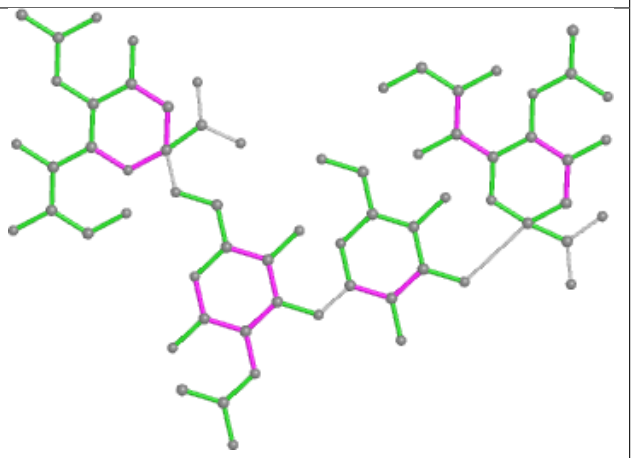


Rings

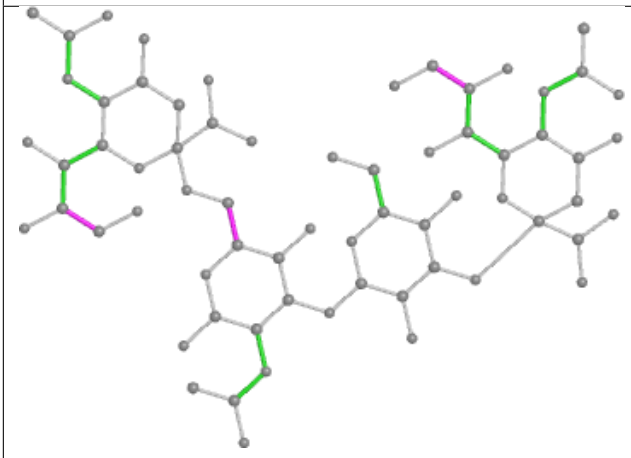
Oligosaccharide Chain I



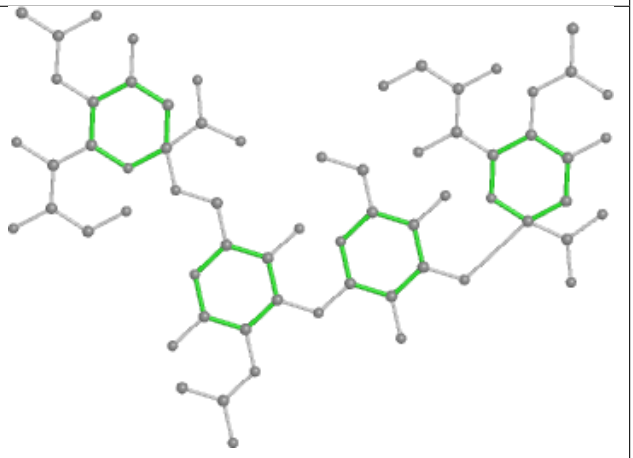
Bond lengths



Bond angles

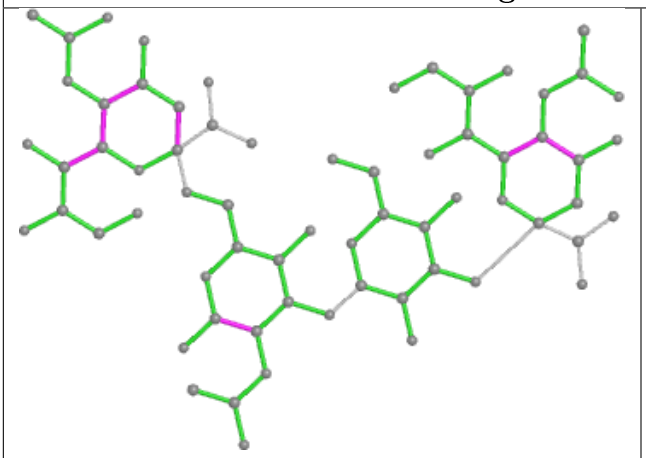


Torsions

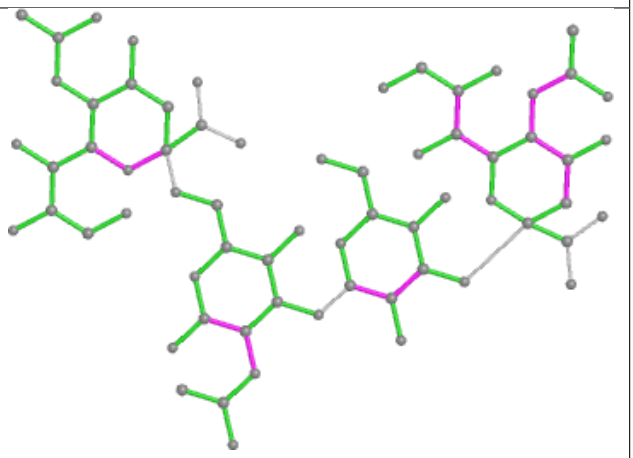


Rings

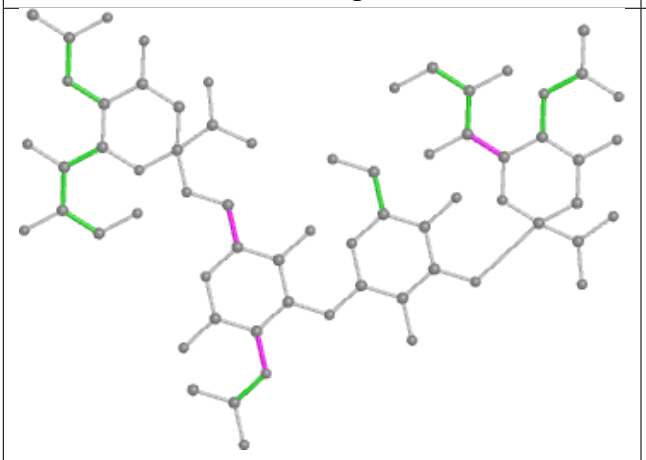
Oligosaccharide Chain J



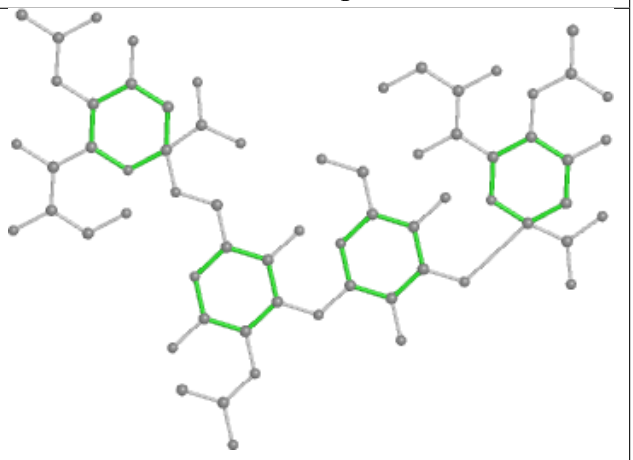
Bond lengths



Bond angles

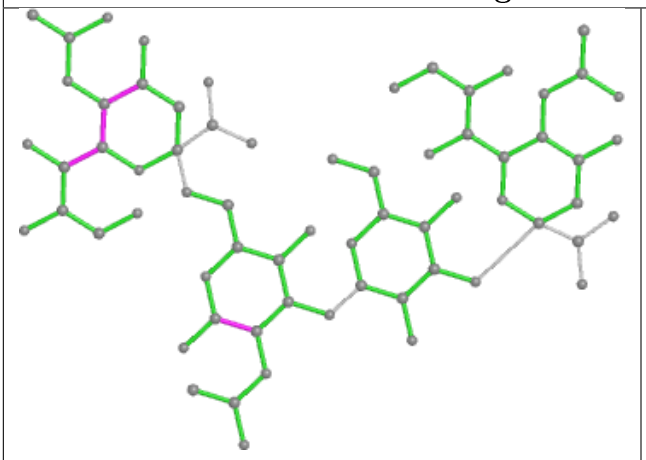


Torsions

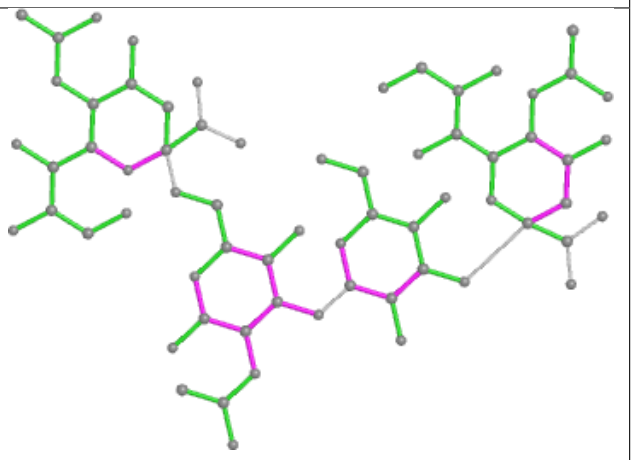


Rings

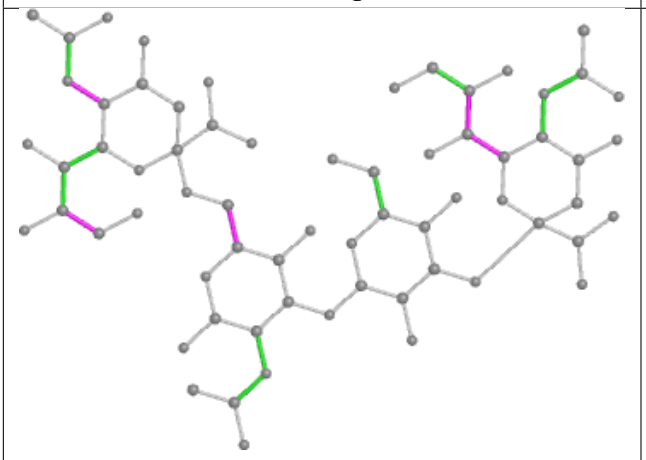
Oligosaccharide Chain K



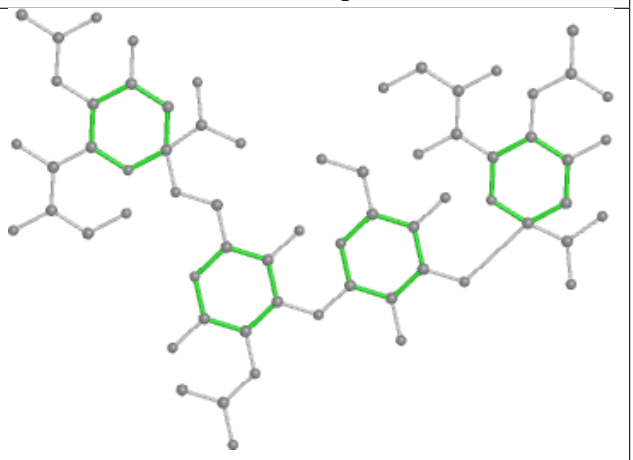
Bond lengths



Bond angles

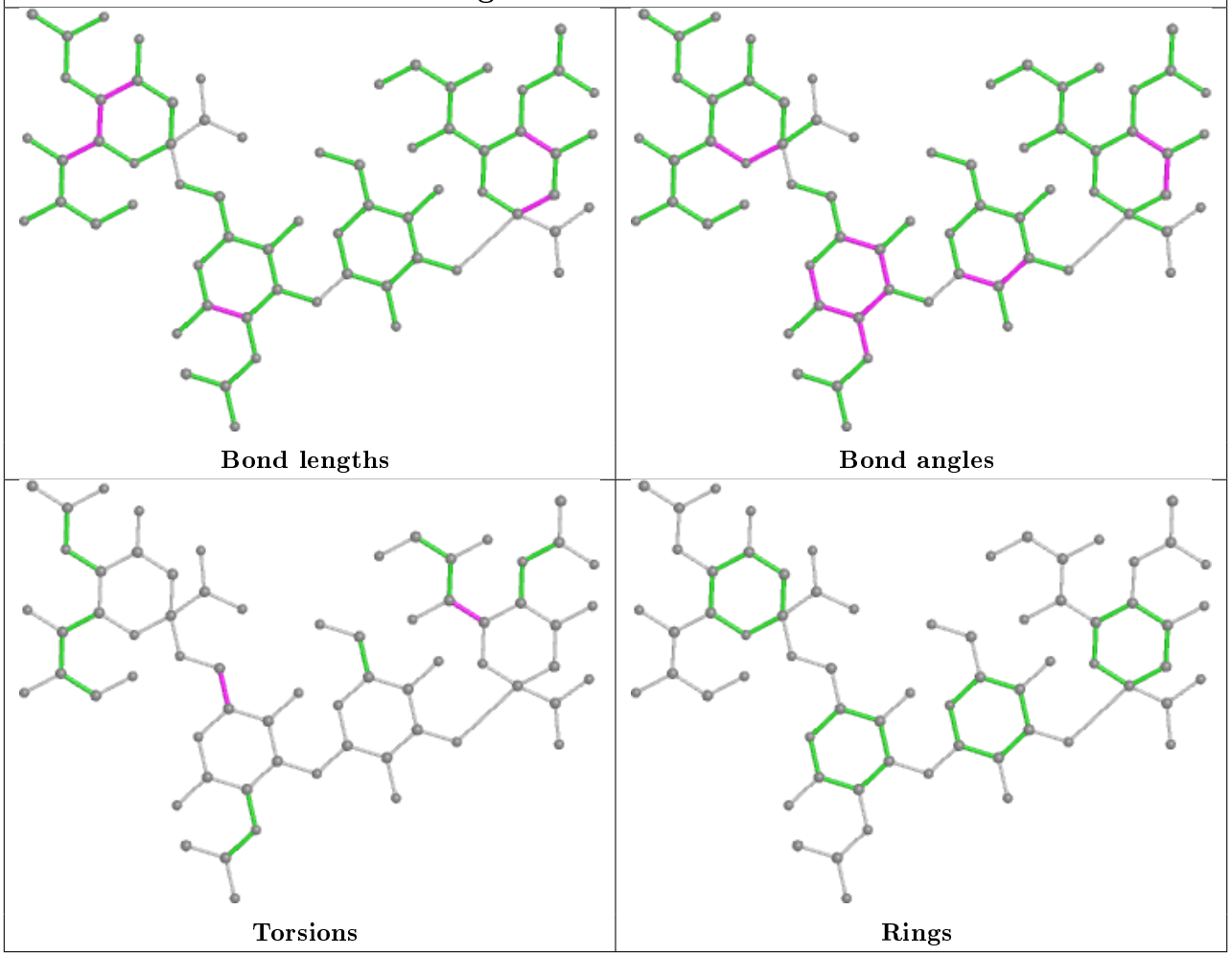


Torsions



Rings

Oligosaccharide Chain L



5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	1
1	D	1
1	C	1

Continued on next page...

Continued from previous page...

Mol	Chain	Number of breaks
1	F	1
1	E	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	336:VAL	C	337:GLN	N	4.77
1	F	336:VAL	C	337:GLN	N	4.21
1	C	336:VAL	C	337:GLN	N	3.33
1	B	336:VAL	C	337:GLN	N	3.13
1	E	336:VAL	C	337:GLN	N	1.19

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.