



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 08:34 AM UTC

PDB ID : 1FLC / pdb_00001flc
Title : X-RAY STRUCTURE OF THE HAEMAGGLUTININ-ESTERASE-FUSION GLYCOPROTEIN OF INFLUENZA C VIRUS
Authors : Rosenthal, P.B.; Zhang, X.; Formanowski, F.; Fitz, W.; Wong, C.H.; Meier-Ewert, H.; Skehel, J.J.; Wiley, D.C.
Deposited on : 1999-02-22
Resolution : 3.20 Å(reported)

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A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

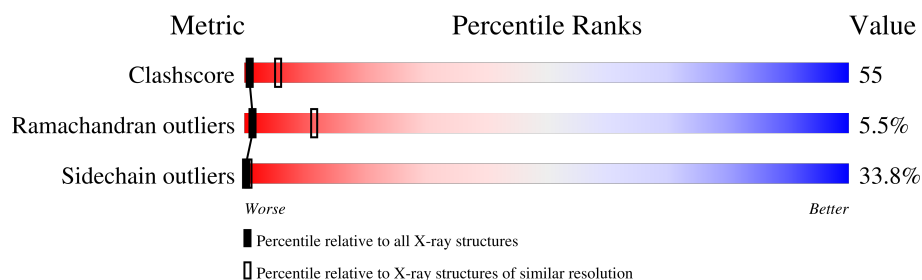
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 Å.

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



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

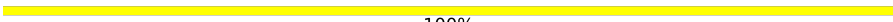
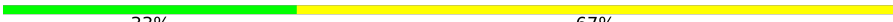
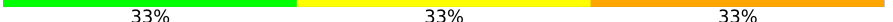
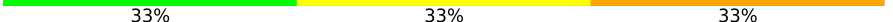
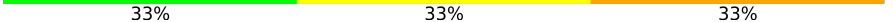
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively.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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	432	35% 38% 22% ..
1	C	432	33% 44% 19% ..
1	E	432	34% 42% 19% ..
2	B	175	22% 33% 34% . 7%
2	D	175	22% 37% 30% . 7%
2	F	175	21% 40% 27% 5% 7%
3	G	3	33% 67%
3	H	3	33% 67%

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Mol	Chain	Length	Quality of chain
3	I	3	 100%
3	J	3	 33% 67%
3	L	3	 33% 67%
3	M	3	 33% 67%
3	O	3	 100%
3	Q	3	 33% 33% 33%
3	R	3	 33% 33% 33%
3	S	3	 33% 33% 33%
3	T	3	 67% 33%
4	K	3	 67% 33%
4	P	3	 33% 67%
4	U	3	 33% 67%
5	N	3	 33% 67%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NAG	G	1	X	-	-	-
3	NAG	L	1	X	-	-	-
3	NAG	Q	1	X	-	-	-
4	NDG	K	2	-	-	X	-
4	MAN	K	3	-	-	X	-
4	NDG	U	2	-	-	X	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 14285 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.

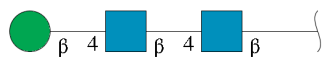
- Molecule 1 is a protein called HAEMAGGLUTININ-ESTERASE-FUSION GLYCOPROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	427	Total	C	N	O	S	0	0	0
			3339	2113	565	636	25			
1	C	427	Total	C	N	O	S	0	0	0
			3338	2112	565	636	25			
1	E	427	Total	C	N	O	S	0	0	0
			3339	2113	565	636	25			

- Molecule 2 is a protein called HAEMAGGLUTININ-ESTERASE-FUSION GLYCOPROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	162	Total	C	N	O	S	0	0	0
			1228	773	206	246	3			
2	D	162	Total	C	N	O	S	0	0	0
			1228	773	206	246	3			
2	F	162	Total	C	N	O	S	0	0	0
			1228	773	206	246	3			

- Molecule 3 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



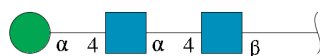
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	G	3	Total	C	N	O	0	0	0
			39	22	2	15			
3	H	3	Total	C	N	O	0	0	0
			39	22	2	15			
3	I	3	Total	C	N	O	0	0	0
			39	22	2	15			

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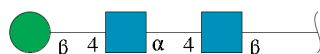
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	J	3	Total	C	N	O	0	0	0
			39	22	2	15			
3	L	3	Total	C	N	O	0	0	0
			39	22	2	15			
3	M	3	Total	C	N	O	0	0	0
			39	22	2	15			
3	O	3	Total	C	N	O	0	0	0
			39	22	2	15			
3	Q	3	Total	C	N	O	0	0	0
			39	22	2	15			
3	R	3	Total	C	N	O	0	0	0
			39	22	2	15			
3	S	3	Total	C	N	O	0	0	0
			39	22	2	15			
3	T	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 4 is an oligosaccharide called alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-alpha-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	K	3	Total	C	N	O	0	0	0
			39	22	2	15			
4	P	3	Total	C	N	O	0	0	0
			39	22	2	15			
4	U	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 5 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-alpha-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



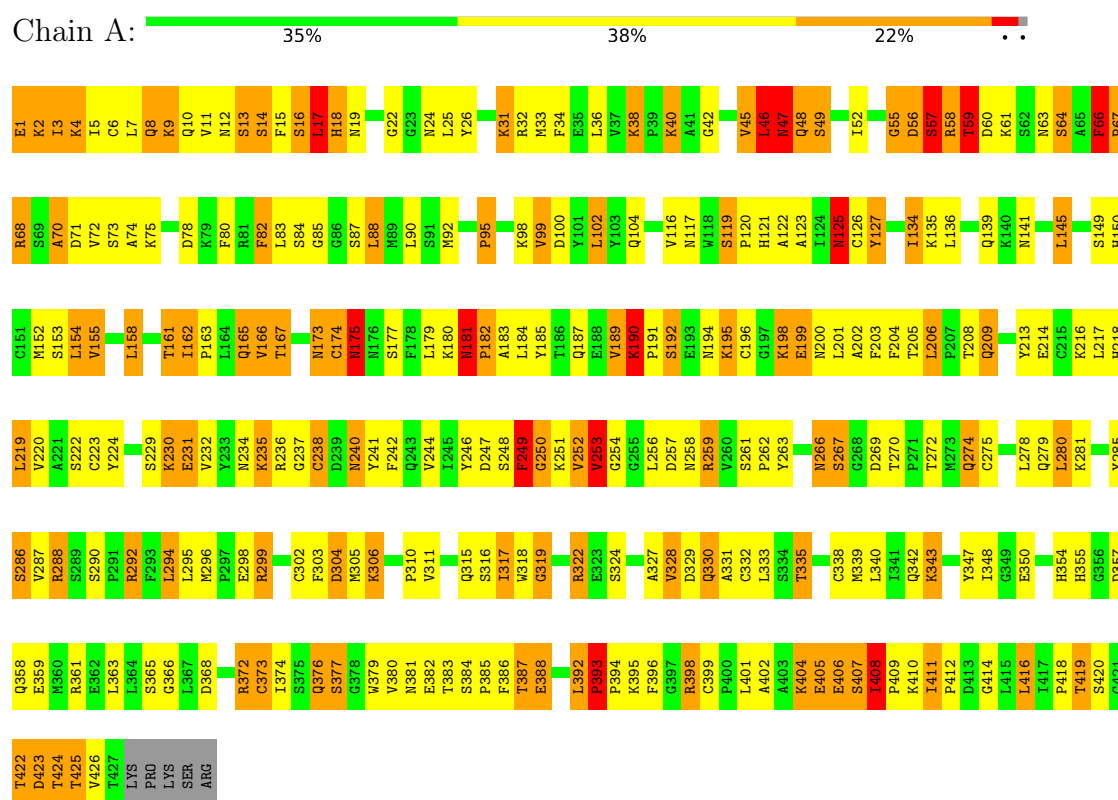
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	N	3	Total	C	N	O	0	0	0
			39	22	2	15			

3 Residue-property plots

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

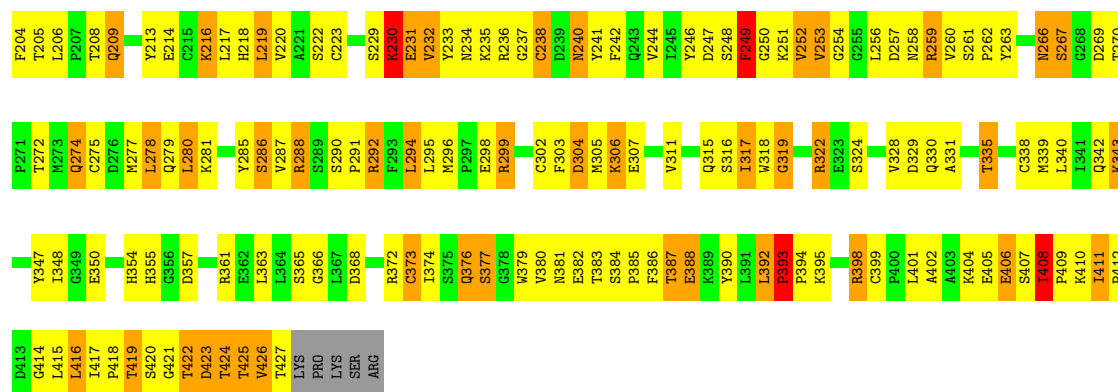
Note EDS was not executed.

• Molecule 1: HAEMAGGLUTININ-ESTERASE-FUSION GLYCOPROTEIN



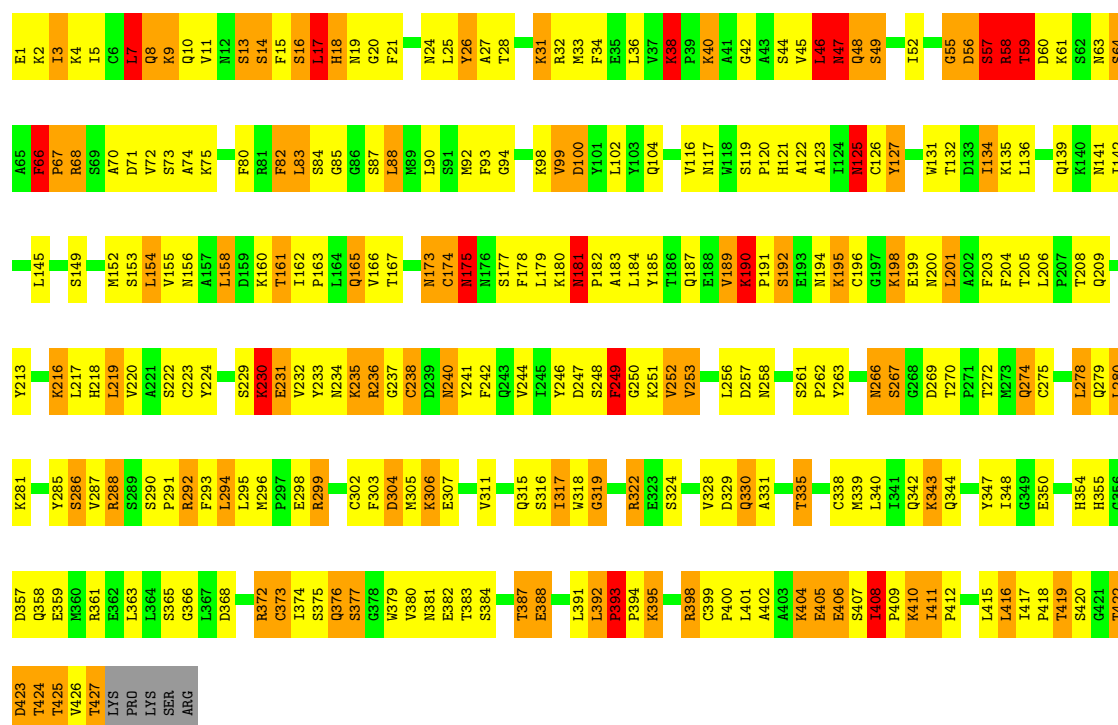
• Molecule 1: HAEMAGGLUTININ-ESTERASE-FUSION GLYCOPROTEIN





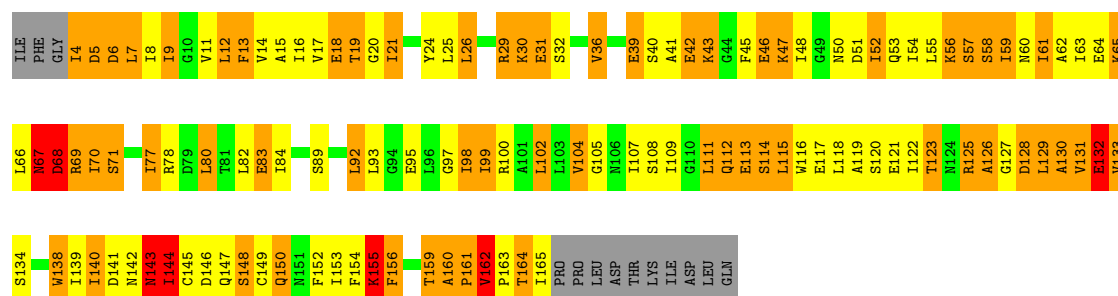
• Molecule 1: HAEMAGGLUTININ-ESTERASE-FUSION GLYCOPROTEIN

Chain E: 34% 42% 19% . .



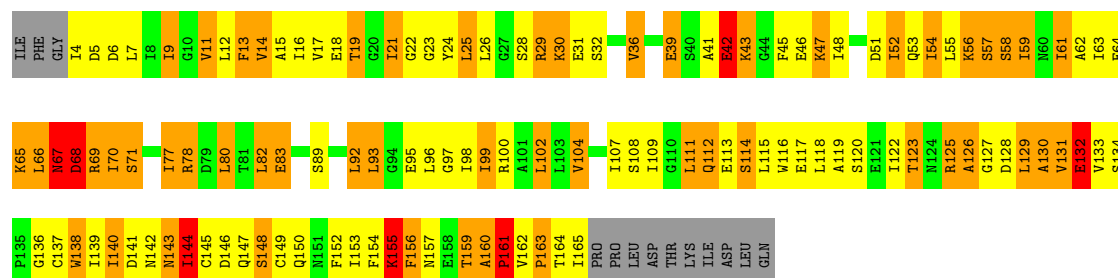
• Molecule 2: HAEMAGGLUTININ-ESTERASE-FUSION GLYCOPROTEIN

Chain B: 22% 33% 34% . 7%

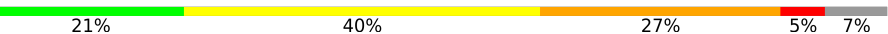


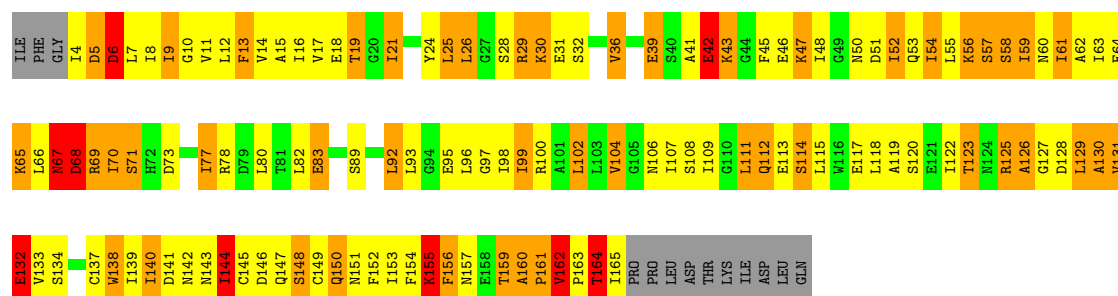
- Molecule 2: HAEMAGGLUTININ-ESTERASE-FUSION GLYCOPROTEIN

Chain D: 



- Molecule 2: HAEMAGGLUTININ-ESTERASE-FUSION GLYCOPROTEIN

Chain F: 

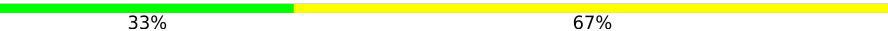


- Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G: 

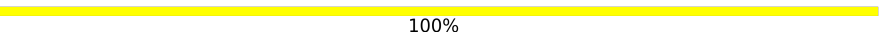


- Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H: 



- Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I: 



- Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:  33% 67%

MAG1
MAG2
BM13

- Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain L:  33% 67%

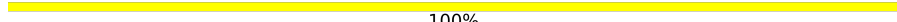
MAG1
MAG2
BM13

- Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:  33% 67%

MAG1
MAG2
BM13

- Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain O:  100%

MAG1
MAG2
BM13

- Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Q:  33% 33% 33%

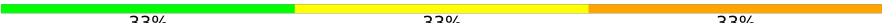
MAG1
MAG2
BM13

- Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain R:  33% 33% 33%

MAG1
MAG2
BM13

- Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain S:  33% 33% 33%



- Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain T:



- Molecule 4: alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-alpha-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:



- Molecule 4: alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-alpha-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain P:



- Molecule 4: alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-alpha-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain U:



- Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-alpha-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain N:



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 43 2 2	Depositor
Cell constants a, b, c, α , β , γ	155.40 Å 155.40 Å 414.40 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 3.20	Depositor
% Data completeness (in resolution range)	99.0 (10.00-3.20)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
Refinement program	X-PLOR 3.54	Depositor
R, R_{free}	0.223 , 0.267	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	14285	wwPDB-VP
Average B, all atoms (Å ²)	59.0	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: NDG, MAN, NAG, BMA

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.85	2/3420 (0.1%)	1.36	58/4622 (1.3%)
1	C	0.84	0/3418	1.37	53/4618 (1.1%)
1	E	0.87	0/3420	1.35	50/4622 (1.1%)
2	B	0.77	0/1241	1.17	9/1678 (0.5%)
2	D	0.74	0/1241	1.22	9/1678 (0.5%)
2	F	0.77	1/1241 (0.1%)	1.28	14/1678 (0.8%)
All	All	0.83	3/13981 (0.0%)	1.32	193/18896 (1.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	C	0	1
1	E	0	1
All	All	0	3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	162	VAL	CA-CB	7.44	1.63	1.54
1	A	155	VAL	CA-CB	-5.30	1.47	1.53
1	A	166	VAL	CA-CB	-5.04	1.48	1.54

All (193) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	69	ARG	N-CA-C	-15.88	96.14	112.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	69	ARG	N-CA-C	-15.38	96.67	112.97
1	A	57	SER	N-CA-C	-13.42	99.32	114.62
1	A	392	LEU	CA-C-N	13.37	134.15	120.38
1	A	392	LEU	C-N-CA	13.37	134.15	120.38
1	E	392	LEU	CA-C-N	13.34	134.12	120.38
1	E	392	LEU	C-N-CA	13.34	134.12	120.38
1	C	57	SER	N-CA-C	-13.09	99.69	114.62
1	E	57	SER	N-CA-C	-12.99	99.81	114.62
1	C	392	LEU	CA-C-N	12.71	133.47	120.38
1	C	392	LEU	C-N-CA	12.71	133.47	120.38
2	B	69	ARG	N-CA-C	-12.59	95.61	112.72
1	A	181	ASN	CA-C-N	-12.35	105.66	119.98
1	A	181	ASN	C-N-CA	-12.35	105.66	119.98
1	A	304	ASP	N-CA-C	-12.26	94.71	110.53
1	C	304	ASP	N-CA-C	-11.92	95.15	110.53
1	E	304	ASP	N-CA-C	-10.72	95.04	110.59
2	F	162	VAL	CA-C-N	10.66	133.17	119.84
2	F	162	VAL	C-N-CA	10.66	133.17	119.84
1	E	393	PRO	CA-C-N	-10.58	106.61	119.84
1	E	393	PRO	C-N-CA	-10.58	106.61	119.84
1	C	181	ASN	CA-C-N	-10.53	106.67	119.84
1	C	181	ASN	C-N-CA	-10.53	106.67	119.84
2	D	160	ALA	CA-C-N	10.44	132.89	119.84
2	D	160	ALA	C-N-CA	10.44	132.89	119.84
1	C	393	PRO	CA-C-N	-10.34	106.92	119.84
1	C	393	PRO	C-N-CA	-10.34	106.92	119.84
1	A	393	PRO	CA-C-N	-10.02	107.32	119.84
1	A	393	PRO	C-N-CA	-10.02	107.32	119.84
1	E	181	ASN	CA-C-N	-9.99	107.35	119.84
1	E	181	ASN	C-N-CA	-9.99	107.35	119.84
1	E	392	LEU	N-CA-C	9.96	122.20	109.65
1	C	392	LEU	N-CA-C	9.78	121.97	109.65
1	A	392	LEU	N-CA-C	9.50	121.62	109.65
1	C	55	GLY	N-CA-C	9.03	128.54	112.10
2	B	127	GLY	N-CA-C	-8.64	102.18	115.66
2	F	127	GLY	N-CA-C	-8.61	104.05	115.32
1	A	55	GLY	N-CA-C	8.34	127.28	112.10
1	E	55	GLY	N-CA-C	8.21	127.04	112.10
2	D	127	GLY	N-CA-C	-8.14	104.66	115.32
1	E	175	ASN	CA-C-N	-7.91	106.43	121.54
1	E	175	ASN	C-N-CA	-7.91	106.43	121.54
1	C	238	CYS	N-CA-C	7.91	123.43	112.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	319	GLY	N-CA-C	-7.91	99.02	112.30
1	A	238	CYS	N-CA-C	7.84	123.33	112.04
1	E	319	GLY	N-CA-C	-7.70	99.36	112.30
2	F	162	VAL	N-CA-C	7.67	125.45	108.88
1	C	319	GLY	N-CA-C	-7.62	99.49	112.30
1	E	238	CYS	N-CA-C	7.61	123.00	112.04
1	C	393	PRO	N-CA-C	7.54	119.89	110.70
1	E	393	PRO	N-CA-C	7.49	119.84	110.70
1	A	249	PHE	N-CA-C	-7.43	99.81	110.59
1	A	175	ASN	CA-C-N	-7.39	107.42	121.54
1	A	175	ASN	C-N-CA	-7.39	107.42	121.54
1	C	175	ASN	CA-C-N	-7.28	107.63	121.54
1	C	175	ASN	C-N-CA	-7.28	107.63	121.54
2	B	160	ALA	CA-C-N	7.27	128.93	119.84
2	B	160	ALA	C-N-CA	7.27	128.93	119.84
1	E	249	PHE	N-CA-C	-7.26	100.06	110.59
1	C	71	ASP	N-CA-C	-7.18	103.68	113.30
1	C	249	PHE	N-CA-C	-7.14	100.24	110.59
1	A	26	TYR	N-CA-C	-7.08	98.78	110.17
1	C	150	HIS	N-CA-C	-7.02	104.70	113.55
1	C	66	PHE	N-CA-C	6.92	125.11	109.81
1	A	393	PRO	N-CA-C	6.91	119.14	110.70
1	C	52	ILE	CA-C-N	-6.87	116.32	121.61
1	C	52	ILE	C-N-CA	-6.87	116.32	121.61
1	A	66	PHE	N-CA-C	6.85	124.95	109.81
2	B	144	ILE	N-CA-C	-6.75	106.01	111.81
1	E	66	PHE	N-CA-C	6.72	124.65	109.81
1	C	216	LYS	N-CA-C	-6.70	105.27	113.50
1	E	383	THR	N-CA-C	6.68	123.41	114.12
1	C	269	ASP	N-CA-C	6.62	120.45	112.38
1	A	213	TYR	N-CA-C	6.60	119.93	110.10
2	F	144	ILE	N-CA-C	-6.59	105.41	111.67
1	A	125	ASN	CA-C-N	-6.57	114.14	123.20
1	A	125	ASN	C-N-CA	-6.57	114.14	123.20
1	C	408	ILE	CA-C-N	6.56	126.54	119.78
1	C	408	ILE	C-N-CA	6.56	126.54	119.78
1	C	376	GLN	N-CA-C	-6.53	105.42	113.19
1	C	125	ASN	CA-C-N	-6.48	114.25	123.20
1	C	125	ASN	C-N-CA	-6.48	114.25	123.20
1	A	71	ASP	N-CA-C	-6.48	104.62	113.30
1	C	205	THR	N-CA-C	6.39	119.21	108.02
1	E	125	ASN	CA-C-N	-6.39	114.38	123.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	125	ASN	C-N-CA	-6.39	114.38	123.20
1	E	269	ASP	N-CA-C	6.30	119.81	111.75
1	A	292	ARG	N-CA-C	6.29	121.76	111.37
1	E	376	GLN	N-CA-C	-6.28	105.71	113.19
1	E	408	ILE	CA-C-N	6.25	126.22	119.78
1	E	408	ILE	C-N-CA	6.25	126.22	119.78
1	A	235	LYS	N-CA-C	-6.24	104.40	111.14
1	E	205	THR	N-CA-C	6.22	118.55	108.34
1	A	150	HIS	N-CA-C	-6.21	105.73	113.55
2	F	5	ASP	N-CA-C	6.17	115.59	108.49
1	E	292	ARG	N-CA-C	6.16	121.53	111.37
1	E	213	TYR	N-CA-C	6.10	119.19	110.10
1	C	383	THR	N-CA-C	6.05	122.54	114.12
1	A	46	LEU	N-CA-C	-6.02	101.02	109.69
1	A	190	LYS	CA-C-N	6.00	125.71	119.05
1	A	190	LYS	C-N-CA	6.00	125.71	119.05
1	E	372	ARG	N-CA-C	-5.97	105.08	112.90
1	A	205	THR	N-CA-C	5.94	118.08	108.34
1	C	292	ARG	N-CA-C	5.92	121.08	111.37
2	F	115	LEU	N-CA-C	-5.83	104.89	112.23
1	E	190	LYS	CA-C-N	5.81	125.50	119.05
1	E	190	LYS	C-N-CA	5.81	125.50	119.05
1	E	71	ASP	N-CA-C	-5.80	105.52	113.30
1	A	383	THR	N-CA-C	5.76	122.12	114.12
1	E	94	GLY	CA-C-N	-5.75	114.46	120.38
1	E	94	GLY	C-N-CA	-5.75	114.46	120.38
1	C	129	LYS	N-CA-C	5.74	117.34	111.14
1	A	304	ASP	CA-C-N	-5.70	113.55	122.49
1	A	304	ASP	C-N-CA	-5.70	113.55	122.49
1	C	190	LYS	CA-C-N	5.68	125.36	119.05
1	C	190	LYS	C-N-CA	5.68	125.36	119.05
1	A	267	SER	N-CA-C	-5.67	104.59	112.30
1	E	59	THR	N-CA-C	-5.66	107.01	114.31
2	B	143	ASN	N-CA-C	-5.65	105.11	112.23
2	B	115	LEU	N-CA-C	-5.64	105.12	112.23
1	C	46	LEU	N-CA-C	-5.63	101.58	109.69
1	A	59	THR	N-CA-C	-5.63	107.05	114.31
1	A	254	GLY	N-CA-C	5.61	118.76	110.63
1	C	259	ARG	N-CA-C	-5.56	106.45	113.18
1	A	47	ASN	N-CA-C	5.55	122.61	110.80
1	E	175	ASN	N-CA-C	-5.54	99.01	110.80
1	A	182	PRO	N-CA-C	-5.51	102.03	110.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	376	GLN	N-CA-C	-5.51	106.40	113.01
1	E	304	ASP	CA-C-N	-5.49	113.87	122.49
1	E	304	ASP	C-N-CA	-5.49	113.87	122.49
1	C	175	ASN	N-CA-C	-5.48	99.12	110.80
1	C	304	ASP	CA-C-N	-5.48	113.88	122.49
1	C	304	ASP	C-N-CA	-5.48	113.88	122.49
1	C	38	LYS	CA-C-N	-5.46	112.89	120.25
1	C	38	LYS	C-N-CA	-5.46	112.89	120.25
1	E	46	LEU	N-CA-C	-5.45	101.15	109.65
1	C	238	CYS	CA-C-N	-5.43	115.12	121.64
1	C	238	CYS	C-N-CA	-5.43	115.12	121.64
1	C	26	TYR	N-CA-C	-5.41	100.89	109.76
2	D	144	ILE	N-CA-C	-5.41	106.53	111.67
2	D	115	LEU	N-CA-C	-5.40	105.43	112.23
1	E	38	LYS	CA-C-N	-5.40	112.97	120.25
1	E	38	LYS	C-N-CA	-5.40	112.97	120.25
1	E	267	SER	N-CA-C	-5.40	104.96	112.30
1	C	213	TYR	N-CA-C	5.38	118.12	110.10
1	E	307	GLU	N-CA-C	5.38	117.25	109.07
2	F	73	ASP	N-CA-C	5.37	118.49	109.95
2	D	71	SER	N-CA-C	5.37	118.07	110.50
1	E	26	TYR	N-CA-C	-5.35	100.98	109.76
1	A	372	ARG	N-CA-C	-5.33	106.63	113.23
1	C	232	VAL	N-CA-C	-5.32	105.32	110.42
1	A	52	ILE	CA-C-N	-5.31	117.52	121.61
1	A	52	ILE	C-N-CA	-5.31	117.52	121.61
1	E	17	LEU	N-CA-C	5.28	118.03	107.62
1	A	40	LYS	N-CA-C	-5.27	102.06	109.96
1	C	47	ASN	N-CA-C	5.25	121.99	110.80
2	F	160	ALA	N-CA-C	5.25	121.42	109.81
1	C	254	GLY	N-CA-C	5.25	118.37	110.18
1	C	307	GLU	N-CA-C	5.25	117.04	109.07
2	F	71	SER	N-CA-C	5.24	117.89	110.50
1	A	269	ASP	N-CA-C	5.24	117.73	111.71
1	E	344	GLN	N-CA-C	-5.21	106.61	113.12
1	E	7	LEU	N-CA-C	-5.20	101.66	109.15
1	C	154	LEU	N-CA-C	-5.19	103.18	110.50
2	D	161	PRO	N-CA-C	5.19	123.16	112.47
2	F	161	PRO	CA-C-N	5.19	131.73	122.13
2	F	161	PRO	C-N-CA	5.19	131.73	122.13
1	A	259	ARG	N-CA-C	-5.19	106.95	113.28
1	A	95	PRO	CA-C-N	5.18	125.43	119.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	95	PRO	C-N-CA	5.18	125.43	119.83
1	A	17	LEU	N-CA-C	5.18	117.88	107.41
1	E	58	ARG	N-CA-C	-5.18	106.80	113.01
1	A	408	ILE	CA-C-N	5.17	125.11	119.78
1	A	408	ILE	C-N-CA	5.17	125.11	119.78
1	A	407	SER	N-CA-C	5.14	119.03	112.34
2	B	71	SER	N-CA-C	5.13	117.73	110.50
1	E	410	LYS	N-CA-C	5.12	117.83	109.59
1	A	206	LEU	CA-C-N	5.09	124.99	119.85
1	A	206	LEU	C-N-CA	5.09	124.99	119.85
1	A	119	SER	N-CA-C	-5.07	104.22	110.31
1	A	70	ALA	N-CA-C	5.07	117.98	110.48
1	C	95	PRO	CA-C-N	5.07	125.31	119.83
1	C	95	PRO	C-N-CA	5.07	125.31	119.83
1	E	235	LYS	N-CA-C	-5.07	105.66	111.14
1	A	175	ASN	N-CA-C	-5.06	100.02	110.80
2	D	93	LEU	N-CA-C	-5.06	105.66	111.07
2	F	150	GLN	N-CA-C	-5.05	105.04	111.11
1	A	162	ILE	CA-C-N	5.03	125.75	120.11
1	A	162	ILE	C-N-CA	5.03	125.75	120.11
1	E	216	LYS	N-CA-C	-5.03	107.00	113.23
1	A	253	VAL	N-CA-C	-5.02	108.40	113.47
2	B	150	GLN	N-CA-C	-5.02	105.09	111.11
1	C	267	SER	N-CA-C	-5.01	105.49	112.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	249	PHE	Sidechain
1	C	249	PHE	Sidechain
1	E	249	PHE	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3339	0	3251	357	0
1	C	3338	0	3245	380	0
1	E	3339	0	3250	363	0
2	B	1228	0	1232	211	0
2	D	1228	0	1232	243	0
2	F	1228	0	1232	199	0
3	G	39	0	34	2	0
3	H	39	0	34	0	0
3	I	39	0	34	0	0
3	J	39	0	34	0	0
3	L	39	0	34	3	0
3	M	39	0	34	0	0
3	O	39	0	34	0	0
3	Q	39	0	34	6	0
3	R	39	0	34	1	0
3	S	39	0	34	1	0
3	T	39	0	34	2	0
4	K	39	0	33	10	0
4	P	39	0	33	5	0
4	U	39	0	33	8	0
5	N	39	0	33	0	0
All	All	14285	0	13948	1554	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 55.

All (1554) 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:55:GLY:HA3	1:A:82:PHE:HB3	1.26	1.17
1:E:55:GLY:HA3	1:E:82:PHE:HB3	1.23	1.17
1:C:55:GLY:HA3	1:C:82:PHE:HB3	1.19	1.16
2:F:126:ALA:HB3	2:F:129:LEU:HG	1.25	1.15
2:B:126:ALA:HB3	2:B:129:LEU:HG	1.21	1.14
2:B:5:ASP:H	2:B:9:ILE:HG23	1.07	1.10
1:C:418:PRO:HD3	2:D:111:LEU:HD13	1.11	1.10
2:D:126:ALA:HB3	2:D:129:LEU:HG	1.28	1.10
1:A:249:PHE:HE2	1:C:252:VAL:HG11	1.07	1.10
1:A:257:ASP:HB2	1:E:249:PHE:CE1	1.88	1.09
2:D:30:LYS:HD2	2:D:32:SER:H	1.19	1.07
2:B:30:LYS:HD2	2:B:32:SER:H	1.21	1.05
1:A:249:PHE:CD2	1:C:252:VAL:HG21	1.91	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:418:PRO:HD3	2:F:111:LEU:HD13	1.31	1.04
4:K:2:NDG:O3	4:K:3:MAN:H5	1.57	1.03
2:B:129:LEU:O	2:B:131:VAL:HG12	1.56	1.03
1:A:2:LYS:HB3	2:B:31:GLU:HB2	1.37	1.03
1:E:377:SER:HB2	1:E:392:LEU:H	1.24	1.02
1:C:294:LEU:HD11	1:C:296:MET:HE3	1.41	1.02
1:A:377:SER:HB2	1:A:392:LEU:H	1.20	1.02
2:F:30:LYS:HD2	2:F:32:SER:H	1.23	1.01
2:F:129:LEU:O	2:F:131:VAL:HG12	1.58	1.01
1:C:10:GLN:NE2	2:D:25:LEU:HD21	1.75	1.01
1:C:55:GLY:CA	1:C:82:PHE:HB3	1.88	1.01
1:C:377:SER:HB2	1:C:392:LEU:H	1.21	1.01
1:E:166:VAL:HG21	1:E:185:TYR:HB3	1.42	1.01
1:E:1:GLU:N	2:F:142:ASN:H	1.59	1.01
1:E:55:GLY:CA	1:E:82:PHE:HB3	1.90	1.01
1:E:294:LEU:HD11	1:E:296:MET:HE3	1.38	1.01
1:A:249:PHE:CE2	1:C:252:VAL:HG11	1.95	1.00
1:A:3:ILE:HA	2:B:30:LYS:HA	1.41	1.00
1:C:249:PHE:HE2	1:E:252:VAL:HG11	1.27	1.00
1:A:55:GLY:CA	1:A:82:PHE:HB3	1.93	0.99
2:D:129:LEU:O	2:D:131:VAL:HG12	1.62	0.98
1:A:249:PHE:HD2	1:C:252:VAL:HG21	1.23	0.97
1:C:5:ILE:HG21	2:D:154:PHE:CD1	1.98	0.97
1:C:418:PRO:HD3	2:D:111:LEU:CD1	1.96	0.96
1:E:166:VAL:CG2	1:E:185:TYR:HB3	1.94	0.96
1:A:8:GLN:HE22	2:B:8:ILE:HA	1.28	0.95
1:A:216:LYS:HD3	1:A:305:MET:H	1.30	0.94
1:C:166:VAL:HG21	1:C:185:TYR:HB3	1.46	0.94
1:C:216:LYS:HD3	1:C:305:MET:H	1.32	0.94
1:C:3:ILE:HD11	2:D:140:ILE:HG22	1.48	0.93
1:C:418:PRO:HG3	2:D:111:LEU:HB3	1.51	0.93
1:E:1:GLU:H2	2:F:142:ASN:H	1.03	0.92
1:C:3:ILE:CD1	2:D:140:ILE:HG22	1.98	0.92
1:A:257:ASP:HB2	1:E:249:PHE:CD1	2.05	0.92
1:A:166:VAL:HG21	1:A:185:TYR:HB3	1.49	0.92
1:C:166:VAL:CG2	1:C:185:TYR:HB3	2.00	0.92
1:A:294:LEU:HD11	1:A:296:MET:HE3	1.51	0.92
1:C:10:GLN:HE21	2:D:25:LEU:HD21	1.34	0.91
1:A:8:GLN:HE22	2:B:8:ILE:CA	1.83	0.91
1:C:3:ILE:CG1	2:D:140:ILE:HG22	2.00	0.91
2:F:129:LEU:HA	2:F:140:ILE:HG12	1.53	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:216:LYS:HD3	1:E:305:MET:H	1.33	0.90
1:A:231:GLU:CD	1:A:231:GLU:N	2.28	0.90
1:A:166:VAL:CG2	1:A:185:TYR:HB3	2.02	0.90
2:D:141:ASP:OD1	2:D:143:ASN:HB2	1.71	0.90
2:B:129:LEU:HA	2:B:140:ILE:HG12	1.54	0.89
1:C:9:LYS:HE2	2:D:112:GLN:HE22	1.36	0.89
1:E:8:GLN:HB3	2:F:25:LEU:HD12	1.55	0.88
1:E:231:GLU:N	1:E:231:GLU:CD	2.30	0.88
2:B:4:ILE:HG22	2:B:9:ILE:HG21	1.55	0.88
1:C:31:LYS:NZ	1:C:411:ILE:HB	1.88	0.88
2:D:129:LEU:HA	2:D:140:ILE:HG12	1.56	0.88
1:A:31:LYS:NZ	1:A:411:ILE:HB	1.88	0.88
2:D:160:ALA:N	2:D:161:PRO:HD3	1.89	0.88
1:E:184:LEU:HD12	1:E:185:TYR:H	1.38	0.88
2:F:4:ILE:HG22	2:F:13:PHE:CD2	2.09	0.87
1:A:422:THR:HG21	2:F:51:ASP:HB3	1.55	0.87
1:C:426:VAL:CG2	2:D:4:ILE:HG23	2.04	0.87
1:A:184:LEU:HD12	1:A:185:TYR:H	1.40	0.87
1:A:230:LYS:HD2	1:A:234:ASN:HD21	1.41	0.86
1:E:31:LYS:NZ	1:E:411:ILE:HB	1.90	0.86
1:C:249:PHE:HD2	1:E:252:VAL:HG21	1.39	0.86
1:C:5:ILE:HG12	2:D:154:PHE:CE2	2.09	0.86
1:E:126:CYS:O	1:E:127:TYR:HB2	1.76	0.86
1:C:231:GLU:N	1:C:231:GLU:CD	2.34	0.86
2:B:126:ALA:HB3	2:B:129:LEU:CG	2.03	0.85
1:E:3:ILE:HD11	2:F:140:ILE:HG22	1.58	0.85
2:F:68:ASP:C	2:F:70:ILE:H	1.85	0.85
1:A:80:PHE:HB3	1:A:82:PHE:CD2	2.11	0.85
1:C:249:PHE:CE2	1:E:252:VAL:HG11	2.12	0.84
1:C:426:VAL:HG21	2:D:4:ILE:HG23	1.59	0.84
2:B:5:ASP:HB2	2:B:9:ILE:HA	1.59	0.84
2:B:5:ASP:N	2:B:9:ILE:HG23	1.90	0.84
1:C:8:GLN:HB3	2:D:25:LEU:HD12	1.58	0.84
1:A:59:THR:HB	1:A:82:PHE:CD2	2.13	0.83
2:B:68:ASP:C	2:B:70:ILE:H	1.83	0.83
1:C:80:PHE:HB3	1:C:82:PHE:CD2	2.13	0.83
1:E:59:THR:HB	1:E:82:PHE:CD2	2.14	0.83
1:A:134:ILE:HD13	1:A:275:CYS:HB2	1.60	0.83
2:B:126:ALA:CB	2:B:129:LEU:HG	2.07	0.83
1:E:249:PHE:CG	1:E:250:GLY:N	2.43	0.83
1:E:45:VAL:C	1:E:46:LEU:HD23	2.04	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:VAL:C	1:A:46:LEU:HD23	2.03	0.82
2:F:126:ALA:HB3	2:F:129:LEU:CG	2.06	0.82
1:C:184:LEU:HD12	1:C:185:TYR:H	1.44	0.82
2:D:126:ALA:HB3	2:D:129:LEU:CG	2.09	0.82
1:E:4:LYS:O	2:F:28:SER:HA	1.79	0.82
1:E:80:PHE:HB3	1:E:82:PHE:CD2	2.14	0.82
2:F:126:ALA:CB	2:F:129:LEU:HG	2.09	0.82
1:C:249:PHE:CD2	1:E:252:VAL:HG21	2.15	0.82
1:E:181:ASN:HB3	1:E:182:PRO:HD3	1.60	0.82
1:C:249:PHE:CG	1:C:250:GLY:N	2.47	0.81
1:A:249:PHE:CG	1:A:250:GLY:N	2.48	0.81
1:C:393:PRO:HB2	1:C:394:PRO:HD3	1.61	0.81
2:D:4:ILE:HG22	2:D:13:PHE:CB	2.10	0.81
1:C:181:ASN:HB3	1:C:182:PRO:HD3	1.62	0.80
1:C:25:LEU:HD11	2:D:107:ILE:CG2	2.11	0.80
1:A:126:CYS:O	1:A:127:TYR:HB2	1.80	0.80
2:D:68:ASP:C	2:D:70:ILE:H	1.86	0.80
2:F:65:LYS:HZ2	2:F:65:LYS:HB2	1.46	0.80
4:U:2:NDG:O3	4:U:3:MAN:H2	1.82	0.80
2:B:131:VAL:HG11	2:B:139:ILE:C	2.07	0.80
1:C:59:THR:HB	1:C:82:PHE:CD2	2.17	0.80
2:D:5:ASP:OD1	2:D:9:ILE:HA	1.80	0.80
1:A:181:ASN:HB3	1:A:182:PRO:HD3	1.62	0.80
1:A:288:ARG:NH1	1:A:288:ARG:HG3	1.97	0.79
1:C:230:LYS:HD2	1:C:234:ASN:HD21	1.45	0.79
1:C:3:ILE:HG13	2:D:140:ILE:O	1.82	0.79
1:C:38:LYS:H	1:C:38:LYS:HD3	1.48	0.79
1:C:420:SER:HB3	1:C:424:THR:OG1	1.83	0.79
1:C:25:LEU:HD11	2:D:107:ILE:HG21	1.62	0.79
1:C:45:VAL:C	1:C:46:LEU:HD23	2.07	0.79
1:E:134:ILE:HD13	1:E:275:CYS:HB2	1.65	0.79
1:A:19:ASN:ND2	4:U:2:NDG:H8C2	1.97	0.79
2:B:125:ARG:C	2:B:129:LEU:HD21	2.08	0.79
1:E:1:GLU:HG2	1:E:2:LYS:N	1.98	0.79
2:D:4:ILE:HG22	2:D:9:ILE:HG21	1.63	0.78
1:E:28:THR:HG21	3:Q:2:NAG:H82	1.64	0.78
1:E:230:LYS:HD2	1:E:234:ASN:HD21	1.48	0.78
1:E:405:GLU:O	1:E:408:ILE:HG23	1.84	0.78
1:C:3:ILE:HG12	2:D:140:ILE:HG22	1.66	0.78
1:C:405:GLU:O	1:C:408:ILE:HG23	1.83	0.78
2:B:131:VAL:HG21	2:B:139:ILE:HB	1.64	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3:ILE:HD11	2:D:140:ILE:CG2	2.13	0.78
1:C:388:GLU:CD	1:C:388:GLU:H	1.90	0.78
2:B:125:ARG:O	2:B:129:LEU:HD21	1.82	0.78
1:E:240:ASN:ND2	1:E:263:TYR:OH	2.15	0.78
2:D:9:ILE:N	2:D:9:ILE:HD13	1.99	0.77
1:E:46:LEU:O	1:E:48:GLN:N	2.17	0.77
1:A:257:ASP:HB2	1:E:249:PHE:HE1	1.46	0.77
1:A:240:ASN:ND2	1:A:263:TYR:OH	2.18	0.77
1:A:22:GLY:N	2:F:106:ASN:OD1	2.18	0.77
1:A:288:ARG:HG3	1:A:288:ARG:HH11	1.49	0.77
2:B:126:ALA:N	2:B:129:LEU:HD11	2.00	0.77
2:D:146:ASP:OD2	2:D:148:SER:HB2	1.85	0.77
1:A:154:LEU:HD22	1:A:155:VAL:N	2.00	0.76
2:B:141:ASP:OD1	2:B:143:ASN:HB2	1.84	0.76
1:C:46:LEU:O	1:C:48:GLN:N	2.18	0.76
2:B:21:ILE:H	2:B:21:ILE:HD12	1.50	0.76
1:C:338:CYS:O	2:D:78:ARG:NH2	2.18	0.76
1:A:319:GLY:H	1:A:354:HIS:CD2	2.04	0.76
1:E:294:LEU:HD11	1:E:296:MET:CE	2.13	0.76
1:E:418:PRO:HD3	2:F:111:LEU:CD1	2.15	0.76
1:C:126:CYS:O	1:C:127:TYR:HB2	1.84	0.76
2:F:7:LEU:HD23	2:F:29:ARG:HH12	1.49	0.76
2:B:5:ASP:O	2:B:9:ILE:HD13	1.84	0.76
1:C:294:LEU:HD11	1:C:296:MET:CE	2.15	0.76
1:A:158:LEU:HD21	1:A:298:GLU:HA	1.67	0.75
2:D:126:ALA:CB	2:D:129:LEU:HG	2.12	0.75
1:E:38:LYS:HD3	1:E:38:LYS:H	1.50	0.75
1:E:420:SER:HB3	1:E:424:THR:OG1	1.86	0.75
1:A:231:GLU:CD	1:A:231:GLU:H	1.91	0.75
1:E:373:CYS:HG	1:E:399:CYS:HG	1.25	0.75
1:C:134:ILE:HD13	1:C:275:CYS:HB2	1.68	0.75
1:A:393:PRO:HB2	1:A:394:PRO:HD3	1.67	0.75
2:B:162:VAL:HG22	2:B:162:VAL:O	1.87	0.75
2:B:129:LEU:O	2:B:131:VAL:N	2.19	0.74
1:C:203:PHE:HD1	1:C:286:SER:HB3	1.51	0.74
1:E:158:LEU:HD21	1:E:298:GLU:HA	1.67	0.74
1:E:154:LEU:HD22	1:E:155:VAL:N	2.03	0.74
2:F:129:LEU:O	2:F:131:VAL:N	2.21	0.74
1:C:5:ILE:O	2:D:138:TRP:CD1	2.40	0.74
1:C:3:ILE:O	2:D:139:ILE:HG23	1.86	0.74
1:E:379:TRP:HZ3	1:E:381:ASN:HB3	1.52	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:131:VAL:HG11	2:F:139:ILE:C	2.12	0.74
1:C:340:LEU:H	1:C:376:GLN:HE22	1.33	0.74
2:D:131:VAL:HG11	2:D:139:ILE:C	2.12	0.74
1:E:388:GLU:CD	1:E:388:GLU:H	1.91	0.74
2:B:4:ILE:HG22	2:B:9:ILE:CG2	2.18	0.74
2:B:131:VAL:CG2	2:B:139:ILE:H	2.01	0.74
2:B:138:TRP:CD1	2:B:138:TRP:N	2.56	0.74
1:C:59:THR:O	1:C:82:PHE:CE2	2.41	0.74
2:B:65:LYS:HB2	2:B:65:LYS:HZ2	1.52	0.74
1:C:163:PRO:HB2	1:C:165:GLN:OE1	1.88	0.74
1:C:158:LEU:HD21	1:C:298:GLU:HA	1.70	0.74
4:K:2:NDG:H4	4:K:3:MAN:H3	1.68	0.74
1:A:163:PRO:HB2	1:A:165:GLN:OE1	1.87	0.73
2:D:65:LYS:HB2	2:D:65:LYS:NZ	2.03	0.73
2:F:55:LEU:HB3	2:F:107:ILE:HD12	1.70	0.73
1:C:60:ASP:HA	1:C:82:PHE:CD1	2.22	0.73
2:B:55:LEU:HB3	2:B:107:ILE:HD12	1.70	0.73
1:C:240:ASN:ND2	1:C:263:TYR:OH	2.20	0.73
1:E:66:PHE:HB3	1:E:67:PRO:HD3	1.70	0.73
1:A:216:LYS:HD3	1:A:305:MET:N	2.02	0.73
1:C:3:ILE:CD1	2:D:140:ILE:H	2.01	0.73
1:E:231:GLU:CD	1:E:231:GLU:H	1.96	0.73
1:A:46:LEU:O	1:A:48:GLN:N	2.22	0.73
2:B:62:ALA:O	2:B:66:LEU:HD13	1.89	0.73
1:E:392:LEU:HD22	1:E:393:PRO:HD2	1.68	0.73
2:F:141:ASP:OD1	2:F:143:ASN:HB2	1.87	0.73
1:C:319:GLY:H	1:C:354:HIS:CD2	2.06	0.73
1:E:31:LYS:HZ1	1:E:411:ILE:HB	1.52	0.73
1:C:379:TRP:HZ3	1:C:381:ASN:HB3	1.54	0.73
2:D:152:PHE:HD2	2:D:153:ILE:HD13	1.54	0.73
2:F:146:ASP:OD2	2:F:148:SER:HB2	1.88	0.72
2:F:9:ILE:HG22	2:F:10:GLY:H	1.53	0.72
1:A:420:SER:HB3	1:A:424:THR:OG1	1.88	0.72
2:D:112:GLN:HE21	2:D:112:GLN:HA	1.53	0.72
2:F:126:ALA:N	2:F:129:LEU:HD11	2.05	0.72
1:A:231:GLU:OE1	1:A:232:VAL:N	2.21	0.72
1:C:154:LEU:HD22	1:C:155:VAL:N	2.03	0.72
1:A:230:LYS:HD2	1:A:234:ASN:ND2	2.04	0.72
2:D:160:ALA:H	2:D:161:PRO:HD3	1.54	0.72
2:F:112:GLN:HE21	2:F:112:GLN:HA	1.53	0.72
1:A:249:PHE:HE2	1:C:252:VAL:CG1	1.94	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:104:GLN:HB2	1:A:153:SER:HB2	1.71	0.71
1:C:5:ILE:O	2:D:138:TRP:HD1	1.73	0.71
1:C:58:ARG:NH1	1:C:354:HIS:O	2.22	0.71
1:C:288:ARG:NH1	1:C:288:ARG:HG3	2.04	0.71
1:E:60:ASP:HA	1:E:82:PHE:CD1	2.25	0.71
1:E:294:LEU:C	1:E:294:LEU:HD22	2.15	0.71
2:F:125:ARG:C	2:F:129:LEU:HD21	2.15	0.71
1:E:216:LYS:HD3	1:E:305:MET:N	2.05	0.71
1:E:217:LEU:HD23	1:E:305:MET:HE2	1.72	0.71
1:A:66:PHE:HB3	1:A:67:PRO:HD3	1.73	0.71
2:B:146:ASP:OD2	2:B:148:SER:HB2	1.91	0.71
1:C:318:TRP:HB3	1:C:322:ARG:HG3	1.72	0.71
2:D:129:LEU:O	2:D:131:VAL:N	2.23	0.71
1:E:28:THR:HB	3:Q:2:NAG:H81	1.73	0.71
1:A:392:LEU:HD22	1:A:393:PRO:HD2	1.70	0.71
1:E:393:PRO:HB2	1:E:394:PRO:HD3	1.71	0.71
1:C:315:GLN:NE2	1:C:343:LYS:H	1.89	0.71
1:E:288:ARG:NH1	1:E:288:ARG:HG3	2.04	0.71
1:A:405:GLU:O	1:A:408:ILE:HG23	1.91	0.71
1:A:66:PHE:O	1:A:67:PRO:C	2.34	0.71
1:E:1:GLU:O	2:F:141:ASP:HA	1.91	0.70
1:A:59:THR:O	1:A:82:PHE:CE2	2.44	0.70
1:C:249:PHE:CE1	1:E:257:ASP:HB2	2.26	0.70
1:E:288:ARG:HG3	1:E:288:ARG:HH11	1.56	0.70
1:E:426:VAL:HG11	2:F:4:ILE:HG21	1.72	0.70
4:P:2:NDG:O3	4:P:3:MAN:H2	1.91	0.70
1:A:2:LYS:O	2:B:31:GLU:N	2.23	0.70
1:C:319:GLY:HA2	1:C:347:TYR:HB3	1.74	0.70
2:D:131:VAL:CG2	2:D:139:ILE:H	2.05	0.70
1:E:319:GLY:H	1:E:354:HIS:CD2	2.09	0.70
2:F:65:LYS:HB2	2:F:65:LYS:NZ	2.04	0.70
2:B:140:ILE:HD12	2:B:141:ASP:H	1.56	0.70
2:D:131:VAL:HG21	2:D:139:ILE:HB	1.74	0.70
2:F:131:VAL:CG2	2:F:139:ILE:H	2.05	0.70
4:K:2:NDG:O7	4:K:2:NDG:C3	2.39	0.70
1:A:388:GLU:H	1:A:388:GLU:CD	1.97	0.70
1:E:376:GLN:HB2	1:E:394:PRO:HD2	1.73	0.70
1:E:418:PRO:HG3	2:F:111:LEU:HB3	1.73	0.70
1:C:288:ARG:HG3	1:C:288:ARG:HH11	1.57	0.69
2:D:21:ILE:HD12	2:D:21:ILE:H	1.57	0.69
2:F:4:ILE:HB	2:F:9:ILE:CD1	2.22	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:152:PHE:HD2	2:F:153:ILE:HD13	1.57	0.69
1:A:8:GLN:NE2	2:B:8:ILE:HA	2.07	0.69
2:B:140:ILE:CD1	2:B:141:ASP:H	2.06	0.69
1:C:420:SER:H	1:C:424:THR:HG21	1.57	0.69
1:E:392:LEU:CD2	1:E:393:PRO:HD2	2.21	0.69
2:F:45:PHE:HA	2:F:48:ILE:HD12	1.74	0.69
1:A:38:LYS:H	1:A:38:LYS:HD3	1.56	0.69
2:B:112:GLN:HE21	2:B:112:GLN:HA	1.56	0.69
1:C:3:ILE:HD13	1:C:5:ILE:CD1	2.23	0.69
1:A:80:PHE:HB3	1:A:82:PHE:CE2	2.26	0.69
2:D:55:LEU:HB3	2:D:107:ILE:HD12	1.73	0.69
2:F:125:ARG:O	2:F:129:LEU:HD21	1.93	0.69
1:C:66:PHE:O	1:C:67:PRO:C	2.31	0.69
1:E:1:GLU:HA	2:F:141:ASP:HA	1.72	0.69
1:C:38:LYS:HD3	1:C:38:LYS:N	2.07	0.69
1:A:60:ASP:HA	1:A:82:PHE:CD1	2.28	0.69
1:A:373:CYS:HG	1:A:399:CYS:HG	1.39	0.69
1:C:216:LYS:HD3	1:C:305:MET:N	2.05	0.69
2:D:125:ARG:C	2:D:129:LEU:HD21	2.18	0.69
1:E:230:LYS:HD2	1:E:234:ASN:ND2	2.08	0.69
1:A:340:LEU:H	1:A:376:GLN:HE22	1.38	0.69
1:E:315:GLN:NE2	1:E:343:LYS:H	1.91	0.69
1:A:9:LYS:O	2:B:15:ALA:N	2.25	0.68
2:F:62:ALA:O	2:F:66:LEU:HD13	1.94	0.68
1:A:379:TRP:HZ3	1:A:381:ASN:HB3	1.58	0.68
2:B:45:PHE:HA	2:B:48:ILE:HD12	1.76	0.68
1:C:426:VAL:HB	2:D:4:ILE:HD13	1.74	0.68
1:E:25:LEU:HD11	2:F:107:ILE:HG21	1.75	0.68
1:E:340:LEU:H	1:E:376:GLN:HE22	1.40	0.68
1:A:31:LYS:HZ3	1:A:31:LYS:HB2	1.58	0.68
1:A:319:GLY:HA2	1:A:347:TYR:HB3	1.75	0.68
2:B:65:LYS:HB2	2:B:65:LYS:NZ	2.08	0.68
1:C:1:GLU:OE1	1:C:2:LYS:HB2	1.94	0.68
1:C:60:ASP:HA	1:C:82:PHE:CE1	2.29	0.68
1:C:230:LYS:HD2	1:C:234:ASN:ND2	2.08	0.68
1:E:9:LYS:HE2	2:F:112:GLN:HE22	1.57	0.68
1:E:247:ASP:O	1:E:249:PHE:O	2.10	0.68
1:A:58:ARG:NH1	1:A:354:HIS:O	2.26	0.68
1:A:315:GLN:NE2	1:A:343:LYS:H	1.90	0.68
1:C:231:GLU:CD	1:C:231:GLU:H	2.01	0.68
1:E:1:GLU:N	2:F:142:ASN:N	2.39	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:425:THR:HB	2:B:16:ILE:HD11	1.73	0.68
1:E:25:LEU:HD11	2:F:107:ILE:CG2	2.24	0.68
2:B:129:LEU:CD2	2:B:153:ILE:HD12	2.24	0.68
1:C:249:PHE:CD1	1:C:250:GLY:N	2.59	0.68
1:C:392:LEU:HD22	1:C:393:PRO:HD2	1.75	0.68
1:A:294:LEU:HD11	1:A:296:MET:CE	2.24	0.68
1:A:376:GLN:HB2	1:A:394:PRO:HD2	1.76	0.68
1:E:59:THR:O	1:E:82:PHE:CE2	2.47	0.68
1:A:252:VAL:HG11	1:E:249:PHE:HE2	1.59	0.67
2:B:19:THR:O	3:G:1:NAG:H82	1.94	0.67
2:D:125:ARG:O	2:D:129:LEU:HD21	1.95	0.67
1:E:163:PRO:HB2	1:E:165:GLN:OE1	1.93	0.67
1:A:119:SER:HB3	1:A:120:PRO:HD2	1.76	0.67
1:A:426:VAL:HG11	2:B:4:ILE:HG12	1.77	0.67
1:C:66:PHE:HB3	1:C:67:PRO:HD3	1.76	0.67
1:E:66:PHE:O	1:E:67:PRO:C	2.32	0.67
2:D:154:PHE:O	2:D:156:PHE:N	2.28	0.67
2:B:122:ILE:HB	2:B:138:TRP:CH2	2.30	0.67
1:C:3:ILE:HD11	2:D:140:ILE:CB	2.24	0.67
2:D:138:TRP:CD1	2:D:138:TRP:N	2.60	0.67
2:F:138:TRP:CD1	2:F:138:TRP:N	2.61	0.67
2:B:152:PHE:HD2	2:B:153:ILE:HD13	1.60	0.67
1:E:60:ASP:HA	1:E:82:PHE:CE1	2.30	0.67
1:A:203:PHE:HD1	1:A:286:SER:HB3	1.60	0.67
2:B:4:ILE:HG23	2:B:13:PHE:CD2	2.30	0.67
1:C:373:CYS:HG	1:C:399:CYS:HG	1.42	0.67
1:E:1:GLU:HA	2:F:141:ASP:CA	2.24	0.67
1:E:231:GLU:OE1	1:E:232:VAL:N	2.25	0.67
2:B:5:ASP:H	2:B:9:ILE:CG2	1.97	0.67
1:E:1:GLU:H1	2:F:142:ASN:CG	2.01	0.67
1:E:1:GLU:CA	2:F:142:ASN:H	2.08	0.67
1:A:217:LEU:HD23	1:A:305:MET:HE2	1.76	0.66
2:F:140:ILE:CD1	2:F:141:ASP:H	2.08	0.66
1:A:249:PHE:CE2	1:C:252:VAL:CG1	2.75	0.66
2:F:122:ILE:HB	2:F:138:TRP:CH2	2.30	0.66
1:A:420:SER:H	1:A:424:THR:HG21	1.59	0.66
1:A:392:LEU:CD2	1:A:393:PRO:HD2	2.26	0.66
1:C:339:MET:HE1	1:C:374:ILE:HD12	1.77	0.66
2:D:45:PHE:HA	2:D:48:ILE:HD12	1.78	0.66
2:D:65:LYS:HB2	2:D:65:LYS:HZ2	1.58	0.66
2:D:125:ARG:NH1	2:D:152:PHE:O	2.28	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:58:ARG:NH2	1:E:317:ILE:O	2.29	0.66
2:F:140:ILE:HD12	2:F:141:ASP:H	1.61	0.66
2:F:131:VAL:HG21	2:F:139:ILE:HB	1.76	0.66
1:E:184:LEU:HD12	1:E:185:TYR:N	2.10	0.65
1:E:420:SER:H	1:E:424:THR:HG21	1.60	0.65
1:A:59:THR:HB	1:A:82:PHE:HD2	1.61	0.65
2:D:62:ALA:O	2:D:66:LEU:HD13	1.96	0.65
2:D:125:ARG:HB3	2:D:129:LEU:HD21	1.77	0.65
2:D:140:ILE:HD12	2:D:141:ASP:H	1.60	0.65
1:E:59:THR:HB	1:E:82:PHE:HD2	1.61	0.65
1:E:181:ASN:HB3	1:E:182:PRO:CD	2.26	0.65
1:E:249:PHE:CD1	1:E:250:GLY:N	2.59	0.65
1:A:33:MET:CE	2:B:100:ARG:HB2	2.26	0.65
1:A:257:ASP:CB	1:E:249:PHE:CE1	2.76	0.65
1:C:217:LEU:HD23	1:C:305:MET:HE2	1.79	0.65
2:D:126:ALA:N	2:D:129:LEU:HD11	2.11	0.65
2:D:140:ILE:CD1	2:D:141:ASP:H	2.08	0.65
1:E:1:GLU:H2	2:F:142:ASN:N	1.86	0.65
1:E:203:PHE:HD1	1:E:286:SER:HB3	1.62	0.65
1:A:318:TRP:HB3	1:A:322:ARG:HG3	1.77	0.65
2:D:122:ILE:HB	2:D:138:TRP:CH2	2.32	0.65
1:C:163:PRO:HG2	1:C:166:VAL:CG1	2.27	0.65
1:C:394:PRO:HG3	2:D:78:ARG:HG3	1.79	0.65
1:E:319:GLY:HA2	1:E:347:TYR:HB3	1.77	0.65
2:F:4:ILE:HB	2:F:9:ILE:HD13	1.79	0.65
2:D:9:ILE:HG21	2:D:13:PHE:HB2	1.79	0.65
1:A:1:GLU:OE1	1:A:1:GLU:N	2.27	0.65
1:C:85:GLY:O	1:C:99:VAL:HG13	1.97	0.65
2:D:30:LYS:HD2	2:D:32:SER:N	2.03	0.65
1:E:1:GLU:CA	2:F:141:ASP:HA	2.26	0.65
1:C:418:PRO:CG	2:D:111:LEU:HB3	2.27	0.65
1:E:10:GLN:HG3	2:F:15:ALA:HB3	1.79	0.65
1:E:31:LYS:HZ3	1:E:31:LYS:HB2	1.61	0.65
2:F:21:ILE:HD12	2:F:21:ILE:H	1.62	0.65
2:B:116:TRP:HZ3	2:D:116:TRP:HH2	1.45	0.64
2:D:102:LEU:CD1	2:F:102:LEU:HD21	2.27	0.64
1:E:80:PHE:HB3	1:E:82:PHE:CE2	2.33	0.64
1:A:80:PHE:CB	1:A:82:PHE:CE2	2.80	0.64
1:C:294:LEU:HD22	1:C:294:LEU:C	2.22	0.64
2:D:30:LYS:CD	2:D:32:SER:H	2.04	0.64
2:D:152:PHE:CD2	2:D:153:ILE:HD13	2.33	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:126:CYS:HA	1:E:173:ASN:HD22	1.63	0.64
1:A:425:THR:CG2	2:B:16:ILE:HD11	2.28	0.64
1:A:47:ASN:O	1:A:49:SER:N	2.30	0.64
1:A:126:CYS:HA	1:A:173:ASN:HD22	1.63	0.64
1:C:416:LEU:HB2	2:D:52:ILE:HD13	1.79	0.64
1:C:416:LEU:HD22	2:D:56:LYS:HD2	1.78	0.64
1:E:38:LYS:HD3	1:E:38:LYS:N	2.10	0.64
1:A:424:THR:HG23	2:B:13:PHE:HA	1.80	0.64
2:F:125:ARG:HB3	2:F:129:LEU:HD21	1.80	0.64
1:C:19:ASN:CG	4:K:2:NDG:H8C2	2.23	0.64
1:C:47:ASN:O	1:C:49:SER:N	2.31	0.64
1:E:104:GLN:HB2	1:E:153:SER:HB2	1.78	0.64
2:F:129:LEU:CD2	2:F:153:ILE:HD12	2.28	0.64
1:C:31:LYS:HZ3	1:C:31:LYS:HB2	1.63	0.64
2:F:5:ASP:OD2	2:F:9:ILE:HA	1.97	0.64
1:A:125:ASN:OD1	1:A:125:ASN:C	2.41	0.63
1:C:5:ILE:HG12	2:D:154:PHE:CD2	2.32	0.63
2:D:4:ILE:HG22	2:D:13:PHE:CG	2.32	0.63
1:C:58:ARG:NH2	1:C:317:ILE:O	2.28	0.63
1:E:58:ARG:NH1	1:E:354:HIS:O	2.30	0.63
1:E:416:LEU:HD22	2:F:56:LYS:HD2	1.80	0.63
1:A:163:PRO:HG2	1:A:166:VAL:CG1	2.28	0.63
1:A:181:ASN:HB3	1:A:182:PRO:CD	2.27	0.63
1:A:249:PHE:CD2	1:C:252:VAL:CG2	2.75	0.63
1:E:249:PHE:CD2	1:E:250:GLY:N	2.65	0.63
1:E:339:MET:HE1	1:E:374:ILE:HD12	1.80	0.63
2:B:116:TRP:CZ3	2:D:116:TRP:HH2	2.16	0.63
1:A:34:PHE:HZ	2:B:66:LEU:HD23	1.63	0.63
1:A:249:PHE:CD1	1:A:250:GLY:N	2.62	0.63
1:A:288:ARG:NH2	1:C:260:VAL:HG12	2.14	0.63
1:A:162:ILE:HG23	1:A:163:PRO:HD2	1.81	0.63
1:C:125:ASN:OD1	1:C:125:ASN:C	2.40	0.63
1:C:376:GLN:HB2	1:C:394:PRO:HD2	1.80	0.63
1:E:17:LEU:C	1:E:17:LEU:HD22	2.23	0.63
2:F:17:VAL:O	2:F:19:THR:N	2.32	0.63
1:E:59:THR:HG21	1:E:80:PHE:CE2	2.34	0.63
1:E:125:ASN:OD1	1:E:125:ASN:C	2.42	0.63
1:C:7:LEU:HD21	2:D:118:LEU:HD13	1.82	0.62
1:C:34:PHE:HE2	2:D:96:LEU:HD13	1.64	0.62
2:D:5:ASP:H	2:D:9:ILE:HD12	1.63	0.62
1:A:288:ARG:HH22	1:C:260:VAL:HG12	1.63	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:181:ASN:HB3	1:C:182:PRO:CD	2.28	0.62
1:C:425:THR:HB	2:D:16:ILE:HD11	1.81	0.62
1:E:66:PHE:HB3	1:E:67:PRO:CD	2.28	0.62
1:E:294:LEU:HD21	1:E:296:MET:HE2	1.80	0.62
4:K:2:NDG:O7	4:K:2:NDG:H3	1.99	0.62
2:B:125:ARG:HB3	2:B:129:LEU:HD21	1.79	0.62
2:B:131:VAL:O	2:B:132:GLU:C	2.42	0.62
1:C:80:PHE:HB3	1:C:82:PHE:CE2	2.34	0.62
2:F:164:THR:HG23	2:F:165:ILE:H	1.64	0.62
2:B:17:VAL:O	2:B:17:VAL:HG23	2.00	0.62
1:A:3:ILE:HD13	1:A:5:ILE:CD1	2.29	0.62
1:E:3:ILE:HD11	2:F:140:ILE:H	1.63	0.62
1:A:190:LYS:HD3	1:A:191:PRO:HD2	1.80	0.62
1:A:319:GLY:H	1:A:354:HIS:HD2	1.47	0.62
1:E:19:ASN:CG	4:P:2:NDG:H8C1	2.25	0.62
1:A:249:PHE:CE2	1:C:252:VAL:HG21	2.34	0.62
2:B:17:VAL:O	2:B:19:THR:N	2.32	0.62
1:C:80:PHE:CB	1:C:82:PHE:CE2	2.82	0.62
2:D:41:ALA:O	2:D:43:LYS:N	2.33	0.62
4:U:1:NAG:O3	4:U:2:NDG:N2	2.33	0.62
1:C:104:GLN:HB2	1:C:153:SER:HB2	1.81	0.62
1:A:60:ASP:HA	1:A:82:PHE:CE1	2.35	0.61
1:C:126:CYS:HA	1:C:173:ASN:HD22	1.63	0.61
1:C:414:GLY:H	2:D:56:LYS:HE3	1.65	0.61
1:E:80:PHE:CB	1:E:82:PHE:CE2	2.83	0.61
1:A:184:LEU:HD12	1:A:185:TYR:N	2.12	0.61
2:B:4:ILE:CG2	2:B:9:ILE:HG21	2.29	0.61
1:C:31:LYS:HZ1	1:C:411:ILE:HB	1.60	0.61
2:F:152:PHE:CD2	2:F:153:ILE:HD13	2.35	0.61
2:F:17:VAL:O	2:F:17:VAL:HG23	2.00	0.61
2:B:125:ARG:NH1	2:B:152:PHE:O	2.34	0.61
1:E:163:PRO:HG2	1:E:166:VAL:CG1	2.30	0.61
1:A:249:PHE:CD2	1:A:250:GLY:N	2.69	0.61
1:A:425:THR:CB	2:B:16:ILE:HD11	2.31	0.61
1:A:426:VAL:HG21	2:B:4:ILE:HG21	1.81	0.61
1:C:59:THR:HB	1:C:82:PHE:HD2	1.63	0.61
1:C:203:PHE:CD1	1:C:286:SER:HB3	2.36	0.61
1:C:392:LEU:CD2	1:C:393:PRO:HD2	2.30	0.61
2:F:8:ILE:O	2:F:8:ILE:HG13	2.01	0.61
1:E:3:ILE:O	2:F:139:ILE:HG23	2.01	0.61
1:E:8:GLN:HB3	2:F:25:LEU:CD1	2.29	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:19:ASN:CB	4:P:2:NDG:H8C1	2.30	0.61
1:E:3:ILE:HD13	1:E:5:ILE:CD1	2.31	0.61
1:E:190:LYS:HD3	1:E:191:PRO:HD2	1.82	0.61
1:E:294:LEU:HD22	1:E:295:LEU:N	2.15	0.61
1:A:31:LYS:HZ2	1:A:411:ILE:HB	1.66	0.60
1:A:357:ASP:O	1:A:361:ARG:HG3	2.01	0.60
1:E:318:TRP:HB3	1:E:322:ARG:HG3	1.82	0.60
2:B:129:LEU:HD23	2:B:153:ILE:HD12	1.82	0.60
2:B:160:ALA:N	2:B:161:PRO:HD3	2.15	0.60
1:C:315:GLN:HE21	1:C:343:LYS:H	1.49	0.60
1:E:1:GLU:CG	1:E:2:LYS:N	2.64	0.60
1:E:24:ASN:H	1:E:419:THR:HG22	1.67	0.60
2:F:125:ARG:NH1	2:F:152:PHE:O	2.34	0.60
1:A:31:LYS:HZ1	1:A:411:ILE:HB	1.61	0.60
2:B:123:THR:HG1	2:B:138:TRP:HZ3	1.48	0.60
1:C:3:ILE:HD11	2:D:140:ILE:H	1.64	0.60
2:D:4:ILE:HG22	2:D:13:PHE:HB2	1.82	0.60
1:E:92:MET:O	1:E:181:ASN:HB2	2.02	0.60
1:A:241:TYR:O	1:A:258:ASN:HB2	2.01	0.60
1:E:376:GLN:CB	1:E:394:PRO:HD2	2.32	0.60
1:C:17:LEU:C	1:C:17:LEU:HD22	2.25	0.60
1:A:5:ILE:HD12	1:A:5:ILE:N	2.16	0.60
1:E:33:MET:HE3	1:E:409:PRO:HB2	1.84	0.60
2:F:131:VAL:O	2:F:132:GLU:C	2.44	0.60
4:U:2:NDG:O7	4:U:2:NDG:C3	2.49	0.60
2:B:131:VAL:HG11	2:B:139:ILE:O	2.01	0.60
2:F:83:GLU:CD	2:F:83:GLU:H	2.08	0.60
2:B:102:LEU:CD1	2:D:102:LEU:HD21	2.31	0.60
2:D:142:ASN:HA	2:D:145:CYS:O	2.01	0.60
1:E:266:ASN:O	1:E:266:ASN:CG	2.44	0.60
1:A:66:PHE:HB3	1:A:67:PRO:CD	2.31	0.59
1:A:261:SER:OG	1:A:262:PRO:HD2	2.03	0.59
1:A:85:GLY:O	1:A:99:VAL:HG13	2.02	0.59
2:B:129:LEU:HD23	2:B:153:ILE:CD1	2.32	0.59
1:C:231:GLU:OE2	1:C:232:VAL:N	2.28	0.59
1:E:59:THR:HG21	1:E:80:PHE:CD2	2.37	0.59
2:D:161:PRO:HG2	2:D:162:VAL:H	1.67	0.59
1:E:85:GLY:O	1:E:99:VAL:HG13	2.02	0.59
1:A:33:MET:HE1	2:B:100:ARG:HB2	1.83	0.59
1:C:10:GLN:O	2:D:23:GLY:N	2.30	0.59
1:C:59:THR:HG21	1:C:80:PHE:CE2	2.38	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:241:TYR:O	1:C:258:ASN:HB2	2.02	0.59
2:D:17:VAL:HG23	2:D:17:VAL:O	2.02	0.59
1:A:331:ALA:O	1:A:335:THR:HG23	2.02	0.59
2:B:159:THR:O	2:B:160:ALA:HB3	2.02	0.59
1:E:46:LEU:HD23	1:E:46:LEU:N	2.16	0.59
2:B:152:PHE:CD2	2:B:153:ILE:HD13	2.37	0.59
2:D:17:VAL:O	2:D:19:THR:N	2.35	0.59
4:K:2:NDG:C4	4:K:3:MAN:H3	2.32	0.59
1:A:13:SER:C	1:A:15:PHE:H	2.11	0.59
1:A:17:LEU:C	1:A:17:LEU:HD22	2.28	0.59
1:A:426:VAL:HG21	2:B:4:ILE:HG12	1.85	0.59
1:C:31:LYS:HZ2	1:C:411:ILE:HB	1.67	0.59
1:C:119:SER:HB3	1:C:120:PRO:HD2	1.84	0.59
1:C:249:PHE:CD2	1:C:250:GLY:N	2.71	0.58
4:U:1:NAG:O3	4:U:2:NDG:C7	2.51	0.58
1:C:18:HIS:CD2	1:C:412:PRO:HB3	2.37	0.58
1:C:5:ILE:HG21	2:D:154:PHE:CE1	2.38	0.58
2:F:154:PHE:O	2:F:156:PHE:N	2.36	0.58
1:A:315:GLN:HE21	1:A:343:LYS:H	1.49	0.58
1:C:3:ILE:HD12	2:D:140:ILE:H	1.68	0.58
1:C:46:LEU:HD23	1:C:46:LEU:N	2.18	0.58
1:C:319:GLY:H	1:C:354:HIS:HD2	1.51	0.58
2:D:29:ARG:HB2	2:D:36:VAL:HG13	1.84	0.58
1:A:294:LEU:C	1:A:294:LEU:HD22	2.28	0.58
1:C:66:PHE:HB3	1:C:67:PRO:CD	2.33	0.58
2:D:9:ILE:HD13	2:D:9:ILE:H	1.68	0.58
2:D:131:VAL:O	2:D:132:GLU:C	2.46	0.58
2:B:47:LYS:HZ1	1:C:423:ASP:CG	2.12	0.58
1:E:3:ILE:CD1	2:F:140:ILE:HG22	2.32	0.58
1:E:66:PHE:O	1:E:68:ARG:N	2.37	0.58
1:E:331:ALA:O	1:E:335:THR:HG23	2.03	0.58
1:C:87:SER:HB3	1:C:90:LEU:HD12	1.86	0.58
1:C:184:LEU:HD12	1:C:185:TYR:N	2.17	0.58
1:C:187:GLN:O	1:C:189:VAL:HG12	2.02	0.58
1:A:266:ASN:CG	1:A:266:ASN:O	2.44	0.58
1:C:230:LYS:O	1:C:234:ASN:N	2.28	0.58
1:C:417:ILE:HA	2:D:24:TYR:OH	2.04	0.58
1:C:163:PRO:HG2	1:C:166:VAL:HG12	1.85	0.58
2:D:61:ILE:N	2:D:61:ILE:HD12	2.19	0.58
1:A:414:GLY:H	2:B:56:LYS:HE3	1.68	0.58
2:B:154:PHE:O	2:B:156:PHE:N	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:126:ALA:O	2:D:129:LEU:HD12	2.04	0.58
1:A:10:GLN:HG3	2:B:15:ALA:HB3	1.84	0.57
1:A:187:GLN:O	1:A:189:VAL:HG12	2.04	0.57
2:B:30:LYS:HD2	2:B:32:SER:N	2.05	0.57
1:A:163:PRO:HG2	1:A:166:VAL:HG12	1.86	0.57
2:B:126:ALA:O	2:B:129:LEU:HD12	2.04	0.57
1:E:315:GLN:HE21	1:E:343:LYS:H	1.50	0.57
1:E:311:VAL:O	1:E:338:CYS:HA	2.04	0.57
2:F:29:ARG:HB2	2:F:36:VAL:HG13	1.85	0.57
2:B:30:LYS:CD	2:B:32:SER:H	2.07	0.57
1:C:33:MET:HE3	1:C:409:PRO:CG	2.34	0.57
1:E:294:LEU:C	1:E:294:LEU:CD2	2.77	0.57
2:F:68:ASP:C	2:F:70:ILE:N	2.56	0.57
2:B:131:VAL:HG21	2:B:139:ILE:CB	2.34	0.57
1:C:92:MET:O	1:C:181:ASN:HB2	2.04	0.57
1:E:1:GLU:C	2:F:141:ASP:HA	2.28	0.57
2:D:68:ASP:C	2:D:70:ILE:N	2.56	0.57
2:F:131:VAL:HG11	2:F:139:ILE:O	2.05	0.57
1:A:244:VAL:CG2	1:E:249:PHE:CE1	2.88	0.57
1:C:13:SER:C	1:C:15:PHE:H	2.12	0.57
2:F:162:VAL:HG13	2:F:164:THR:H	1.69	0.57
2:B:41:ALA:O	2:B:43:LYS:N	2.38	0.57
1:C:162:ILE:HG23	1:C:163:PRO:HD2	1.86	0.57
1:C:393:PRO:O	1:C:395:LYS:HG2	2.05	0.57
2:D:129:LEU:CD2	2:D:153:ILE:HD12	2.34	0.57
1:E:18:HIS:CD2	1:E:412:PRO:HB3	2.39	0.57
1:E:416:LEU:HB2	2:F:52:ILE:HD13	1.86	0.57
1:A:104:GLN:CB	1:A:153:SER:HB2	2.35	0.57
1:A:149:SER:OG	1:A:303:PHE:HB3	2.05	0.57
2:B:29:ARG:HB2	2:B:36:VAL:HG13	1.87	0.57
2:B:125:ARG:O	2:B:126:ALA:HB2	2.05	0.57
2:D:163:PRO:O	2:D:165:ILE:N	2.37	0.57
1:E:13:SER:C	1:E:15:PHE:H	2.11	0.57
2:B:141:ASP:HB3	2:B:144:ILE:HG12	1.87	0.56
2:D:21:ILE:H	2:D:21:ILE:CD1	2.15	0.56
2:D:161:PRO:O	2:D:162:VAL:HG13	2.05	0.56
1:E:1:GLU:HA	2:F:142:ASN:N	2.20	0.56
2:F:7:LEU:N	2:F:7:LEU:HD22	2.19	0.56
2:F:41:ALA:O	2:F:43:LYS:N	2.38	0.56
1:A:33:MET:HE3	1:A:409:PRO:HB2	1.85	0.56
1:C:331:ALA:O	1:C:335:THR:HG23	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:83:GLU:CD	2:D:83:GLU:H	2.13	0.56
2:D:102:LEU:HD13	2:F:102:LEU:HD21	1.86	0.56
2:F:131:VAL:HG21	2:F:139:ILE:H	1.71	0.56
1:A:18:HIS:CD2	1:A:412:PRO:HB3	2.41	0.56
1:A:59:THR:HG21	1:A:80:PHE:CD2	2.40	0.56
1:A:322:ARG:HD2	1:A:354:HIS:CE1	2.39	0.56
2:B:83:GLU:CD	2:B:83:GLU:H	2.14	0.56
2:D:125:ARG:O	2:D:126:ALA:HB2	2.05	0.56
1:E:47:ASN:O	1:E:49:SER:N	2.38	0.56
2:F:7:LEU:HD23	2:F:29:ARG:NH1	2.20	0.56
2:F:9:ILE:HG22	2:F:10:GLY:N	2.18	0.56
2:F:125:ARG:O	2:F:126:ALA:HB2	2.04	0.56
2:F:163:PRO:C	2:F:164:THR:HG22	2.29	0.56
1:E:379:TRP:CZ3	1:E:381:ASN:HB3	2.39	0.56
1:A:339:MET:HE1	1:A:374:ILE:HD12	1.87	0.56
1:E:119:SER:HB3	1:E:120:PRO:HD2	1.87	0.56
4:U:1:NAG:O3	4:U:2:NDG:C8	2.53	0.56
1:C:66:PHE:O	1:C:68:ARG:N	2.38	0.56
1:C:66:PHE:CE1	1:C:70:ALA:HB2	2.41	0.56
2:F:97:GLY:O	2:F:100:ARG:HB3	2.04	0.56
1:A:46:LEU:HD23	1:A:46:LEU:N	2.18	0.56
1:A:59:THR:HG21	1:A:80:PHE:CE2	2.40	0.56
2:B:13:PHE:N	2:B:13:PHE:CD1	2.74	0.56
1:C:278:LEU:HD22	1:C:280:LEU:CD1	2.36	0.56
2:F:129:LEU:HD23	2:F:153:ILE:HD12	1.86	0.56
1:A:154:LEU:HD22	1:A:155:VAL:H	1.68	0.56
1:A:174:CYS:O	1:A:175:ASN:C	2.49	0.56
1:C:294:LEU:HD22	1:C:295:LEU:N	2.21	0.56
1:E:319:GLY:H	1:E:354:HIS:HD2	1.51	0.56
2:B:102:LEU:HD13	2:D:102:LEU:HD21	1.87	0.56
1:C:393:PRO:HB2	1:C:394:PRO:CD	2.34	0.56
1:C:416:LEU:O	2:D:52:ILE:HD11	2.06	0.56
2:F:129:LEU:HD23	2:F:153:ILE:CD1	2.36	0.56
1:A:249:PHE:HD2	1:C:252:VAL:CG2	2.09	0.56
1:C:278:LEU:HD22	1:C:280:LEU:HD11	1.87	0.56
2:D:122:ILE:O	2:D:125:ARG:HB2	2.06	0.56
1:E:357:ASP:O	1:E:361:ARG:HG3	2.06	0.56
1:C:311:VAL:O	1:C:338:CYS:HA	2.05	0.55
1:E:187:GLN:O	1:E:189:VAL:HG12	2.06	0.55
2:D:30:LYS:HE3	2:D:32:SER:HB3	1.88	0.55
1:A:231:GLU:N	1:A:231:GLU:OE1	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:33:MET:HE3	1:C:409:PRO:HB2	1.88	0.55
2:D:43:LYS:HB3	2:D:155:LYS:O	2.07	0.55
1:E:278:LEU:HD22	1:E:280:LEU:HD11	1.88	0.55
1:A:58:ARG:NH2	1:A:317:ILE:O	2.35	0.55
1:A:311:VAL:O	1:A:338:CYS:HA	2.06	0.55
2:B:122:ILE:O	2:B:125:ARG:HB2	2.06	0.55
1:C:304:ASP:C	1:C:304:ASP:OD1	2.49	0.55
2:D:4:ILE:CG2	2:D:9:ILE:HG13	2.36	0.55
1:A:66:PHE:O	1:A:68:ARG:N	2.39	0.55
1:E:422:THR:OG1	1:E:423:ASP:N	2.39	0.55
1:C:80:PHE:HB2	1:C:82:PHE:CE2	2.41	0.55
1:C:247:ASP:O	1:C:249:PHE:O	2.24	0.55
2:D:22:GLY:O	3:L:1:NAG:H61	2.07	0.55
1:E:163:PRO:HG2	1:E:166:VAL:HG12	1.88	0.55
2:F:126:ALA:O	2:F:129:LEU:HD12	2.07	0.55
1:A:190:LYS:CD	1:A:191:PRO:HD2	2.37	0.55
1:A:92:MET:O	1:A:181:ASN:HB2	2.06	0.55
1:A:203:PHE:CE2	1:C:262:PRO:HB3	2.42	0.55
1:A:376:GLN:CB	1:A:394:PRO:HD2	2.37	0.55
2:B:47:LYS:NZ	1:C:423:ASP:OD2	2.35	0.55
1:E:162:ILE:HG23	1:E:163:PRO:HD2	1.89	0.55
1:A:339:MET:HE1	1:A:374:ILE:HB	1.89	0.55
2:F:43:LYS:HB3	2:F:155:LYS:O	2.07	0.55
1:A:3:ILE:HD12	1:A:3:ILE:C	2.32	0.55
1:E:294:LEU:CD1	1:E:296:MET:HE3	2.26	0.55
1:A:1:GLU:C	1:A:3:ILE:H	2.14	0.54
1:A:244:VAL:HG21	1:E:249:PHE:CE1	2.42	0.54
1:C:59:THR:HG21	1:C:80:PHE:CD2	2.42	0.54
1:C:424:THR:O	2:D:13:PHE:HB3	2.07	0.54
1:E:174:CYS:O	1:E:175:ASN:C	2.50	0.54
2:B:7:LEU:HD13	2:B:36:VAL:HG21	1.89	0.54
1:C:5:ILE:HG21	2:D:154:PHE:CG	2.40	0.54
1:A:10:GLN:HG3	2:B:15:ALA:CB	2.36	0.54
1:C:55:GLY:C	1:C:82:PHE:HB3	2.32	0.54
2:D:123:THR:HG1	2:D:138:TRP:HZ3	1.55	0.54
1:A:1:GLU:O	1:A:3:ILE:HG13	2.08	0.54
2:D:148:SER:OG	2:D:160:ALA:HB3	2.08	0.54
1:A:249:PHE:CE1	1:C:244:VAL:CG2	2.90	0.54
1:A:333:LEU:HA	2:B:78:ARG:NH2	2.22	0.54
2:B:163:PRO:C	2:B:165:ILE:H	2.15	0.54
2:F:123:THR:HG1	2:F:138:TRP:HZ3	1.53	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:161:PRO:C	2:B:162:VAL:HG12	2.33	0.54
1:C:249:PHE:HE1	1:E:257:ASP:HB2	1.70	0.54
1:E:33:MET:HE3	1:E:409:PRO:CG	2.37	0.54
4:U:2:NDG:O7	4:U:2:NDG:H3	2.06	0.54
1:A:55:GLY:C	1:A:82:PHE:HB3	2.33	0.54
2:B:160:ALA:H	2:B:161:PRO:HD3	1.72	0.54
1:C:190:LYS:HD3	1:C:191:PRO:HD2	1.89	0.54
1:E:87:SER:HB3	1:E:90:LEU:HD12	1.90	0.54
1:E:339:MET:HE1	1:E:374:ILE:HB	1.90	0.54
1:E:393:PRO:O	1:E:395:LYS:HG2	2.08	0.54
1:A:266:ASN:C	1:A:266:ASN:ND2	2.66	0.54
1:C:24:ASN:H	1:C:419:THR:HG22	1.73	0.54
2:F:164:THR:O	2:F:165:ILE:CB	2.56	0.54
1:A:181:ASN:O	1:A:182:PRO:C	2.46	0.54
2:B:30:LYS:HE3	2:B:32:SER:HB3	1.90	0.54
2:B:131:VAL:HG21	2:B:139:ILE:H	1.71	0.54
2:B:147:GLN:O	2:B:148:SER:C	2.51	0.54
1:C:422:THR:OG1	1:C:423:ASP:N	2.41	0.54
4:K:2:NDG:H4	4:K:3:MAN:C3	2.30	0.54
1:A:38:LYS:HD3	1:A:38:LYS:N	2.16	0.53
1:A:247:ASP:O	1:A:249:PHE:O	2.26	0.53
1:A:319:GLY:N	1:A:354:HIS:CD2	2.76	0.53
2:D:13:PHE:N	2:D:13:PHE:CD1	2.75	0.53
1:E:1:GLU:CA	2:F:142:ASN:N	2.70	0.53
1:A:319:GLY:N	1:A:354:HIS:HD2	2.07	0.53
2:B:148:SER:OG	2:B:160:ALA:HB3	2.08	0.53
1:E:116:VAL:HG13	1:E:117:ASN:N	2.23	0.53
1:A:294:LEU:HD22	1:A:295:LEU:N	2.23	0.53
1:C:1:GLU:CA	2:D:142:ASN:OD1	2.57	0.53
1:C:393:PRO:O	1:C:395:LYS:N	2.40	0.53
2:D:119:ALA:HA	2:D:138:TRP:HH2	1.73	0.53
1:E:154:LEU:HD22	1:E:155:VAL:H	1.72	0.53
2:F:64:GLU:OE1	2:F:65:LYS:N	2.41	0.53
1:C:5:ILE:HD12	1:C:5:ILE:N	2.23	0.53
1:C:266:ASN:O	1:C:266:ASN:CG	2.49	0.53
2:D:64:GLU:OE1	2:D:65:LYS:N	2.41	0.53
2:D:131:VAL:HG21	2:D:139:ILE:H	1.72	0.53
1:E:20:GLY:HA3	2:F:104:VAL:HG12	1.89	0.53
1:E:241:TYR:O	1:E:258:ASN:HB2	2.09	0.53
1:E:241:TYR:O	1:E:242:PHE:HB3	2.08	0.53
1:A:3:ILE:HD13	1:A:5:ILE:HD13	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:154:LEU:HD22	1:C:155:VAL:H	1.71	0.53
2:F:7:LEU:HD22	2:F:7:LEU:H	1.74	0.53
2:F:147:GLN:O	2:F:148:SER:C	2.52	0.53
1:A:249:PHE:CZ	1:C:244:VAL:HG11	2.43	0.53
2:D:129:LEU:HD12	2:D:130:ALA:H	1.73	0.53
1:A:68:ARG:CZ	1:A:68:ARG:HB3	2.39	0.53
1:A:393:PRO:O	1:A:395:LYS:HG2	2.08	0.53
2:D:129:LEU:HD23	2:D:153:ILE:CD1	2.39	0.53
1:E:5:ILE:N	1:E:5:ILE:HD12	2.23	0.53
2:F:61:ILE:N	2:F:61:ILE:HD12	2.24	0.53
1:A:203:PHE:CD1	1:A:286:SER:HB3	2.43	0.53
2:B:97:GLY:O	2:B:100:ARG:HB3	2.07	0.53
2:B:129:LEU:HD12	2:B:130:ALA:H	1.71	0.53
1:C:232:VAL:O	1:C:235:LYS:HB2	2.09	0.53
1:A:162:ILE:HD12	1:A:162:ILE:N	2.24	0.53
2:B:57:SER:O	2:B:61:ILE:HD13	2.09	0.53
1:C:261:SER:OG	1:C:262:PRO:HD2	2.08	0.53
1:C:288:ARG:HH11	1:C:288:ARG:CG	2.22	0.53
1:C:294:LEU:HD21	1:C:296:MET:HE2	1.91	0.53
1:C:318:TRP:CB	1:C:322:ARG:HG3	2.37	0.53
1:E:304:ASP:C	1:E:304:ASP:OD1	2.52	0.53
1:A:425:THR:HB	2:B:16:ILE:CD1	2.37	0.53
1:C:4:LYS:HA	2:D:138:TRP:O	2.09	0.53
1:C:155:VAL:O	1:C:299:ARG:HG2	2.09	0.52
2:D:154:PHE:O	2:D:155:LYS:C	2.52	0.52
1:A:278:LEU:HD22	1:A:280:LEU:HD11	1.91	0.52
1:A:304:ASP:OD1	1:A:304:ASP:C	2.52	0.52
1:C:174:CYS:O	1:C:175:ASN:C	2.52	0.52
2:D:125:ARG:O	2:D:126:ALA:CB	2.58	0.52
1:E:31:LYS:NZ	1:E:31:LYS:HB2	2.24	0.52
1:E:294:LEU:HD21	1:E:296:MET:CE	2.39	0.52
1:A:288:ARG:HH11	1:A:288:ARG:CG	2.15	0.52
2:B:61:ILE:HD12	2:B:61:ILE:N	2.25	0.52
1:C:357:ASP:O	1:C:361:ARG:HG3	2.09	0.52
2:F:62:ALA:O	2:F:65:LYS:HB3	2.09	0.52
1:A:12:ASN:HB3	2:B:20:GLY:O	2.09	0.52
1:C:411:ILE:HG13	2:D:63:ILE:HD11	1.92	0.52
1:E:190:LYS:HD2	1:E:192:SER:OG	2.09	0.52
1:A:294:LEU:HD21	1:A:296:MET:HE2	1.91	0.52
2:B:59:ILE:HG22	2:B:63:ILE:HD11	1.90	0.52
1:E:149:SER:OG	1:E:303:PHE:HB3	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:278:LEU:HD22	1:E:280:LEU:CD1	2.39	0.52
1:E:80:PHE:HB2	1:E:82:PHE:CE2	2.44	0.52
1:A:47:ASN:C	1:A:49:SER:H	2.18	0.52
1:C:424:THR:HG23	2:D:13:PHE:HA	1.90	0.52
2:D:141:ASP:HB3	2:D:144:ILE:HG12	1.91	0.52
1:E:66:PHE:CB	1:E:67:PRO:CD	2.87	0.52
1:A:80:PHE:HB2	1:A:82:PHE:CE2	2.45	0.52
2:F:149:CYS:O	2:F:153:ILE:HG12	2.09	0.52
1:A:125:ASN:O	1:A:173:ASN:HB2	2.10	0.52
1:A:190:LYS:HD2	1:A:192:SER:OG	2.09	0.52
1:A:252:VAL:HG21	1:E:249:PHE:HD2	1.74	0.52
1:C:163:PRO:HG2	1:C:166:VAL:HG11	1.91	0.52
2:D:131:VAL:HG11	2:D:139:ILE:O	2.09	0.52
1:E:206:LEU:HB3	1:E:218:HIS:CD2	2.45	0.52
1:C:294:LEU:C	1:C:294:LEU:CD2	2.83	0.51
2:D:92:LEU:HA	2:D:95:GLU:HG3	1.92	0.51
1:E:256:LEU:HD12	1:E:257:ASP:N	2.24	0.51
1:A:425:THR:HG22	2:B:16:ILE:HD11	1.93	0.51
1:C:100:ASP:C	1:C:100:ASP:OD1	2.53	0.51
1:E:55:GLY:C	1:E:82:PHE:HB3	2.33	0.51
1:E:317:ILE:HG22	1:E:324:SER:HB3	1.91	0.51
2:F:13:PHE:CD1	2:F:13:PHE:N	2.77	0.51
1:C:149:SER:OG	1:C:303:PHE:HB3	2.10	0.51
1:E:230:LYS:O	1:E:234:ASN:N	2.30	0.51
1:E:232:VAL:O	1:E:235:LYS:HB2	2.10	0.51
1:A:8:GLN:NE2	2:B:9:ILE:H	2.08	0.51
1:A:19:ASN:CG	4:U:2:NDG:H8C2	2.35	0.51
1:A:181:ASN:O	1:A:183:ALA:N	2.44	0.51
1:C:47:ASN:C	1:C:49:SER:H	2.18	0.51
1:C:414:GLY:N	2:D:56:LYS:HE3	2.26	0.51
2:D:160:ALA:N	2:D:161:PRO:CD	2.68	0.51
1:A:87:SER:HB3	1:A:90:LEU:HD12	1.92	0.51
1:A:256:LEU:HD12	1:A:257:ASP:N	2.26	0.51
1:A:354:HIS:C	1:A:355:HIS:ND1	2.69	0.51
2:B:68:ASP:C	2:B:70:ILE:N	2.52	0.51
1:C:339:MET:HE1	1:C:374:ILE:HB	1.92	0.51
1:E:68:ARG:HB3	1:E:68:ARG:CZ	2.40	0.51
1:E:190:LYS:CD	1:E:191:PRO:HD2	2.39	0.51
1:A:116:VAL:HG13	1:A:117:ASN:N	2.26	0.51
1:A:406:GLU:CD	1:A:406:GLU:H	2.19	0.51
1:E:241:TYR:CG	1:E:242:PHE:N	2.79	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:5:ASP:OD1	2:F:6:ASP:N	2.43	0.51
2:F:142:ASN:HA	2:F:145:CYS:O	2.11	0.51
1:A:422:THR:OG1	1:A:423:ASP:N	2.43	0.51
2:B:138:TRP:CD1	2:B:138:TRP:H	2.29	0.51
1:E:11:VAL:HG22	1:E:15:PHE:HB3	1.92	0.51
1:A:162:ILE:N	1:A:162:ILE:CD1	2.74	0.51
1:C:93:PHE:CD1	1:C:93:PHE:N	2.78	0.51
2:D:41:ALA:C	2:D:43:LYS:H	2.19	0.51
2:D:59:ILE:HG22	2:D:63:ILE:HD11	1.92	0.51
1:A:247:ASP:OD1	1:A:249:PHE:O	2.29	0.51
1:C:3:ILE:HD13	1:C:5:ILE:HD13	1.93	0.51
1:C:121:HIS:C	1:C:123:ALA:N	2.69	0.51
1:C:390:TYR:CE2	2:D:82:LEU:HG	2.45	0.51
1:E:1:GLU:HA	2:F:141:ASP:CG	2.35	0.51
1:E:141:ASN:HD22	1:E:279:GLN:HE21	1.58	0.51
1:E:198:LYS:O	1:E:199:GLU:C	2.54	0.51
1:A:163:PRO:HG2	1:A:166:VAL:HG11	1.93	0.51
1:A:266:ASN:O	1:A:266:ASN:ND2	2.44	0.51
2:B:125:ARG:O	2:B:126:ALA:CB	2.58	0.51
1:C:66:PHE:CD2	1:C:67:PRO:HD3	2.46	0.51
1:C:376:GLN:CB	1:C:394:PRO:HD2	2.41	0.51
2:F:119:ALA:HA	2:F:138:TRP:HH2	1.76	0.51
2:F:125:ARG:O	2:F:126:ALA:CB	2.59	0.51
1:A:8:GLN:NE2	2:B:9:ILE:N	2.58	0.50
1:C:322:ARG:HD2	1:C:354:HIS:CE1	2.46	0.50
2:D:159:THR:O	2:D:160:ALA:HB3	2.11	0.50
1:E:3:ILE:CD1	2:F:140:ILE:H	2.25	0.50
1:A:58:ARG:HD2	1:A:347:TYR:OH	2.11	0.50
1:A:158:LEU:HD21	1:A:298:GLU:CA	2.39	0.50
1:A:206:LEU:HB3	1:A:218:HIS:CD2	2.46	0.50
1:E:15:PHE:CD2	1:E:16:SER:N	2.80	0.50
1:A:198:LYS:O	1:A:199:GLU:C	2.54	0.50
1:A:241:TYR:CG	1:A:242:PHE:N	2.80	0.50
2:B:43:LYS:HB3	2:B:155:LYS:O	2.11	0.50
2:B:99:ILE:HG12	2:B:99:ILE:O	2.11	0.50
2:D:107:ILE:O	2:D:108:SER:C	2.54	0.50
1:E:125:ASN:O	1:E:173:ASN:HB2	2.11	0.50
1:E:393:PRO:O	1:E:395:LYS:N	2.44	0.50
1:A:24:ASN:H	1:A:419:THR:HG22	1.77	0.50
1:A:66:PHE:CB	1:A:67:PRO:CD	2.89	0.50
1:A:135:LYS:O	1:A:139:GLN:HG2	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:249:PHE:CE2	1:C:252:VAL:CB	2.95	0.50
2:B:21:ILE:HD12	2:B:21:ILE:N	2.23	0.50
1:E:3:ILE:HD13	1:E:5:ILE:HD13	1.94	0.50
1:E:66:PHE:CB	1:E:67:PRO:HD3	2.39	0.50
1:A:393:PRO:O	1:A:395:LYS:N	2.44	0.50
1:C:222:SER:HB2	1:C:278:LEU:HD12	1.94	0.50
1:C:398:ARG:NH1	2:D:70:ILE:O	2.44	0.50
2:D:4:ILE:HG21	2:D:9:ILE:HG13	1.93	0.50
1:E:121:HIS:C	1:E:123:ALA:N	2.66	0.50
2:F:122:ILE:O	2:F:125:ARG:HB2	2.11	0.50
4:K:2:NDG:O3	4:K:2:NDG:O7	2.27	0.50
1:A:11:VAL:HG22	1:A:15:PHE:HB3	1.94	0.50
1:A:45:VAL:O	1:A:46:LEU:HD23	2.12	0.50
2:B:8:ILE:HG13	2:B:8:ILE:O	2.10	0.50
2:D:5:ASP:CG	2:D:9:ILE:HA	2.37	0.50
2:D:62:ALA:O	2:D:65:LYS:HB3	2.12	0.50
1:E:28:THR:CG2	3:Q:2:NAG:H82	2.37	0.50
2:F:59:ILE:HG22	2:F:63:ILE:HD11	1.94	0.50
2:B:43:LYS:HD3	2:B:156:PHE:HB2	1.94	0.50
1:E:10:GLN:HE21	2:F:25:LEU:HD21	1.76	0.50
2:F:159:THR:O	2:F:160:ALA:HB3	2.11	0.50
1:C:6:CYS:HA	2:D:136:GLY:O	2.12	0.50
2:D:129:LEU:HD23	2:D:153:ILE:HD12	1.93	0.50
1:A:33:MET:HE3	1:A:409:PRO:CG	2.42	0.50
1:C:11:VAL:HG22	1:C:15:PHE:HB3	1.94	0.50
2:D:161:PRO:CG	2:D:162:VAL:H	2.22	0.50
2:B:162:VAL:O	2:B:162:VAL:CG2	2.60	0.49
1:C:317:ILE:HG22	1:C:324:SER:HB3	1.94	0.49
1:C:319:GLY:N	1:C:354:HIS:CD2	2.78	0.49
1:C:398:ARG:NH1	1:C:398:ARG:HG2	2.27	0.49
1:E:3:ILE:HG13	2:F:140:ILE:O	2.10	0.49
1:A:232:VAL:O	1:A:235:LYS:HB2	2.11	0.49
2:F:148:SER:HB3	2:F:160:ALA:O	2.11	0.49
1:C:38:LYS:O	1:C:38:LYS:NZ	2.44	0.49
2:D:43:LYS:HD3	2:D:156:PHE:HB2	1.93	0.49
1:A:10:GLN:HA	2:B:15:ALA:HB3	1.95	0.49
1:A:418:PRO:HD3	2:B:111:LEU:HD13	1.94	0.49
2:B:118:LEU:O	2:B:119:ALA:C	2.55	0.49
2:B:119:ALA:O	2:B:120:SER:C	2.54	0.49
1:C:247:ASP:OD1	1:C:249:PHE:O	2.31	0.49
1:C:377:SER:HB2	1:C:392:LEU:N	2.07	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:4:ILE:HA	2:D:13:PHE:CD2	2.47	0.49
2:D:21:ILE:HA	3:L:1:NAG:O7	2.13	0.49
1:E:121:HIS:C	1:E:123:ALA:H	2.21	0.49
1:A:189:VAL:HG23	1:A:196:CYS:HA	1.94	0.49
1:A:253:VAL:O	1:A:278:LEU:HD21	2.13	0.49
1:E:135:LYS:O	1:E:139:GLN:HG2	2.13	0.49
1:E:231:GLU:N	1:E:231:GLU:OE1	2.45	0.49
2:F:148:SER:OG	2:F:160:ALA:HB3	2.11	0.49
3:T:1:NAG:H61	3:T:2:NAG:C7	2.41	0.49
2:B:41:ALA:C	2:B:43:LYS:H	2.20	0.49
1:C:1:GLU:CA	2:D:142:ASN:N	2.75	0.49
1:C:34:PHE:CE2	2:D:96:LEU:HD13	2.46	0.49
1:C:74:ALA:O	1:C:75:LYS:C	2.54	0.49
1:E:10:GLN:NE2	2:F:25:LEU:HD21	2.27	0.49
2:B:119:ALA:HA	2:B:138:TRP:HH2	1.76	0.49
1:C:8:GLN:O	2:D:24:TYR:HA	2.13	0.49
1:C:192:SER:C	1:C:194:ASN:H	2.20	0.49
1:E:162:ILE:N	1:E:162:ILE:HD12	2.27	0.49
2:B:39:GLU:OE1	2:B:155:LYS:HE3	2.13	0.49
1:C:410:LYS:C	1:C:411:ILE:HD13	2.38	0.49
2:D:5:ASP:OD2	2:D:9:ILE:HG23	2.12	0.49
1:A:333:LEU:HD11	1:A:340:LEU:HD23	1.93	0.49
1:A:377:SER:HB2	1:A:392:LEU:N	2.06	0.49
1:C:181:ASN:O	1:C:183:ALA:N	2.46	0.49
2:D:57:SER:O	2:D:61:ILE:HD13	2.13	0.49
2:D:119:ALA:O	2:D:120:SER:C	2.54	0.49
1:E:155:VAL:O	1:E:299:ARG:HG2	2.12	0.49
1:E:288:ARG:HH11	1:E:288:ARG:CG	2.24	0.49
1:A:252:VAL:HG11	1:E:249:PHE:CE2	2.44	0.49
1:A:426:VAL:HG11	2:B:4:ILE:CG1	2.42	0.49
1:C:319:GLY:N	1:C:354:HIS:HD2	2.10	0.49
1:E:189:VAL:HG23	1:E:196:CYS:HA	1.95	0.49
1:E:393:PRO:HB2	1:E:394:PRO:CD	2.42	0.49
2:F:4:ILE:CG1	2:F:5:ASP:N	2.74	0.49
2:F:43:LYS:HD3	2:F:156:PHE:HB2	1.95	0.49
1:A:422:THR:C	1:A:424:THR:H	2.20	0.48
1:C:66:PHE:CB	1:C:67:PRO:CD	2.91	0.48
1:C:231:GLU:HA	1:C:234:ASN:HB2	1.94	0.48
2:D:4:ILE:HA	2:D:13:PHE:CE2	2.48	0.48
1:E:401:LEU:N	1:E:401:LEU:HD12	2.28	0.48
1:C:125:ASN:O	1:C:173:ASN:HB2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:373:CYS:HG	1:C:399:CYS:CB	2.25	0.48
2:D:4:ILE:HB	2:D:9:ILE:CG1	2.43	0.48
2:D:4:ILE:HB	2:D:9:ILE:HG13	1.93	0.48
1:A:66:PHE:CB	1:A:67:PRO:HD3	2.41	0.48
1:A:68:ARG:HA	1:A:350:GLU:OE2	2.14	0.48
1:C:20:GLY:HA3	2:D:104:VAL:HG12	1.93	0.48
1:C:385:PRO:HG2	1:C:386:PHE:CD2	2.49	0.48
1:E:247:ASP:OD1	1:E:249:PHE:O	2.31	0.48
2:F:30:LYS:CD	2:F:32:SER:H	2.10	0.48
2:F:41:ALA:C	2:F:43:LYS:H	2.21	0.48
2:F:154:PHE:O	2:F:155:LYS:C	2.56	0.48
1:A:5:ILE:CD1	1:A:5:ILE:N	2.76	0.48
1:A:246:TYR:HA	1:A:251:LYS:O	2.13	0.48
1:A:257:ASP:CB	1:E:249:PHE:CD1	2.88	0.48
1:C:219:LEU:C	1:C:219:LEU:CD2	2.86	0.48
1:C:249:PHE:CD1	1:E:257:ASP:HB2	2.48	0.48
1:E:20:GLY:C	4:P:1:NAG:H83	2.38	0.48
1:E:319:GLY:N	1:E:354:HIS:HD2	2.11	0.48
2:F:8:ILE:HG23	2:F:36:VAL:CG1	2.44	0.48
2:F:119:ALA:O	2:F:120:SER:C	2.56	0.48
1:A:318:TRP:CB	1:A:322:ARG:HG3	2.44	0.48
1:C:10:GLN:HG3	2:D:15:ALA:HB3	1.95	0.48
1:C:85:GLY:O	1:C:99:VAL:CG1	2.61	0.48
1:E:19:ASN:CG	4:P:2:NDG:C8	2.86	0.48
1:E:329:ASP:HA	1:E:340:LEU:CD2	2.44	0.48
2:F:92:LEU:HA	2:F:95:GLU:HG3	1.95	0.48
1:A:3:ILE:HD12	1:A:4:LYS:N	2.29	0.48
2:B:154:PHE:O	2:B:155:LYS:C	2.54	0.48
2:D:4:ILE:CG2	2:D:9:ILE:HG21	2.38	0.48
2:D:4:ILE:HB	2:D:9:ILE:HD12	1.96	0.48
2:D:61:ILE:CD1	2:D:61:ILE:H	2.26	0.48
2:F:30:LYS:HE3	2:F:32:SER:HB3	1.95	0.48
1:A:203:PHE:CD1	1:C:262:PRO:HD3	2.49	0.48
1:A:278:LEU:HD22	1:A:280:LEU:CD1	2.43	0.48
1:A:410:LYS:C	1:A:411:ILE:HD13	2.39	0.48
2:B:64:GLU:OE1	2:B:65:LYS:N	2.47	0.48
1:C:135:LYS:O	1:C:139:GLN:HG2	2.12	0.48
1:C:379:TRP:CZ3	1:C:381:ASN:HB3	2.42	0.48
2:F:21:ILE:H	2:F:21:ILE:CD1	2.20	0.48
1:A:234:ASN:HA	1:A:237:GLY:O	2.14	0.48
1:C:66:PHE:CB	1:C:67:PRO:HD3	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:266:ASN:C	1:E:266:ASN:ND2	2.70	0.48
1:C:354:HIS:C	1:C:355:HIS:ND1	2.72	0.48
1:E:33:MET:HE3	1:E:409:PRO:CB	2.43	0.48
1:E:121:HIS:O	1:E:123:ALA:N	2.46	0.48
1:A:192:SER:C	1:A:194:ASN:H	2.22	0.47
1:C:374:ILE:HG13	1:C:374:ILE:O	2.14	0.47
1:E:331:ALA:O	1:E:335:THR:CG2	2.62	0.47
1:E:366:GLY:C	1:E:368:ASP:H	2.21	0.47
1:A:66:PHE:CD2	1:A:67:PRO:HD3	2.49	0.47
1:A:121:HIS:C	1:A:123:ALA:N	2.72	0.47
1:A:385:PRO:HG2	1:A:386:PHE:CD2	2.48	0.47
2:B:125:ARG:HB3	2:B:129:LEU:CD2	2.45	0.47
2:F:131:VAL:HG21	2:F:139:ILE:CB	2.44	0.47
1:A:294:LEU:C	1:A:294:LEU:CD2	2.87	0.47
1:A:401:LEU:HD11	2:B:70:ILE:HD11	1.95	0.47
2:B:164:THR:O	2:B:164:THR:HG22	2.14	0.47
1:E:203:PHE:CD1	1:E:286:SER:HB3	2.45	0.47
1:E:247:ASP:OD1	1:E:247:ASP:C	2.54	0.47
1:E:424:THR:HG23	2:F:13:PHE:HA	1.97	0.47
1:A:244:VAL:HG22	1:E:249:PHE:CE1	2.49	0.47
2:B:43:LYS:O	2:B:46:GLU:HB2	2.14	0.47
1:C:68:ARG:CZ	1:C:68:ARG:HB3	2.45	0.47
1:E:28:THR:HB	3:Q:2:NAG:C8	2.43	0.47
1:E:38:LYS:O	1:E:38:LYS:NZ	2.47	0.47
1:E:374:ILE:HG13	1:E:374:ILE:O	2.13	0.47
2:F:129:LEU:HD12	2:F:130:ALA:H	1.78	0.47
1:A:66:PHE:CE1	1:A:70:ALA:HB2	2.49	0.47
1:A:423:ASP:CG	2:F:47:LYS:NZ	2.73	0.47
2:B:5:ASP:CB	2:B:9:ILE:HA	2.38	0.47
2:D:41:ALA:C	2:D:43:LYS:N	2.72	0.47
1:E:26:TYR:OH	1:E:425:THR:HG21	2.14	0.47
1:E:68:ARG:HA	1:E:350:GLU:OE2	2.15	0.47
1:E:163:PRO:HG2	1:E:166:VAL:HG11	1.95	0.47
2:F:54:ILE:O	2:F:57:SER:HB3	2.14	0.47
2:F:162:VAL:HA	2:F:163:PRO:HD3	1.47	0.47
1:A:74:ALA:O	1:A:75:LYS:C	2.56	0.47
1:A:161:THR:C	1:A:162:ILE:HD12	2.40	0.47
1:A:229:SER:C	1:A:231:GLU:OE1	2.58	0.47
1:C:80:PHE:HB2	1:C:82:PHE:HE2	1.79	0.47
1:C:198:LYS:O	1:C:199:GLU:C	2.58	0.47
2:F:154:PHE:O	2:F:156:PHE:CD2	2.67	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:LYS:NZ	1:A:31:LYS:HB2	2.28	0.47
1:A:152:MET:HE3	1:A:152:MET:HB2	1.86	0.47
1:A:219:LEU:C	1:A:219:LEU:CD2	2.87	0.47
1:A:329:ASP:HA	1:A:340:LEU:CD2	2.45	0.47
1:C:121:HIS:O	1:C:123:ALA:N	2.48	0.47
2:D:67:ASN:OD1	2:D:67:ASN:N	2.48	0.47
1:E:47:ASN:C	1:E:49:SER:H	2.22	0.47
1:E:127:TYR:N	1:E:173:ASN:ND2	2.62	0.47
1:A:34:PHE:HZ	2:B:66:LEU:CD2	2.28	0.47
1:A:304:ASP:OD1	1:A:306:LYS:HB2	2.14	0.47
1:A:329:ASP:HA	1:A:340:LEU:HD22	1.96	0.47
2:B:6:ASP:HB2	2:B:7:LEU:H	1.43	0.47
1:C:5:ILE:CG1	2:D:154:PHE:CE2	2.91	0.47
1:C:388:GLU:CD	1:C:388:GLU:N	2.68	0.47
2:D:147:GLN:O	2:D:148:SER:C	2.57	0.47
1:E:231:GLU:HA	1:E:234:ASN:HB2	1.97	0.47
1:A:1:GLU:O	1:A:3:ILE:N	2.41	0.46
1:A:1:GLU:HA	2:B:141:ASP:HA	1.98	0.46
1:C:10:GLN:HE22	2:D:25:LEU:HD21	1.74	0.46
1:C:33:MET:HE3	1:C:409:PRO:CB	2.44	0.46
1:C:160:LYS:HG3	1:C:162:ILE:CD1	2.45	0.46
1:C:387:THR:O	1:C:402:ALA:HA	2.15	0.46
1:C:398:ARG:HG2	1:C:398:ARG:HH11	1.80	0.46
2:D:77:ILE:HD12	2:D:77:ILE:H	1.80	0.46
1:A:25:LEU:HD23	1:A:418:PRO:HA	1.97	0.46
1:A:149:SER:HB3	1:A:304:ASP:O	2.15	0.46
1:A:377:SER:CB	1:A:392:LEU:H	2.09	0.46
2:B:21:ILE:H	2:B:21:ILE:CD1	2.12	0.46
1:C:127:TYR:N	1:C:173:ASN:ND2	2.63	0.46
1:C:181:ASN:O	1:C:182:PRO:C	2.55	0.46
1:E:31:LYS:HZ2	1:E:31:LYS:C	2.24	0.46
1:E:387:THR:HG22	1:E:400:PRO:HB2	1.96	0.46
2:F:164:THR:OG1	2:F:165:ILE:N	2.46	0.46
1:A:222:SER:HB2	1:A:278:LEU:HD12	1.96	0.46
1:A:374:ILE:O	1:A:374:ILE:HG13	2.14	0.46
2:B:93:LEU:HD23	2:B:93:LEU:HA	1.74	0.46
2:B:131:VAL:HG22	2:B:139:ILE:H	1.78	0.46
1:C:190:LYS:CD	1:C:191:PRO:HD2	2.46	0.46
1:C:398:ARG:HH11	1:C:398:ARG:CG	2.29	0.46
1:E:178:PHE:CD2	1:E:179:LEU:N	2.83	0.46
1:E:181:ASN:O	1:E:182:PRO:C	2.55	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:331:ALA:O	1:A:335:THR:CG2	2.63	0.46
1:C:223:CYS:HA	1:C:274:GLN:O	2.16	0.46
1:C:422:THR:C	1:C:424:THR:H	2.23	0.46
1:E:329:ASP:HA	1:E:340:LEU:HD22	1.97	0.46
1:C:156:ASN:HA	1:C:299:ARG:HG2	1.98	0.46
1:E:219:LEU:C	1:E:219:LEU:CD2	2.88	0.46
2:F:107:ILE:O	2:F:108:SER:C	2.59	0.46
1:A:379:TRP:CZ3	1:A:381:ASN:HB3	2.46	0.46
2:B:4:ILE:HG22	2:B:9:ILE:HD12	1.97	0.46
2:B:102:LEU:HD11	2:D:102:LEU:HD21	1.98	0.46
2:B:149:CYS:O	2:B:153:ILE:HG12	2.15	0.46
1:C:241:TYR:O	1:C:242:PHE:HB3	2.15	0.46
1:E:80:PHE:HB2	1:E:82:PHE:HE2	1.81	0.46
2:F:163:PRO:O	2:F:164:THR:HG22	2.16	0.46
1:A:8:GLN:HE22	2:B:8:ILE:CB	2.28	0.46
1:A:15:PHE:CD2	1:A:16:SER:N	2.84	0.46
1:A:257:ASP:CG	1:A:259:ARG:HE	2.24	0.46
2:B:99:ILE:HD13	2:B:99:ILE:C	2.41	0.46
1:C:246:TYR:HA	1:C:251:LYS:O	2.16	0.46
1:E:401:LEU:HD11	2:F:70:ILE:HD11	1.97	0.46
1:A:42:GLY:HA2	1:A:363:LEU:HD22	1.98	0.46
1:A:141:ASN:HD22	1:A:279:GLN:HE21	1.64	0.46
1:A:230:LYS:O	1:A:234:ASN:N	2.33	0.46
1:A:249:PHE:CE1	1:C:244:VAL:HG22	2.51	0.46
1:E:201:LEU:C	1:E:201:LEU:CD2	2.89	0.46
1:A:223:CYS:HA	1:A:274:GLN:O	2.15	0.46
1:A:281:LYS:O	1:A:285:TYR:OH	2.29	0.46
2:B:142:ASN:HA	2:B:145:CYS:O	2.16	0.46
1:C:163:PRO:HD3	1:C:202:ALA:HB2	1.96	0.46
2:D:61:ILE:N	2:D:61:ILE:CD1	2.79	0.46
1:E:66:PHE:CD2	1:E:67:PRO:HD3	2.50	0.46
1:E:192:SER:C	1:E:194:ASN:H	2.24	0.46
2:B:92:LEU:HA	2:B:95:GLU:HG3	1.97	0.46
2:B:125:ARG:C	2:B:129:LEU:HD11	2.40	0.46
1:C:1:GLU:CA	2:D:142:ASN:H	2.28	0.46
2:D:146:ASP:O	2:D:147:GLN:C	2.58	0.46
1:E:354:HIS:C	1:E:355:HIS:ND1	2.73	0.46
1:E:398:ARG:NH1	1:E:398:ARG:HG2	2.30	0.46
1:A:393:PRO:HB2	1:A:394:PRO:CD	2.40	0.45
1:A:426:VAL:CG2	2:B:4:ILE:HG21	2.44	0.45
1:C:4:LYS:O	2:D:28:SER:HA	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:7:LEU:HD13	1:C:7:LEU:HA	1.73	0.45
1:C:162:ILE:N	1:C:162:ILE:HD12	2.31	0.45
1:C:414:GLY:O	2:D:56:LYS:NZ	2.41	0.45
2:D:149:CYS:O	2:D:153:ILE:N	2.36	0.45
1:E:7:LEU:HD13	1:E:7:LEU:HA	1.74	0.45
1:E:222:SER:HB2	1:E:278:LEU:HD12	1.98	0.45
1:A:249:PHE:CE1	1:C:257:ASP:HB2	2.51	0.45
2:B:5:ASP:CG	2:B:9:ILE:CG2	2.89	0.45
2:B:41:ALA:C	2:B:43:LYS:N	2.74	0.45
1:C:68:ARG:HA	1:C:350:GLU:OE2	2.16	0.45
2:D:9:ILE:H	2:D:9:ILE:CD1	2.24	0.45
1:E:88:LEU:N	1:E:88:LEU:HD23	2.31	0.45
2:F:77:ILE:HD12	2:F:77:ILE:H	1.81	0.45
1:A:100:ASP:C	1:A:100:ASP:OD1	2.60	0.45
1:A:398:ARG:NH1	1:A:398:ARG:HG2	2.31	0.45
1:C:5:ILE:HB	2:D:154:PHE:CZ	2.52	0.45
1:C:189:VAL:HG23	1:C:196:CYS:HA	1.98	0.45
2:F:41:ALA:C	2:F:43:LYS:N	2.75	0.45
1:A:158:LEU:N	1:A:158:LEU:CD2	2.79	0.45
1:C:315:GLN:HG3	1:C:317:ILE:HD13	1.99	0.45
1:E:74:ALA:O	1:E:75:LYS:C	2.59	0.45
1:E:406:GLU:CD	1:E:406:GLU:H	2.24	0.45
2:B:56:LYS:O	2:B:59:ILE:HG12	2.16	0.45
1:C:3:ILE:HD11	2:D:140:ILE:N	2.29	0.45
2:D:4:ILE:HB	2:D:9:ILE:CD1	2.47	0.45
1:E:104:GLN:CB	1:E:153:SER:HB2	2.46	0.45
1:A:127:TYR:N	1:A:173:ASN:ND2	2.64	0.45
1:A:252:VAL:HG21	1:E:249:PHE:CD2	2.51	0.45
2:B:65:LYS:NZ	2:B:65:LYS:CB	2.76	0.45
1:C:31:LYS:CE	1:C:411:ILE:HB	2.47	0.45
1:C:68:ARG:H	1:C:68:ARG:HG2	1.48	0.45
1:C:249:PHE:CE1	1:E:244:VAL:CG2	2.99	0.45
1:C:296:MET:HE3	1:C:296:MET:HB2	1.81	0.45
2:D:118:LEU:O	2:D:119:ALA:C	2.58	0.45
1:E:1:GLU:HA	2:F:141:ASP:C	2.41	0.45
1:E:373:CYS:HG	1:E:399:CYS:CB	2.29	0.45
2:F:7:LEU:HB2	2:F:36:VAL:HG11	1.99	0.45
2:F:141:ASP:HB3	2:F:144:ILE:HG12	1.98	0.45
1:A:374:ILE:O	1:A:395:LYS:HA	2.17	0.45
2:B:154:PHE:O	2:B:156:PHE:CD2	2.70	0.45
1:E:1:GLU:CG	1:E:2:LYS:H	2.29	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:242:PHE:CD1	1:E:242:PHE:C	2.94	0.45
1:E:246:TYR:HA	1:E:251:LYS:O	2.16	0.45
2:F:126:ALA:HB3	2:F:129:LEU:CD2	2.47	0.45
2:B:62:ALA:O	2:B:65:LYS:HB3	2.16	0.45
2:B:131:VAL:HG21	2:B:139:ILE:N	2.31	0.45
1:C:88:LEU:N	1:C:88:LEU:HD23	2.30	0.45
1:C:329:ASP:HA	1:C:340:LEU:HD22	1.98	0.45
1:E:87:SER:O	1:E:88:LEU:C	2.59	0.45
2:F:57:SER:O	2:F:61:ILE:HD13	2.17	0.45
1:A:33:MET:HE3	1:A:409:PRO:CB	2.46	0.45
1:A:38:LYS:HD3	1:A:38:LYS:O	2.17	0.45
1:A:329:ASP:O	1:A:330:GLN:C	2.58	0.45
2:B:5:ASP:CG	2:B:9:ILE:HG23	2.42	0.45
2:B:120:SER:OG	2:B:121:GLU:N	2.49	0.45
2:B:126:ALA:O	2:B:129:LEU:CD1	2.65	0.45
1:C:38:LYS:O	1:C:38:LYS:CD	2.65	0.45
1:C:58:ARG:HD2	1:C:347:TYR:OH	2.16	0.45
1:C:256:LEU:HD12	1:C:257:ASP:N	2.31	0.45
2:D:131:VAL:HG21	2:D:139:ILE:CB	2.43	0.45
1:E:34:PHE:HE2	2:F:96:LEU:HD13	1.82	0.45
2:F:4:ILE:HG22	2:F:13:PHE:CE2	2.51	0.45
1:A:202:ALA:HB3	1:A:296:MET:HE1	1.98	0.45
1:A:319:GLY:CA	1:A:354:HIS:HD2	2.30	0.45
2:B:68:ASP:HB3	2:B:70:ILE:HB	1.98	0.45
1:C:75:LYS:O	1:C:78:ASP:HB2	2.17	0.45
1:C:424:THR:HG22	2:D:14:VAL:CG1	2.47	0.45
1:E:31:LYS:HZ2	1:E:411:ILE:HB	1.80	0.45
1:E:66:PHE:CE1	1:E:70:ALA:HB2	2.52	0.45
1:E:152:MET:HE3	1:E:152:MET:HB2	1.89	0.45
1:A:4:LYS:C	1:A:5:ILE:HD12	2.40	0.44
1:A:358:GLN:O	1:A:359:GLU:C	2.59	0.44
2:B:50:ASN:O	2:B:53:GLN:HB2	2.18	0.44
1:E:31:LYS:NZ	1:E:31:LYS:CB	2.80	0.44
1:E:134:ILE:O	1:E:135:LYS:C	2.58	0.44
1:E:425:THR:HB	2:F:16:ILE:HD11	1.99	0.44
2:F:42:GLU:H	2:F:42:GLU:HG2	1.58	0.44
2:B:107:ILE:O	2:B:108:SER:C	2.60	0.44
2:B:126:ALA:HB3	2:B:129:LEU:CD2	2.47	0.44
2:B:146:ASP:O	2:B:147:GLN:C	2.61	0.44
1:C:7:LEU:CD2	2:D:118:LEU:HD13	2.47	0.44
1:C:294:LEU:HD21	1:C:296:MET:CE	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:93:PHE:N	1:E:93:PHE:CD1	2.85	0.44
1:E:149:SER:HB3	1:E:304:ASP:O	2.17	0.44
1:E:224:TYR:CE1	1:E:274:GLN:HB3	2.52	0.44
2:F:4:ILE:HD12	2:F:5:ASP:H	1.81	0.44
2:F:61:ILE:CD1	2:F:61:ILE:H	2.30	0.44
2:F:149:CYS:HA	2:F:152:PHE:HB3	1.98	0.44
1:A:68:ARG:H	1:A:68:ARG:HG2	1.51	0.44
2:B:4:ILE:HG23	2:B:13:PHE:CG	2.53	0.44
2:B:141:ASP:HB3	2:B:144:ILE:CG1	2.47	0.44
1:C:121:HIS:C	1:C:123:ALA:H	2.26	0.44
1:C:180:LYS:HD2	1:C:299:ARG:NH2	2.33	0.44
1:C:266:ASN:C	1:C:266:ASN:ND2	2.74	0.44
1:E:28:THR:CB	3:Q:2:NAG:C8	2.96	0.44
1:E:174:CYS:C	1:E:175:ASN:O	2.58	0.44
1:E:190:LYS:HD3	1:E:190:LYS:HA	1.74	0.44
1:E:374:ILE:O	1:E:395:LYS:HA	2.16	0.44
1:E:426:VAL:HG22	1:E:427:THR:N	2.32	0.44
1:A:158:LEU:HD21	1:A:298:GLU:C	2.42	0.44
1:A:322:ARG:CD	1:A:354:HIS:CE1	3.00	0.44
1:C:161:THR:HG23	1:C:203:PHE:HB2	1.99	0.44
2:D:149:CYS:HA	2:D:152:PHE:HB3	2.00	0.44
1:E:234:ASN:HA	1:E:237:GLY:O	2.17	0.44
1:C:25:LEU:HD23	1:C:418:PRO:HA	1.99	0.44
1:C:174:CYS:SG	1:C:178:PHE:HA	2.57	0.44
1:C:234:ASN:HA	1:C:237:GLY:O	2.17	0.44
1:E:181:ASN:O	1:E:183:ALA:N	2.51	0.44
2:F:58:SER:O	2:F:59:ILE:C	2.60	0.44
2:F:125:ARG:HB3	2:F:129:LEU:CD2	2.47	0.44
2:F:138:TRP:CD1	2:F:138:TRP:H	2.35	0.44
1:C:116:VAL:HG13	1:C:117:ASN:N	2.31	0.44
1:C:204:PHE:HE1	1:C:206:LEU:HD21	1.82	0.44
1:C:376:GLN:HG3	1:C:376:GLN:O	2.18	0.44
1:E:174:CYS:SG	1:E:178:PHE:HA	2.57	0.44
1:E:322:ARG:HD2	1:E:354:HIS:CE1	2.52	0.44
2:F:67:ASN:OD1	2:F:67:ASN:N	2.50	0.44
1:A:3:ILE:HD11	2:B:140:ILE:O	2.17	0.44
1:A:216:LYS:CD	1:A:305:MET:H	2.15	0.44
1:A:387:THR:O	1:A:402:ALA:HA	2.18	0.44
1:C:5:ILE:CG2	2:D:154:PHE:CE1	3.01	0.44
1:C:36:LEU:HA	1:C:36:LEU:HD23	1.70	0.44
1:C:242:PHE:CD1	1:C:242:PHE:C	2.96	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:131:VAL:HG22	2:D:139:ILE:H	1.82	0.44
1:A:36:LEU:HA	1:A:36:LEU:HD23	1.70	0.44
1:A:38:LYS:O	1:A:38:LYS:CD	2.66	0.44
1:A:161:THR:HG23	1:A:203:PHE:HB2	2.00	0.44
1:C:406:GLU:CD	1:C:406:GLU:H	2.26	0.44
2:D:97:GLY:O	2:D:100:ARG:HB3	2.17	0.44
1:E:28:THR:HG21	3:Q:2:NAG:C8	2.43	0.44
1:E:42:GLY:HA2	1:E:363:LEU:HD22	1.99	0.44
2:F:111:LEU:HD23	2:F:111:LEU:HA	1.77	0.44
1:A:33:MET:HE2	2:B:100:ARG:HB2	1.98	0.44
1:A:38:LYS:HA	1:A:388:GLU:OE2	2.18	0.44
2:D:141:ASP:HB3	2:D:144:ILE:CG1	2.48	0.44
1:E:21:PHE:CD2	2:F:102:LEU:HD23	2.53	0.44
2:F:59:ILE:H	2:F:59:ILE:HG12	1.47	0.44
1:A:3:ILE:HD11	2:B:140:ILE:N	2.33	0.43
2:B:155:LYS:O	2:B:156:PHE:HB2	2.18	0.43
1:C:318:TRP:HA	1:C:318:TRP:CE3	2.53	0.43
1:C:331:ALA:O	1:C:335:THR:CG2	2.66	0.43
1:E:216:LYS:CD	1:E:305:MET:H	2.17	0.43
1:E:318:TRP:CB	1:E:322:ARG:HG3	2.46	0.43
1:E:366:GLY:C	1:E:368:ASP:N	2.73	0.43
2:F:47:LYS:O	2:F:48:ILE:C	2.61	0.43
1:C:38:LYS:HD3	1:C:38:LYS:O	2.18	0.43
1:C:141:ASN:HD22	1:C:279:GLN:HE21	1.65	0.43
1:C:161:THR:C	1:C:162:ILE:HD12	2.43	0.43
1:C:408:ILE:HD12	1:C:409:PRO:HD2	1.99	0.43
2:D:47:LYS:O	2:D:48:ILE:C	2.61	0.43
2:D:55:LEU:HD21	1:E:422:THR:HG22	1.99	0.43
1:E:230:LYS:O	1:E:233:TYR:N	2.51	0.43
1:E:261:SER:OG	1:E:262:PRO:HD2	2.18	0.43
2:F:132:GLU:HG2	2:F:138:TRP:CE3	2.53	0.43
1:A:1:GLU:N	1:A:1:GLU:CD	2.75	0.43
1:A:13:SER:CB	2:B:18:GLU:O	2.67	0.43
1:A:266:ASN:N	1:A:266:ASN:HD22	2.14	0.43
2:B:102:LEU:HB3	1:C:21:PHE:CE1	2.53	0.43
1:C:52:ILE:HG12	1:C:53:GLY:N	2.32	0.43
1:C:104:GLN:CB	1:C:153:SER:HB2	2.46	0.43
2:D:9:ILE:HG21	2:D:13:PHE:CB	2.48	0.43
1:E:5:ILE:HG23	2:F:26:LEU:HG	2.00	0.43
1:C:257:ASP:CG	1:C:259:ARG:HE	2.26	0.43
2:D:4:ILE:HG22	2:D:13:PHE:HB3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:4:ILE:CB	2:D:9:ILE:HG13	2.48	0.43
2:D:42:GLU:H	2:D:42:GLU:HG2	1.59	0.43
1:E:3:ILE:C	1:E:3:ILE:HD12	2.43	0.43
1:E:296:MET:HE3	1:E:296:MET:HB2	1.85	0.43
2:F:118:LEU:O	2:F:119:ALA:C	2.60	0.43
2:F:132:GLU:CG	2:F:138:TRP:CE3	3.01	0.43
1:A:416:LEU:HB2	2:B:52:ILE:HD13	2.01	0.43
1:C:28:THR:HB	3:L:2:NAG:C8	2.48	0.43
1:C:401:LEU:N	1:C:401:LEU:HD12	2.33	0.43
2:D:102:LEU:HD11	2:F:102:LEU:HD21	1.98	0.43
2:D:111:LEU:HA	2:D:111:LEU:HD23	1.80	0.43
2:F:147:GLN:O	2:F:150:GLN:HB2	2.19	0.43
4:K:2:NDG:O3	4:K:3:MAN:C5	2.47	0.43
1:A:80:PHE:HB2	1:A:82:PHE:HE2	1.81	0.43
1:A:404:LYS:H	1:A:404:LYS:HG2	1.32	0.43
2:D:59:ILE:H	2:D:59:ILE:HG12	1.52	0.43
2:F:147:GLN:O	2:F:150:GLN:N	2.51	0.43
1:A:66:PHE:CD1	1:A:66:PHE:C	2.96	0.43
2:B:61:ILE:H	2:B:61:ILE:CD1	2.32	0.43
1:C:44:SER:OG	1:C:45:VAL:N	2.51	0.43
1:C:158:LEU:HD21	1:C:298:GLU:CA	2.45	0.43
1:C:206:LEU:HB3	1:C:218:HIS:CD2	2.53	0.43
1:C:230:LYS:O	1:C:233:TYR:N	2.52	0.43
1:C:426:VAL:HG23	2:D:4:ILE:HG23	1.93	0.43
2:D:61:ILE:HD12	2:D:61:ILE:H	1.82	0.43
2:D:149:CYS:O	2:D:150:GLN:C	2.62	0.43
1:E:141:ASN:O	1:E:142:ILE:C	2.59	0.43
1:E:266:ASN:O	1:E:266:ASN:ND2	2.52	0.43
1:E:410:LYS:C	1:E:411:ILE:HD13	2.43	0.43
1:A:88:LEU:HD23	1:A:88:LEU:N	2.34	0.43
1:A:249:PHE:CE1	1:C:244:VAL:HG21	2.53	0.43
2:B:77:ILE:HD12	2:B:77:ILE:H	1.83	0.43
1:C:152:MET:HE3	1:C:152:MET:HB2	1.93	0.43
1:C:190:LYS:HD2	1:C:192:SER:OG	2.18	0.43
1:C:377:SER:CB	1:C:392:LEU:H	2.10	0.43
2:D:58:SER:O	2:D:59:ILE:C	2.62	0.43
1:E:204:PHE:CD1	1:E:204:PHE:C	2.97	0.43
1:E:229:SER:C	1:E:231:GLU:OE1	2.61	0.43
1:E:387:THR:O	1:E:402:ALA:HA	2.19	0.43
1:E:392:LEU:HA	1:E:393:PRO:HD2	1.56	0.43
2:F:125:ARG:C	2:F:129:LEU:HD11	2.42	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:317:ILE:HG22	1:A:324:SER:HB3	1.99	0.43
1:A:398:ARG:HH11	1:A:398:ARG:CG	2.32	0.43
2:B:131:VAL:CG1	2:B:139:ILE:H	2.31	0.43
1:C:27:ALA:HA	1:C:415:LEU:O	2.19	0.43
2:D:107:ILE:HD13	2:D:107:ILE:HA	1.83	0.43
2:D:126:ALA:O	2:D:129:LEU:CD1	2.66	0.43
1:E:38:LYS:O	1:E:38:LYS:CD	2.67	0.43
1:E:161:THR:C	1:E:162:ILE:HD12	2.43	0.43
1:E:194:ASN:O	1:E:194:ASN:ND2	2.52	0.43
1:E:223:CYS:HA	1:E:274:GLN:O	2.18	0.43
2:B:115:LEU:HD23	2:B:115:LEU:HA	1.74	0.43
2:D:39:GLU:OE1	2:D:155:LYS:HE3	2.19	0.43
2:D:55:LEU:HD12	2:D:111:LEU:HG	2.01	0.43
2:D:147:GLN:O	2:D:150:GLN:HB2	2.19	0.43
1:E:241:TYR:CD2	1:E:242:PHE:N	2.87	0.43
1:E:253:VAL:O	1:E:278:LEU:HD21	2.19	0.43
1:E:404:LYS:HB2	1:E:406:GLU:HG2	2.00	0.43
2:F:53:GLN:O	2:F:54:ILE:C	2.61	0.43
1:A:135:LYS:HD3	1:A:327:ALA:HB3	2.00	0.42
1:A:209:GLN:HG2	1:A:214:GLU:HA	2.00	0.42
1:A:231:GLU:HA	1:A:234:ASN:HB2	2.01	0.42
2:B:47:LYS:CE	1:C:423:ASP:CG	2.92	0.42
2:B:147:GLN:O	2:B:150:GLN:HB2	2.17	0.42
1:C:42:GLY:HA2	1:C:363:LEU:HD22	2.00	0.42
1:C:318:TRP:CG	1:C:322:ARG:HG3	2.54	0.42
1:C:347:TYR:HE2	1:C:354:HIS:C	2.27	0.42
2:D:9:ILE:HG21	2:D:13:PHE:CG	2.53	0.42
2:D:129:LEU:HD22	2:D:153:ILE:HG23	2.00	0.42
1:E:13:SER:C	1:E:15:PHE:N	2.76	0.42
1:E:338:CYS:O	2:F:78:ARG:NH2	2.52	0.42
1:C:329:ASP:HA	1:C:340:LEU:CD2	2.49	0.42
2:D:67:ASN:O	2:D:68:ASP:O	2.37	0.42
1:A:242:PHE:CD1	1:A:242:PHE:C	2.96	0.42
2:B:47:LYS:O	2:B:48:ILE:C	2.62	0.42
1:C:229:SER:C	1:C:231:GLU:OE2	2.62	0.42
1:C:249:PHE:CE1	1:E:244:VAL:HG21	2.54	0.42
2:D:132:GLU:CG	2:D:138:TRP:CE3	3.02	0.42
2:D:161:PRO:C	2:D:162:VAL:HG13	2.45	0.42
1:E:156:ASN:HA	1:E:299:ARG:HG2	2.01	0.42
1:E:162:ILE:N	1:E:162:ILE:CD1	2.82	0.42
2:F:141:ASP:O	2:F:144:ILE:HG12	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:36:LEU:HA	1:E:36:LEU:HD23	1.69	0.42
1:E:56:ASP:HB3	1:E:57:SER:H	1.29	0.42
1:E:85:GLY:O	1:E:99:VAL:CG1	2.68	0.42
1:E:319:GLY:N	1:E:354:HIS:CD2	2.81	0.42
1:E:398:ARG:CG	1:E:398:ARG:HH11	2.32	0.42
2:F:146:ASP:O	2:F:147:GLN:C	2.61	0.42
1:A:11:VAL:HG12	2:B:16:ILE:HA	2.01	0.42
1:A:158:LEU:N	1:A:158:LEU:HD22	2.34	0.42
1:A:203:PHE:HE1	1:C:260:VAL:O	2.03	0.42
2:B:149:CYS:O	2:B:150:GLN:C	2.61	0.42
1:C:294:LEU:CD1	1:C:296:MET:HE3	2.29	0.42
2:D:93:LEU:HA	2:D:93:LEU:HD23	1.68	0.42
1:E:398:ARG:HG2	1:E:398:ARG:HH11	1.85	0.42
2:F:68:ASP:HB3	2:F:70:ILE:HB	2.01	0.42
2:F:129:LEU:HD22	2:F:153:ILE:HG23	2.01	0.42
1:A:1:GLU:C	1:A:3:ILE:N	2.78	0.42
1:A:134:ILE:O	1:A:135:LYS:C	2.63	0.42
1:A:190:LYS:HE2	1:A:192:SER:OG	2.20	0.42
1:A:247:ASP:OD1	1:A:247:ASP:C	2.63	0.42
2:B:104:VAL:HG12	2:B:105:GLY:N	2.33	0.42
1:C:209:GLN:HG2	1:C:214:GLU:HA	2.01	0.42
1:C:366:GLY:C	1:C:368:ASP:H	2.28	0.42
1:C:374:ILE:O	1:C:395:LYS:HA	2.19	0.42
2:D:47:LYS:HZ1	1:E:423:ASP:CG	2.28	0.42
2:D:138:TRP:CD1	2:D:138:TRP:H	2.35	0.42
1:E:100:ASP:OD1	1:E:100:ASP:C	2.62	0.42
1:E:158:LEU:CD2	1:E:298:GLU:HA	2.43	0.42
1:E:392:LEU:HA	1:E:392:LEU:HD23	1.72	0.42
2:F:122:ILE:HB	2:F:138:TRP:HH2	1.83	0.42
1:A:189:VAL:HG23	1:A:195:LYS:O	2.19	0.42
1:A:296:MET:HE3	1:A:296:MET:HB2	1.88	0.42
1:A:315:GLN:HG3	1:A:317:ILE:HD13	2.01	0.42
1:A:328:VAL:O	1:A:329:ASP:C	2.63	0.42
1:A:401:LEU:HD12	1:A:401:LEU:N	2.33	0.42
2:B:41:ALA:HB1	2:B:155:LYS:HA	2.02	0.42
1:C:15:PHE:CD2	1:C:16:SER:N	2.87	0.42
1:C:149:SER:HB3	1:C:304:ASP:O	2.19	0.42
1:C:190:LYS:HD3	1:C:190:LYS:HA	1.75	0.42
2:D:126:ALA:HB3	2:D:129:LEU:CD2	2.50	0.42
1:E:358:GLN:O	1:E:359:GLU:C	2.62	0.42
2:F:47:LYS:HZ2	2:F:47:LYS:HG2	1.46	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:13:SER:HB2	2:B:18:GLU:O	2.20	0.42
1:A:85:GLY:O	1:A:99:VAL:CG1	2.67	0.42
1:A:158:LEU:CD2	1:A:298:GLU:C	2.93	0.42
2:B:4:ILE:HG22	2:B:9:ILE:CG1	2.49	0.42
1:C:31:LYS:NZ	1:C:31:LYS:HB2	2.32	0.42
1:C:38:LYS:H	1:C:38:LYS:CD	2.26	0.42
1:C:366:GLY:C	1:C:368:ASP:N	2.78	0.42
2:D:45:PHE:O	2:D:47:LYS:N	2.53	0.42
2:D:131:VAL:HG21	2:D:139:ILE:N	2.34	0.42
1:E:38:LYS:HD3	1:E:38:LYS:O	2.20	0.42
1:E:131:TRP:O	1:E:132:THR:C	2.63	0.42
1:E:266:ASN:N	1:E:266:ASN:HD22	2.18	0.42
1:A:72:VAL:HG23	1:A:73:SER:O	2.19	0.42
1:C:82:PHE:CD1	1:C:82:PHE:C	2.98	0.42
1:C:253:VAL:O	1:C:278:LEU:HD21	2.20	0.42
2:D:30:LYS:CE	2:D:32:SER:HB3	2.49	0.42
1:E:18:HIS:HD2	1:E:412:PRO:HD3	1.85	0.42
1:E:31:LYS:CE	1:E:411:ILE:HB	2.49	0.42
1:E:158:LEU:HD21	1:E:298:GLU:CA	2.43	0.42
1:E:304:ASP:OD1	1:E:306:LYS:HB2	2.20	0.42
2:F:61:ILE:N	2:F:61:ILE:CD1	2.83	0.42
2:F:67:ASN:O	2:F:68:ASP:O	2.38	0.42
2:F:99:ILE:O	2:F:99:ILE:HG12	2.20	0.42
1:A:166:VAL:HG22	1:A:167:THR:N	2.35	0.42
1:C:304:ASP:OD1	1:C:306:LYS:HB2	2.20	0.42
1:C:417:ILE:HG12	2:D:24:TYR:CZ	2.55	0.42
2:F:99:ILE:HD13	2:F:99:ILE:C	2.44	0.42
1:A:174:CYS:C	1:A:175:ASN:O	2.60	0.41
1:C:195:LYS:HD2	1:C:195:LYS:HA	1.41	0.41
1:C:241:TYR:CG	1:C:242:PHE:N	2.87	0.41
1:C:319:GLY:CA	1:C:354:HIS:HD2	2.32	0.41
2:D:157:ASN:O	2:D:159:THR:HG23	2.20	0.41
1:E:190:LYS:HA	1:E:191:PRO:HD2	1.82	0.41
2:F:112:GLN:C	2:F:114:SER:N	2.76	0.41
1:A:10:GLN:HG2	2:B:17:VAL:HG22	2.02	0.41
1:A:331:ALA:O	1:A:332:CYS:C	2.63	0.41
2:B:149:CYS:O	2:B:153:ILE:N	2.41	0.41
1:C:31:LYS:NZ	1:C:31:LYS:C	2.78	0.41
1:C:171:ALA:N	1:C:177:SER:O	2.49	0.41
1:C:281:LYS:O	1:C:285:TYR:OH	2.26	0.41
2:D:132:GLU:HG2	2:D:138:TRP:CE3	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:149:CYS:O	2:D:153:ILE:HG12	2.21	0.41
2:F:155:LYS:O	2:F:156:PHE:HB2	2.20	0.41
1:A:82:PHE:CD1	1:A:82:PHE:C	2.98	0.41
1:A:304:ASP:OD1	1:A:306:LYS:N	2.53	0.41
2:B:123:THR:OG1	2:B:138:TRP:HZ3	2.02	0.41
2:D:51:ASP:O	2:D:55:LEU:HG	2.20	0.41
1:E:17:LEU:C	1:E:17:LEU:CD2	2.93	0.41
2:F:50:ASN:O	2:F:53:GLN:HB2	2.20	0.41
1:A:18:HIS:ND1	1:A:18:HIS:N	2.68	0.41
1:A:75:LYS:O	1:A:78:ASP:HB2	2.20	0.41
1:A:95:PRO:HA	1:A:179:LEU:HD23	2.01	0.41
2:B:80:LEU:HD12	2:B:80:LEU:HA	1.88	0.41
2:B:132:GLU:CG	2:B:138:TRP:CE3	3.04	0.41
2:D:68:ASP:HB3	2:D:70:ILE:HB	2.02	0.41
1:E:72:VAL:HG23	1:E:73:SER:O	2.20	0.41
1:E:160:LYS:HG3	1:E:162:ILE:CD1	2.50	0.41
2:F:21:ILE:HD12	2:F:21:ILE:N	2.33	0.41
1:A:56:ASP:HB3	1:A:57:SER:H	1.26	0.41
2:B:112:GLN:C	2:B:114:SER:N	2.74	0.41
2:B:140:ILE:HD12	2:B:141:ASP:N	2.31	0.41
1:C:219:LEU:C	1:C:219:LEU:HD22	2.45	0.41
2:F:131:VAL:HG21	2:F:139:ILE:N	2.34	0.41
2:F:157:ASN:O	2:F:159:THR:HG23	2.20	0.41
1:A:83:LEU:O	1:A:84:SER:C	2.64	0.41
1:A:145:LEU:HD12	1:A:145:LEU:HA	1.88	0.41
1:C:13:SER:C	1:C:15:PHE:N	2.77	0.41
1:C:66:PHE:HE1	1:C:70:ALA:HB2	1.86	0.41
2:D:61:ILE:HG22	2:D:62:ALA:N	2.35	0.41
2:D:65:LYS:NZ	2:D:65:LYS:CB	2.74	0.41
1:E:257:ASP:OD1	1:E:257:ASP:C	2.61	0.41
1:E:330:GLN:NE2	3:S:2:NAG:H83	2.35	0.41
1:E:377:SER:CB	1:E:392:LEU:H	2.11	0.41
2:F:126:ALA:O	2:F:129:LEU:CD1	2.68	0.41
1:A:366:GLY:C	1:A:368:ASP:N	2.78	0.41
1:A:398:ARG:HG2	1:A:398:ARG:HH11	1.85	0.41
2:B:58:SER:O	2:B:59:ILE:C	2.64	0.41
1:C:141:ASN:O	1:C:142:ILE:C	2.64	0.41
1:E:40:LYS:N	1:E:379:TRP:O	2.51	0.41
1:E:294:LEU:CD2	1:E:295:LEU:N	2.80	0.41
1:E:404:LYS:H	1:E:404:LYS:HG2	1.34	0.41
1:A:5:ILE:HG22	1:A:6:CYS:N	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:204:PHE:CD1	1:A:204:PHE:C	2.99	0.41
1:A:224:TYR:CE1	1:A:274:GLN:HB3	2.56	0.41
2:B:39:GLU:HG2	2:B:40:SER:N	2.34	0.41
2:B:51:ASP:O	2:B:55:LEU:HG	2.20	0.41
2:B:113:GLU:HB3	1:C:421:GLY:HA3	2.03	0.41
1:C:34:PHE:HE2	2:D:96:LEU:CD1	2.29	0.41
1:C:158:LEU:N	1:C:158:LEU:CD2	2.83	0.41
1:C:190:LYS:HE2	1:C:192:SER:OG	2.20	0.41
1:C:194:ASN:ND2	1:C:194:ASN:O	2.54	0.41
2:D:99:ILE:HD13	2:D:99:ILE:C	2.45	0.41
2:D:154:PHE:O	2:D:156:PHE:CD2	2.74	0.41
1:E:281:LYS:O	1:E:285:TYR:OH	2.31	0.41
2:F:55:LEU:HD12	2:F:111:LEU:HG	2.02	0.41
2:F:61:ILE:HD12	2:F:61:ILE:H	1.86	0.41
3:G:1:NAG:H5	3:G:2:NAG:C7	2.50	0.41
1:A:31:LYS:CE	1:A:411:ILE:HB	2.49	0.41
1:A:102:LEU:HD21	1:A:104:GLN:NE2	2.35	0.41
1:A:411:ILE:HD13	1:A:411:ILE:N	2.36	0.41
2:B:59:ILE:HG12	2:B:59:ILE:H	1.49	0.41
2:B:67:ASN:O	2:B:68:ASP:O	2.38	0.41
2:B:149:CYS:HA	2:B:152:PHE:HB3	2.02	0.41
1:C:17:LEU:C	1:C:17:LEU:CD2	2.93	0.41
1:C:66:PHE:CD1	1:C:66:PHE:C	2.96	0.41
1:C:102:LEU:HD21	1:C:104:GLN:NE2	2.35	0.41
1:C:190:LYS:HA	1:C:191:PRO:HD2	1.80	0.41
1:C:191:PRO:O	1:C:194:ASN:N	2.50	0.41
1:C:231:GLU:N	1:C:231:GLU:OE2	2.52	0.41
1:C:247:ASP:OD1	1:C:247:ASP:C	2.64	0.41
1:C:296:MET:HE2	1:C:296:MET:CA	2.50	0.41
2:D:80:LEU:HD12	2:D:80:LEU:HA	1.93	0.41
2:D:119:ALA:HA	2:D:138:TRP:CH2	2.55	0.41
2:D:125:ARG:HB3	2:D:129:LEU:CD2	2.45	0.41
1:E:18:HIS:ND1	1:E:18:HIS:N	2.68	0.41
1:E:31:LYS:NZ	1:E:31:LYS:C	2.79	0.41
1:E:44:SER:OG	1:E:45:VAL:N	2.54	0.41
1:E:219:LEU:C	1:E:219:LEU:HD22	2.46	0.41
1:E:366:GLY:O	1:E:368:ASP:N	2.54	0.41
2:F:59:ILE:O	2:F:60:ASN:C	2.64	0.41
2:F:134:SER:OG	2:F:137:CYS:HB2	2.21	0.41
4:K:2:NDG:C4	4:K:3:MAN:C3	2.97	0.41
1:A:155:VAL:O	1:A:299:ARG:HG2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:219:LEU:C	1:A:219:LEU:HD22	2.46	0.41
1:A:416:LEU:O	2:B:24:TYR:OH	2.09	0.41
1:C:25:LEU:HD23	1:C:25:LEU:HA	1.86	0.41
1:C:55:GLY:C	1:C:82:PHE:CB	2.93	0.41
1:C:57:SER:C	1:C:59:THR:N	2.79	0.41
1:C:216:LYS:CD	1:C:305:MET:H	2.18	0.41
2:D:5:ASP:N	2:D:9:ILE:HD12	2.33	0.41
2:D:21:ILE:HD12	2:D:21:ILE:N	2.29	0.41
2:D:112:GLN:C	2:D:114:SER:N	2.76	0.41
1:E:33:MET:HE3	1:E:409:PRO:HG2	2.03	0.41
1:E:217:LEU:CD2	1:E:305:MET:HE2	2.47	0.41
1:E:315:GLN:HG3	1:E:317:ILE:HD13	2.03	0.41
1:E:319:GLY:CA	1:E:354:HIS:HD2	2.33	0.41
1:A:11:VAL:N	2:B:15:ALA:O	2.38	0.40
2:B:59:ILE:O	2:B:60:ASN:C	2.64	0.40
1:C:132:THR:O	1:C:133:ASP:C	2.64	0.40
1:C:158:LEU:CD2	1:C:298:GLU:HA	2.47	0.40
1:C:392:LEU:HD23	1:C:392:LEU:HA	1.81	0.40
1:E:27:ALA:HA	1:E:415:LEU:O	2.22	0.40
1:E:38:LYS:H	1:E:38:LYS:CD	2.28	0.40
2:F:51:ASP:O	2:F:55:LEU:HG	2.20	0.40
2:F:93:LEU:HD23	2:F:93:LEU:HA	1.70	0.40
3:T:1:NAG:O4	3:T:2:NAG:O7	2.39	0.40
1:A:310:PRO:HB3	1:A:396:PHE:CE1	2.56	0.40
1:A:366:GLY:C	1:A:368:ASP:H	2.27	0.40
2:B:118:LEU:HD23	2:B:118:LEU:HA	1.94	0.40
2:B:119:ALA:O	2:B:122:ILE:N	2.55	0.40
2:D:53:GLN:O	2:D:54:ILE:C	2.64	0.40
2:D:125:ARG:C	2:D:129:LEU:HD11	2.46	0.40
1:E:25:LEU:HA	1:E:25:LEU:HD23	1.86	0.40
1:E:189:VAL:HG23	1:E:195:LYS:O	2.22	0.40
1:E:375:SER:HB2	1:E:395:LYS:HB3	2.03	0.40
1:E:391:LEU:HD23	1:E:391:LEU:HA	1.84	0.40
2:F:39:GLU:OE1	2:F:155:LYS:HE3	2.22	0.40
1:A:18:HIS:HD2	1:A:412:PRO:HD3	1.87	0.40
1:A:31:LYS:NZ	1:A:31:LYS:CB	2.85	0.40
2:B:132:GLU:HG2	2:B:138:TRP:CE3	2.56	0.40
1:C:189:VAL:HG23	1:C:195:LYS:O	2.22	0.40
2:D:134:SER:OG	2:D:137:CYS:HB2	2.21	0.40
1:E:83:LEU:O	1:E:84:SER:C	2.64	0.40
1:E:236:ARG:NH2	1:E:293:PHE:HZ	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:147:GLN:HG3	2:F:151:ASN:OD1	2.21	0.40
1:A:121:HIS:C	1:A:123:ALA:H	2.29	0.40
1:A:249:PHE:CE2	1:C:252:VAL:CG2	3.04	0.40
1:A:420:SER:HB2	2:B:12:LEU:O	2.21	0.40
2:B:26:LEU:HD12	2:B:26:LEU:HA	1.95	0.40
2:B:128:ASP:O	2:B:140:ILE:HD11	2.21	0.40
2:B:129:LEU:HD22	2:B:153:ILE:HG23	2.04	0.40
2:B:133:VAL:HB	2:B:134:SER:H	1.65	0.40
1:C:363:LEU:HA	1:C:363:LEU:HD23	1.71	0.40
2:D:118:LEU:HD23	2:D:118:LEU:HA	1.89	0.40
1:E:57:SER:C	1:E:59:THR:H	2.28	0.40
1:E:66:PHE:CD1	1:E:66:PHE:C	2.98	0.40
1:E:417:ILE:HA	2:F:24:TYR:OH	2.21	0.40
3:R:1:NAG:H61	3:R:2:NAG:C7	2.52	0.40
1:A:195:LYS:HA	1:A:195:LYS:HD2	1.47	0.40
2:B:98:ILE:C	2:B:100:ARG:N	2.77	0.40
2:D:11:VAL:O	2:D:11:VAL:HG13	2.20	0.40
2:D:41:ALA:HB1	2:D:155:LYS:HA	2.03	0.40
2:D:123:THR:OG1	2:D:138:TRP:HZ3	2.04	0.40
1:E:25:LEU:HD23	1:E:418:PRO:HA	2.03	0.40
1:E:58:ARG:HD2	1:E:347:TYR:OH	2.20	0.40
1:E:158:LEU:CD2	1:E:158:LEU:N	2.84	0.40
1:E:161:THR:HG23	1:E:203:PHE:HB2	2.02	0.40
2:F:30:LYS:HD2	2:F:32:SER:N	2.08	0.40

There are no symmetry-related clashes.

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	425/432 (98%)	359 (84%)	49 (12%)	17 (4%)	2 17

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	425/432 (98%)	359 (84%)	50 (12%)	16 (4%)	2	18
1	E	425/432 (98%)	358 (84%)	51 (12%)	16 (4%)	2	18
2	B	160/175 (91%)	113 (71%)	32 (20%)	15 (9%)	0	3
2	D	160/175 (91%)	111 (69%)	32 (20%)	17 (11%)	0	2
2	F	160/175 (91%)	115 (72%)	29 (18%)	16 (10%)	0	2
All	All	1755/1821 (96%)	1415 (81%)	243 (14%)	97 (6%)	1	11

All (97) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	47	ASN
1	A	48	GLN
1	A	66	PHE
1	A	393	PRO
2	B	18	GLU
2	B	42	GLU
2	B	68	ASP
2	B	126	ALA
2	B	130	ALA
2	B	132	GLU
2	B	155	LYS
1	C	2	LYS
1	C	47	ASN
1	C	48	GLN
1	C	66	PHE
1	C	393	PRO
2	D	18	GLU
2	D	42	GLU
2	D	68	ASP
2	D	126	ALA
2	D	130	ALA
2	D	132	GLU
2	D	155	LYS
2	D	161	PRO
2	D	163	PRO
2	D	164	THR
1	E	47	ASN
1	E	48	GLN
1	E	66	PHE
1	E	393	PRO

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Mol	Chain	Res	Type
2	F	18	GLU
2	F	68	ASP
2	F	126	ALA
2	F	130	ALA
2	F	132	GLU
2	F	155	LYS
2	F	161	PRO
2	F	162	VAL
2	F	164	THR
1	A	64	SER
1	A	422	THR
2	B	67	ASN
2	B	133	VAL
2	B	156	PHE
1	C	64	SER
1	C	422	THR
2	D	67	ASN
2	D	133	VAL
1	E	64	SER
1	E	422	THR
2	F	42	GLU
2	F	67	ASN
2	F	133	VAL
2	F	156	PHE
1	A	2	LYS
1	A	177	SER
2	B	46	GLU
2	B	161	PRO
1	C	122	ALA
1	C	177	SER
1	C	407	SER
2	D	46	GLU
2	D	156	PHE
1	E	122	ALA
1	E	177	SER
1	E	407	SER
2	F	46	GLU
1	A	14	SER
1	A	407	SER
2	B	162	VAL
1	C	14	SER
1	C	230	LYS

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Mol	Chain	Res	Type
2	D	66	LEU
1	E	14	SER
1	E	230	LYS
1	A	4	LYS
1	A	122	ALA
1	A	181	ASN
2	B	164	THR
1	C	181	ASN
2	D	6	ASP
1	E	127	TYR
2	F	6	ASP
1	A	127	TYR
1	E	181	ASN
1	A	3	ILE
1	A	250	GLY
2	F	61	ILE
1	C	3	ILE
2	D	61	ILE
1	A	67	PRO
2	B	61	ILE
1	C	291	PRO
1	E	3	ILE
1	E	67	PRO
1	E	291	PRO
1	C	67	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	369/374 (99%)	262 (71%)	107 (29%)	0	1
1	C	368/374 (98%)	259 (70%)	109 (30%)	0	1
1	E	369/374 (99%)	259 (70%)	110 (30%)	0	1
2	B	134/147 (91%)	70 (52%)	64 (48%)	0	0
2	D	134/147 (91%)	74 (55%)	60 (45%)	0	0

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	F	134/147 (91%)	74 (55%)	60 (45%)	0	0
All	All	1508/1563 (96%)	998 (66%)	510 (34%)	0	1

All (510) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	GLU
1	A	7	LEU
1	A	8	GLN
1	A	9	LYS
1	A	13	SER
1	A	14	SER
1	A	16	SER
1	A	17	LEU
1	A	18	HIS
1	A	31	LYS
1	A	32	ARG
1	A	38	LYS
1	A	40	LYS
1	A	45	VAL
1	A	46	LEU
1	A	47	ASN
1	A	49	SER
1	A	56	ASP
1	A	57	SER
1	A	58	ARG
1	A	59	THR
1	A	61	LYS
1	A	63	ASN
1	A	64	SER
1	A	68	ARG
1	A	82	PHE
1	A	88	LEU
1	A	98	LYS
1	A	99	VAL
1	A	102	LEU
1	A	125	ASN
1	A	134	ILE
1	A	136	LEU
1	A	145	LEU
1	A	154	LEU
1	A	158	LEU

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Mol	Chain	Res	Type
1	A	161	THR
1	A	165	GLN
1	A	167	THR
1	A	173	ASN
1	A	174	CYS
1	A	175	ASN
1	A	180	LYS
1	A	189	VAL
1	A	190	LYS
1	A	192	SER
1	A	195	LYS
1	A	198	LYS
1	A	199	GLU
1	A	200	ASN
1	A	201	LEU
1	A	208	THR
1	A	209	GLN
1	A	219	LEU
1	A	220	VAL
1	A	230	LYS
1	A	231	GLU
1	A	236	ARG
1	A	238	CYS
1	A	240	ASN
1	A	248	SER
1	A	252	VAL
1	A	253	VAL
1	A	266	ASN
1	A	267	SER
1	A	270	THR
1	A	272	THR
1	A	274	GLN
1	A	280	LEU
1	A	286	SER
1	A	287	VAL
1	A	288	ARG
1	A	290	SER
1	A	292	ARG
1	A	294	LEU
1	A	299	ARG
1	A	302	CYS
1	A	306	LYS

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Mol	Chain	Res	Type
1	A	316	SER
1	A	317	ILE
1	A	322	ARG
1	A	328	VAL
1	A	330	GLN
1	A	335	THR
1	A	342	GLN
1	A	343	LYS
1	A	348	ILE
1	A	365	SER
1	A	372	ARG
1	A	373	CYS
1	A	377	SER
1	A	380	VAL
1	A	382	GLU
1	A	384	SER
1	A	387	THR
1	A	388	GLU
1	A	398	ARG
1	A	404	LYS
1	A	405	GLU
1	A	406	GLU
1	A	408	ILE
1	A	411	ILE
1	A	416	LEU
1	A	419	THR
1	A	423	ASP
1	A	424	THR
1	A	425	THR
2	B	4	ILE
2	B	5	ASP
2	B	6	ASP
2	B	7	LEU
2	B	9	ILE
2	B	11	VAL
2	B	12	LEU
2	B	13	PHE
2	B	14	VAL
2	B	19	THR
2	B	21	ILE
2	B	25	LEU
2	B	26	LEU

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Mol	Chain	Res	Type
2	B	29	ARG
2	B	30	LYS
2	B	31	GLU
2	B	36	VAL
2	B	39	GLU
2	B	42	GLU
2	B	43	LYS
2	B	47	LYS
2	B	52	ILE
2	B	54	ILE
2	B	56	LYS
2	B	57	SER
2	B	58	SER
2	B	59	ILE
2	B	65	LYS
2	B	67	ASN
2	B	68	ASP
2	B	69	ARG
2	B	70	ILE
2	B	71	SER
2	B	77	ILE
2	B	80	LEU
2	B	82	LEU
2	B	83	GLU
2	B	84	ILE
2	B	89	SER
2	B	92	LEU
2	B	98	ILE
2	B	99	ILE
2	B	102	LEU
2	B	104	VAL
2	B	109	ILE
2	B	111	LEU
2	B	112	GLN
2	B	113	GLU
2	B	114	SER
2	B	117	GLU
2	B	123	THR
2	B	125	ARG
2	B	128	ASP
2	B	129	LEU
2	B	131	VAL

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Mol	Chain	Res	Type
2	B	132	GLU
2	B	138	TRP
2	B	140	ILE
2	B	143	ASN
2	B	144	ILE
2	B	148	SER
2	B	155	LYS
2	B	159	THR
2	B	162	VAL
1	C	7	LEU
1	C	8	GLN
1	C	9	LYS
1	C	13	SER
1	C	14	SER
1	C	16	SER
1	C	17	LEU
1	C	18	HIS
1	C	31	LYS
1	C	32	ARG
1	C	38	LYS
1	C	40	LYS
1	C	46	LEU
1	C	47	ASN
1	C	49	SER
1	C	56	ASP
1	C	57	SER
1	C	58	ARG
1	C	59	THR
1	C	61	LYS
1	C	63	ASN
1	C	64	SER
1	C	68	ARG
1	C	82	PHE
1	C	88	LEU
1	C	98	LYS
1	C	99	VAL
1	C	102	LEU
1	C	125	ASN
1	C	134	ILE
1	C	136	LEU
1	C	145	LEU
1	C	154	LEU

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Mol	Chain	Res	Type
1	C	158	LEU
1	C	161	THR
1	C	165	GLN
1	C	167	THR
1	C	170	THR
1	C	173	ASN
1	C	174	CYS
1	C	175	ASN
1	C	180	LYS
1	C	189	VAL
1	C	190	LYS
1	C	192	SER
1	C	195	LYS
1	C	198	LYS
1	C	199	GLU
1	C	200	ASN
1	C	201	LEU
1	C	208	THR
1	C	209	GLN
1	C	219	LEU
1	C	220	VAL
1	C	230	LYS
1	C	231	GLU
1	C	236	ARG
1	C	238	CYS
1	C	240	ASN
1	C	248	SER
1	C	252	VAL
1	C	253	VAL
1	C	266	ASN
1	C	267	SER
1	C	270	THR
1	C	272	THR
1	C	274	GLN
1	C	277	MET
1	C	278	LEU
1	C	280	LEU
1	C	286	SER
1	C	287	VAL
1	C	288	ARG
1	C	290	SER
1	C	292	ARG

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Mol	Chain	Res	Type
1	C	294	LEU
1	C	299	ARG
1	C	302	CYS
1	C	306	LYS
1	C	316	SER
1	C	317	ILE
1	C	322	ARG
1	C	328	VAL
1	C	330	GLN
1	C	335	THR
1	C	342	GLN
1	C	343	LYS
1	C	348	ILE
1	C	365	SER
1	C	372	ARG
1	C	373	CYS
1	C	377	SER
1	C	380	VAL
1	C	382	GLU
1	C	384	SER
1	C	387	THR
1	C	388	GLU
1	C	398	ARG
1	C	404	LYS
1	C	406	GLU
1	C	408	ILE
1	C	411	ILE
1	C	416	LEU
1	C	419	THR
1	C	423	ASP
1	C	424	THR
1	C	425	THR
1	C	426	VAL
1	C	427	THR
2	D	7	LEU
2	D	9	ILE
2	D	11	VAL
2	D	12	LEU
2	D	13	PHE
2	D	14	VAL
2	D	19	THR
2	D	21	ILE

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Mol	Chain	Res	Type
2	D	25	LEU
2	D	26	LEU
2	D	29	ARG
2	D	30	LYS
2	D	31	GLU
2	D	36	VAL
2	D	39	GLU
2	D	42	GLU
2	D	43	LYS
2	D	47	LYS
2	D	52	ILE
2	D	54	ILE
2	D	56	LYS
2	D	57	SER
2	D	58	SER
2	D	59	ILE
2	D	65	LYS
2	D	67	ASN
2	D	68	ASP
2	D	69	ARG
2	D	70	ILE
2	D	71	SER
2	D	77	ILE
2	D	78	ARG
2	D	80	LEU
2	D	82	LEU
2	D	83	GLU
2	D	89	SER
2	D	92	LEU
2	D	98	ILE
2	D	99	ILE
2	D	102	LEU
2	D	104	VAL
2	D	109	ILE
2	D	111	LEU
2	D	112	GLN
2	D	113	GLU
2	D	114	SER
2	D	117	GLU
2	D	123	THR
2	D	125	ARG
2	D	128	ASP

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Mol	Chain	Res	Type
2	D	129	LEU
2	D	131	VAL
2	D	132	GLU
2	D	138	TRP
2	D	140	ILE
2	D	143	ASN
2	D	144	ILE
2	D	148	SER
2	D	155	LYS
2	D	159	THR
1	E	7	LEU
1	E	8	GLN
1	E	9	LYS
1	E	13	SER
1	E	14	SER
1	E	16	SER
1	E	17	LEU
1	E	18	HIS
1	E	31	LYS
1	E	32	ARG
1	E	38	LYS
1	E	40	LYS
1	E	46	LEU
1	E	47	ASN
1	E	49	SER
1	E	52	ILE
1	E	56	ASP
1	E	57	SER
1	E	58	ARG
1	E	59	THR
1	E	61	LYS
1	E	63	ASN
1	E	64	SER
1	E	68	ARG
1	E	82	PHE
1	E	83	LEU
1	E	88	LEU
1	E	98	LYS
1	E	99	VAL
1	E	100	ASP
1	E	102	LEU
1	E	125	ASN

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Mol	Chain	Res	Type
1	E	134	ILE
1	E	136	LEU
1	E	145	LEU
1	E	154	LEU
1	E	158	LEU
1	E	161	THR
1	E	165	GLN
1	E	167	THR
1	E	173	ASN
1	E	174	CYS
1	E	175	ASN
1	E	180	LYS
1	E	189	VAL
1	E	190	LYS
1	E	192	SER
1	E	195	LYS
1	E	198	LYS
1	E	200	ASN
1	E	201	LEU
1	E	208	THR
1	E	209	GLN
1	E	219	LEU
1	E	220	VAL
1	E	230	LYS
1	E	231	GLU
1	E	236	ARG
1	E	238	CYS
1	E	240	ASN
1	E	248	SER
1	E	252	VAL
1	E	253	VAL
1	E	266	ASN
1	E	267	SER
1	E	270	THR
1	E	272	THR
1	E	274	GLN
1	E	278	LEU
1	E	280	LEU
1	E	286	SER
1	E	287	VAL
1	E	288	ARG
1	E	290	SER

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Mol	Chain	Res	Type
1	E	292	ARG
1	E	294	LEU
1	E	299	ARG
1	E	302	CYS
1	E	306	LYS
1	E	316	SER
1	E	317	ILE
1	E	322	ARG
1	E	328	VAL
1	E	330	GLN
1	E	335	THR
1	E	342	GLN
1	E	343	LYS
1	E	348	ILE
1	E	365	SER
1	E	372	ARG
1	E	373	CYS
1	E	377	SER
1	E	380	VAL
1	E	382	GLU
1	E	384	SER
1	E	387	THR
1	E	388	GLU
1	E	395	LYS
1	E	398	ARG
1	E	404	LYS
1	E	405	GLU
1	E	406	GLU
1	E	408	ILE
1	E	411	ILE
1	E	416	LEU
1	E	419	THR
1	E	423	ASP
1	E	424	THR
1	E	425	THR
1	E	427	THR
2	F	6	ASP
2	F	9	ILE
2	F	11	VAL
2	F	12	LEU
2	F	13	PHE
2	F	14	VAL

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Mol	Chain	Res	Type
2	F	19	THR
2	F	21	ILE
2	F	25	LEU
2	F	26	LEU
2	F	29	ARG
2	F	30	LYS
2	F	31	GLU
2	F	36	VAL
2	F	39	GLU
2	F	42	GLU
2	F	43	LYS
2	F	47	LYS
2	F	52	ILE
2	F	54	ILE
2	F	56	LYS
2	F	57	SER
2	F	58	SER
2	F	59	ILE
2	F	65	LYS
2	F	67	ASN
2	F	68	ASP
2	F	69	ARG
2	F	70	ILE
2	F	71	SER
2	F	77	ILE
2	F	80	LEU
2	F	82	LEU
2	F	83	GLU
2	F	89	SER
2	F	92	LEU
2	F	98	ILE
2	F	99	ILE
2	F	102	LEU
2	F	104	VAL
2	F	109	ILE
2	F	111	LEU
2	F	112	GLN
2	F	113	GLU
2	F	114	SER
2	F	117	GLU
2	F	123	THR
2	F	125	ARG

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Mol	Chain	Res	Type
2	F	128	ASP
2	F	129	LEU
2	F	131	VAL
2	F	132	GLU
2	F	138	TRP
2	F	140	ILE
2	F	144	ILE
2	F	148	SER
2	F	155	LYS
2	F	159	THR
2	F	162	VAL
2	F	164	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (62) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	GLN
1	A	18	HIS
1	A	63	ASN
1	A	104	GLN
1	A	121	HIS
1	A	139	GLN
1	A	141	ASN
1	A	173	ASN
1	A	194	ASN
1	A	209	GLN
1	A	234	ASN
1	A	240	ASN
1	A	266	ASN
1	A	315	GLN
1	A	330	GLN
1	A	342	GLN
1	A	354	HIS
1	A	376	GLN
2	B	53	GLN
2	B	112	GLN
2	B	143	ASN
2	B	150	GLN
2	B	157	ASN
1	C	8	GLN
1	C	10	GLN
1	C	18	HIS

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Mol	Chain	Res	Type
1	C	63	ASN
1	C	139	GLN
1	C	141	ASN
1	C	173	ASN
1	C	194	ASN
1	C	209	GLN
1	C	234	ASN
1	C	240	ASN
1	C	266	ASN
1	C	315	GLN
1	C	330	GLN
1	C	342	GLN
1	C	354	HIS
1	C	376	GLN
2	D	112	GLN
2	D	150	GLN
2	D	157	ASN
1	E	10	GLN
1	E	18	HIS
1	E	63	ASN
1	E	139	GLN
1	E	141	ASN
1	E	173	ASN
1	E	194	ASN
1	E	209	GLN
1	E	234	ASN
1	E	240	ASN
1	E	266	ASN
1	E	315	GLN
1	E	330	GLN
1	E	342	GLN
1	E	354	HIS
1	E	376	GLN
2	F	112	GLN
2	F	143	ASN
2	F	150	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 ⓘ

45 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	$\# Z > 2$
3	NAG	G	1	3,1	14,14,15	0.70	0	17,19,21	1.32	2 (11%)
3	NAG	G	2	3	14,14,15	0.71	0	17,19,21	1.73	2 (11%)
3	BMA	G	3	3	11,11,12	1.11	0	15,15,17	0.72	0
3	NAG	H	1	3,1	14,14,15	0.65	0	17,19,21	1.16	2 (11%)
3	NAG	H	2	3	14,14,15	0.63	0	17,19,21	0.83	1 (5%)
3	BMA	H	3	3	11,11,12	0.90	0	15,15,17	0.40	0
3	NAG	I	1	3,1	14,14,15	0.70	1 (7%)	17,19,21	1.12	2 (11%)
3	NAG	I	2	3	14,14,15	0.64	0	17,19,21	1.12	2 (11%)
3	BMA	I	3	3	11,11,12	0.96	1 (9%)	15,15,17	0.74	1 (6%)
3	NAG	J	1	3,1	14,14,15	0.75	0	17,19,21	1.18	1 (5%)
3	NAG	J	2	3	14,14,15	0.54	0	17,19,21	0.83	1 (5%)
3	BMA	J	3	3	11,11,12	0.81	0	15,15,17	0.39	0
4	NAG	K	1	2,4	14,14,15	0.52	0	17,19,21	1.31	3 (17%)
4	NDG	K	2	4	14,14,15	0.98	1 (7%)	17,19,21	1.49	2 (11%)
4	MAN	K	3	4	11,11,12	0.83	0	15,15,17	0.35	0
3	NAG	L	1	3,1	14,14,15	0.58	0	17,19,21	1.66	3 (17%)
3	NAG	L	2	3	14,14,15	0.67	0	17,19,21	0.86	1 (5%)
3	BMA	L	3	3	11,11,12	0.80	0	15,15,17	0.47	0
3	NAG	M	1	3,1	14,14,15	0.78	0	17,19,21	1.26	2 (11%)
3	NAG	M	2	3	14,14,15	0.68	0	17,19,21	0.92	1 (5%)
3	BMA	M	3	3	11,11,12	0.88	0	15,15,17	0.60	0
5	NAG	N	1	5,1	14,14,15	0.98	0	17,19,21	0.97	1 (5%)
5	NDG	N	2	5	14,14,15	0.96	1 (7%)	17,19,21	0.92	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	BMA	N	3	5	11,11,12	0.96	0	15,15,17	0.58	0
3	NAG	O	1	3,1	14,14,15	0.76	0	17,19,21	1.40	2 (11%)
3	NAG	O	2	3	14,14,15	0.62	0	17,19,21	1.10	1 (5%)
3	BMA	O	3	3	11,11,12	0.63	0	15,15,17	0.76	1 (6%)
4	NAG	P	1	2,4	14,14,15	0.81	0	17,19,21	1.24	3 (17%)
4	NDG	P	2	4	14,14,15	1.07	1 (7%)	17,19,21	1.26	2 (11%)
4	MAN	P	3	4	11,11,12	0.89	0	15,15,17	0.40	0
3	NAG	Q	1	3,1	14,14,15	0.90	1 (7%)	17,19,21	1.31	3 (17%)
3	NAG	Q	2	3	14,14,15	0.61	0	17,19,21	1.01	1 (5%)
3	BMA	Q	3	3	11,11,12	0.91	0	15,15,17	0.35	0
3	NAG	R	1	3,1	14,14,15	0.63	0	17,19,21	0.93	1 (5%)
3	NAG	R	2	3	14,14,15	0.90	0	17,19,21	0.78	0
3	BMA	R	3	3	11,11,12	0.82	0	15,15,17	0.50	0
3	NAG	S	1	3,1	14,14,15	0.53	0	17,19,21	0.90	0
3	NAG	S	2	3	14,14,15	0.78	0	17,19,21	1.34	3 (17%)
3	BMA	S	3	3	11,11,12	0.92	1 (9%)	15,15,17	0.62	0
3	NAG	T	1	3,1	14,14,15	0.57	0	17,19,21	1.02	2 (11%)
3	NAG	T	2	3	14,14,15	0.54	0	17,19,21	0.74	0
3	BMA	T	3	3	11,11,12	0.93	1 (9%)	15,15,17	0.44	0
4	NAG	U	1	2,4	14,14,15	0.49	0	17,19,21	1.45	2 (11%)
4	NDG	U	2	4	14,14,15	1.13	1 (7%)	17,19,21	1.91	5 (29%)
4	MAN	U	3	4	11,11,12	0.89	0	15,15,17	0.59	0

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
3	NAG	G	1	3,1	1/1/5/7	1/6/23/26	0/1/1/1
3	NAG	G	2	3	-	0/6/23/26	0/1/1/1
3	BMA	G	3	3	-	1/2/19/22	0/1/1/1
3	NAG	H	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	H	2	3	-	1/6/23/26	0/1/1/1
3	BMA	H	3	3	-	2/2/19/22	0/1/1/1
3	NAG	I	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	I	2	3	-	2/6/23/26	0/1/1/1
3	BMA	I	3	3	-	2/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	J	1	3,1	-	1/6/23/26	0/1/1/1
3	NAG	J	2	3	-	2/6/23/26	0/1/1/1
3	BMA	J	3	3	-	2/2/19/22	0/1/1/1
4	NAG	K	1	2,4	-	1/6/23/26	0/1/1/1
4	NDG	K	2	4	-	3/6/23/26	0/1/1/1
4	MAN	K	3	4	-	2/2/19/22	0/1/1/1
3	NAG	L	1	3,1	1/1/5/7	1/6/23/26	0/1/1/1
3	NAG	L	2	3	-	2/6/23/26	0/1/1/1
3	BMA	L	3	3	-	0/2/19/22	0/1/1/1
3	NAG	M	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	M	2	3	-	0/6/23/26	0/1/1/1
3	BMA	M	3	3	-	2/2/19/22	0/1/1/1
5	NAG	N	1	5,1	-	0/6/23/26	0/1/1/1
5	NDG	N	2	5	-	1/6/23/26	0/1/1/1
5	BMA	N	3	5	-	0/2/19/22	0/1/1/1
3	NAG	O	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	O	2	3	-	0/6/23/26	0/1/1/1
3	BMA	O	3	3	-	2/2/19/22	0/1/1/1
4	NAG	P	1	2,4	-	0/6/23/26	0/1/1/1
4	NDG	P	2	4	-	0/6/23/26	0/1/1/1
4	MAN	P	3	4	-	2/2/19/22	0/1/1/1
3	NAG	Q	1	3,1	1/1/5/7	0/6/23/26	0/1/1/1
3	NAG	Q	2	3	-	2/6/23/26	0/1/1/1
3	BMA	Q	3	3	-	1/2/19/22	0/1/1/1
3	NAG	R	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	R	2	3	-	2/6/23/26	0/1/1/1
3	BMA	R	3	3	-	2/2/19/22	0/1/1/1
3	NAG	S	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	S	2	3	-	2/6/23/26	0/1/1/1
3	BMA	S	3	3	-	2/2/19/22	0/1/1/1
3	NAG	T	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	T	2	3	-	0/6/23/26	0/1/1/1
3	BMA	T	3	3	-	2/2/19/22	0/1/1/1
4	NAG	U	1	2,4	-	0/6/23/26	0/1/1/1
4	NDG	U	2	4	-	2/6/23/26	0/1/1/1
4	MAN	U	3	4	-	0/2/19/22	0/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	U	2	NDG	C1-C2	3.34	1.56	1.52
4	K	2	NDG	C1-C2	3.12	1.56	1.52
4	P	2	NDG	C1-C2	2.76	1.56	1.52
3	Q	1	NAG	C1-C2	2.65	1.56	1.52
3	I	3	BMA	C4-C5	2.53	1.58	1.53
3	T	3	BMA	C2-C3	2.25	1.55	1.52
5	N	2	NDG	O5-C5	2.22	1.47	1.43
3	S	3	BMA	C2-C3	2.18	1.55	1.52
3	I	1	NAG	C1-C2	2.01	1.55	1.52

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	2	NAG	C4-C3-C2	-5.37	103.15	111.02
4	U	2	NDG	C3-C4-C5	-5.24	100.73	110.23
3	L	1	NAG	C4-C3-C2	-5.01	103.67	111.02
4	K	2	NDG	C3-C4-C5	-4.39	102.27	110.23
3	O	1	NAG	C2-N2-C7	-3.76	117.86	122.90
4	U	1	NAG	C3-C4-C5	-3.49	103.90	110.23
3	O	2	NAG	C2-N2-C7	-3.46	118.27	122.90
3	M	1	NAG	C2-N2-C7	-3.41	118.33	122.90
3	G	2	NAG	C2-N2-C7	-3.35	118.41	122.90
4	P	1	NAG	C2-N2-C7	-3.10	118.75	122.90
3	O	1	NAG	O5-C1-C2	-3.07	106.55	111.29
3	S	2	NAG	C2-N2-C7	-2.90	119.02	122.90
3	G	1	NAG	C2-N2-C7	-2.89	119.03	122.90
3	R	1	NAG	C2-N2-C7	-2.89	119.03	122.90
3	L	1	NAG	C1-O5-C5	2.86	116.02	112.19
3	L	1	NAG	C2-N2-C7	-2.83	119.10	122.90
4	U	2	NDG	C6-C5-C4	2.83	119.96	113.02
3	G	1	NAG	C4-C3-C2	-2.76	106.97	111.02
4	P	1	NAG	C3-C4-C5	-2.72	105.31	110.23
3	M	1	NAG	O5-C1-C2	-2.68	107.14	111.29
4	U	2	NDG	C4-C3-C2	-2.66	107.12	111.02
4	U	1	NAG	C6-C5-C4	2.61	119.42	113.02
4	K	1	NAG	C3-C4-C5	-2.60	105.51	110.23
4	P	2	NDG	C4-C3-C2	-2.59	107.23	111.02
3	L	2	NAG	C2-N2-C7	-2.56	119.47	122.90
4	K	1	NAG	C2-N2-C7	-2.53	119.50	122.90
3	M	2	NAG	C2-N2-C7	-2.53	119.51	122.90
3	J	1	NAG	C2-N2-C7	-2.52	119.52	122.90
3	T	1	NAG	C2-N2-C7	-2.51	119.54	122.90
3	Q	1	NAG	C1-C2-N2	2.48	114.34	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	N	1	NAG	C2-N2-C7	-2.48	119.58	122.90
3	I	2	NAG	C2-N2-C7	-2.47	119.58	122.90
3	I	1	NAG	C2-N2-C7	-2.47	119.60	122.90
4	P	2	NDG	C2-N2-C7	-2.42	119.66	122.90
3	H	1	NAG	C2-N2-C7	-2.41	119.67	122.90
4	K	2	NDG	C6-C5-C4	2.41	118.93	113.02
3	H	1	NAG	O5-C5-C6	-2.36	103.06	107.66
3	I	1	NAG	C1-C2-N2	2.35	114.14	110.43
3	S	2	NAG	C3-C4-C5	2.33	114.45	110.23
3	Q	1	NAG	C2-N2-C7	-2.31	119.80	122.90
3	Q	2	NAG	C2-N2-C7	-2.26	119.87	122.90
3	T	1	NAG	C4-C3-C2	-2.26	107.71	111.02
3	H	2	NAG	C2-N2-C7	-2.23	119.92	122.90
4	U	2	NDG	O4-C4-C5	2.20	114.75	109.32
3	I	2	NAG	C3-C4-C5	2.19	114.21	110.23
4	U	2	NDG	C1-C2-N2	2.19	113.88	110.43
3	J	2	NAG	C2-N2-C7	-2.14	120.03	122.90
3	O	3	BMA	C2-C3-C4	-2.13	107.11	110.86
3	S	2	NAG	O5-C1-C2	-2.13	108.00	111.29
4	P	1	NAG	C1-C2-N2	-2.10	107.12	110.43
3	Q	1	NAG	O7-C7-C8	-2.09	118.34	122.05
4	K	1	NAG	C1-C2-N2	-2.08	107.15	110.43
3	I	3	BMA	C3-C4-C5	2.02	113.89	110.23

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	G	1	NAG	C1
3	L	1	NAG	C1
3	Q	1	NAG	C1

All (57) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	K	2	NDG	C3-C2-N2-C7
4	U	2	NDG	C3-C2-N2-C7
3	R	3	BMA	O5-C5-C6-O6
3	L	2	NAG	O5-C5-C6-O6
3	T	3	BMA	O5-C5-C6-O6
3	I	3	BMA	O5-C5-C6-O6
3	M	3	BMA	O5-C5-C6-O6
3	I	2	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	S	3	BMA	O5-C5-C6-O6
4	K	3	MAN	O5-C5-C6-O6
4	P	3	MAN	O5-C5-C6-O6
3	L	2	NAG	C4-C5-C6-O6
3	R	3	BMA	C4-C5-C6-O6
3	Q	2	NAG	O5-C5-C6-O6
4	K	2	NDG	C4-C5-C6-O6
3	R	2	NAG	O5-C5-C6-O6
3	M	3	BMA	C4-C5-C6-O6
3	Q	2	NAG	C4-C5-C6-O6
3	R	1	NAG	O5-C5-C6-O6
3	I	2	NAG	C4-C5-C6-O6
3	R	2	NAG	C4-C5-C6-O6
3	S	3	BMA	C4-C5-C6-O6
3	R	1	NAG	C4-C5-C6-O6
3	T	3	BMA	C4-C5-C6-O6
3	I	3	BMA	C4-C5-C6-O6
3	O	3	BMA	O5-C5-C6-O6
4	K	2	NDG	O5-C5-C6-O6
4	K	3	MAN	C4-C5-C6-O6
3	L	1	NAG	O5-C5-C6-O6
3	O	3	BMA	C4-C5-C6-O6
3	H	1	NAG	O5-C5-C6-O6
3	M	1	NAG	O5-C5-C6-O6
3	S	1	NAG	O5-C5-C6-O6
3	H	3	BMA	C4-C5-C6-O6
3	H	1	NAG	C4-C5-C6-O6
3	M	1	NAG	C4-C5-C6-O6
3	J	3	BMA	C4-C5-C6-O6
3	J	3	BMA	O5-C5-C6-O6
3	S	1	NAG	C4-C5-C6-O6
3	Q	3	BMA	O5-C5-C6-O6
3	H	3	BMA	O5-C5-C6-O6
3	S	2	NAG	C4-C5-C6-O6
3	S	2	NAG	O5-C5-C6-O6
3	G	3	BMA	O5-C5-C6-O6
3	G	1	NAG	O5-C5-C6-O6
4	P	3	MAN	C4-C5-C6-O6
3	H	2	NAG	O5-C5-C6-O6
3	I	1	NAG	C4-C5-C6-O6
3	J	2	NAG	C4-C5-C6-O6
3	I	1	NAG	O5-C5-C6-O6

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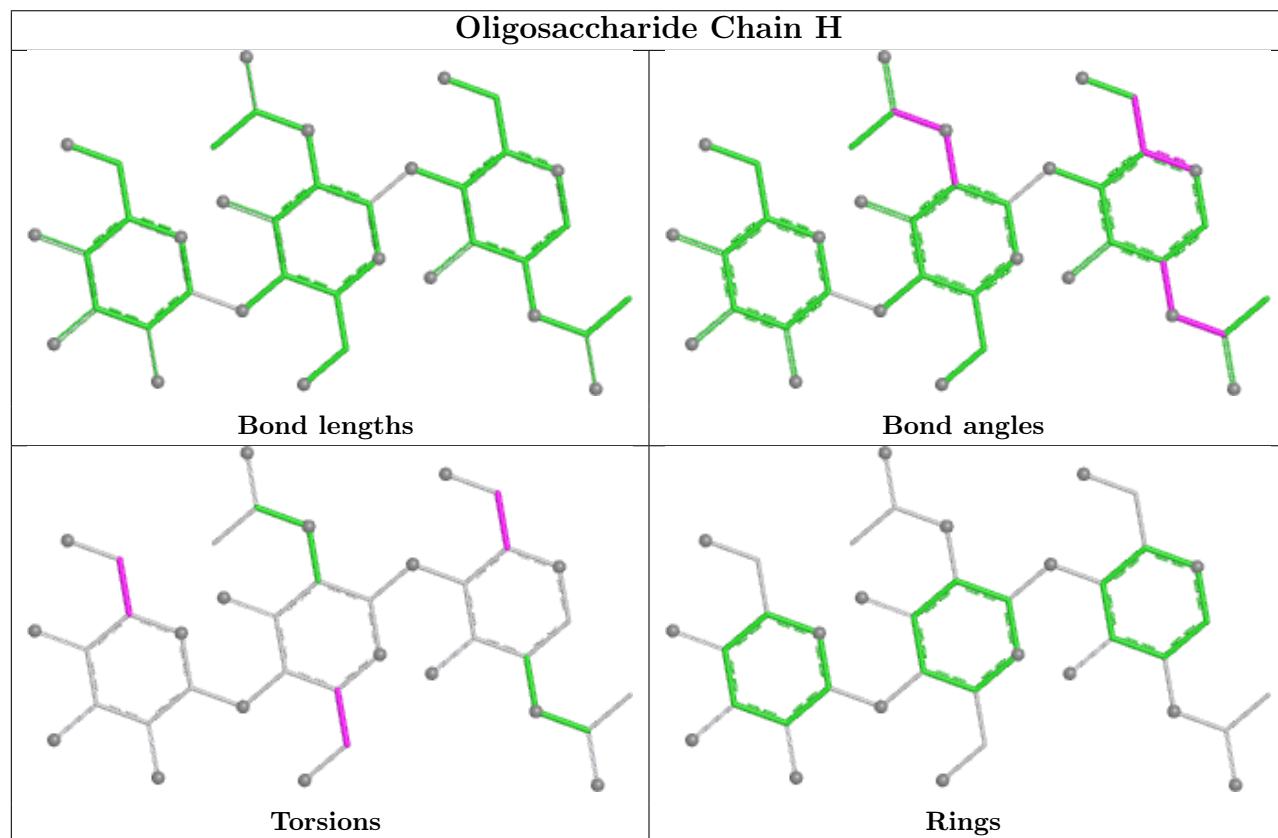
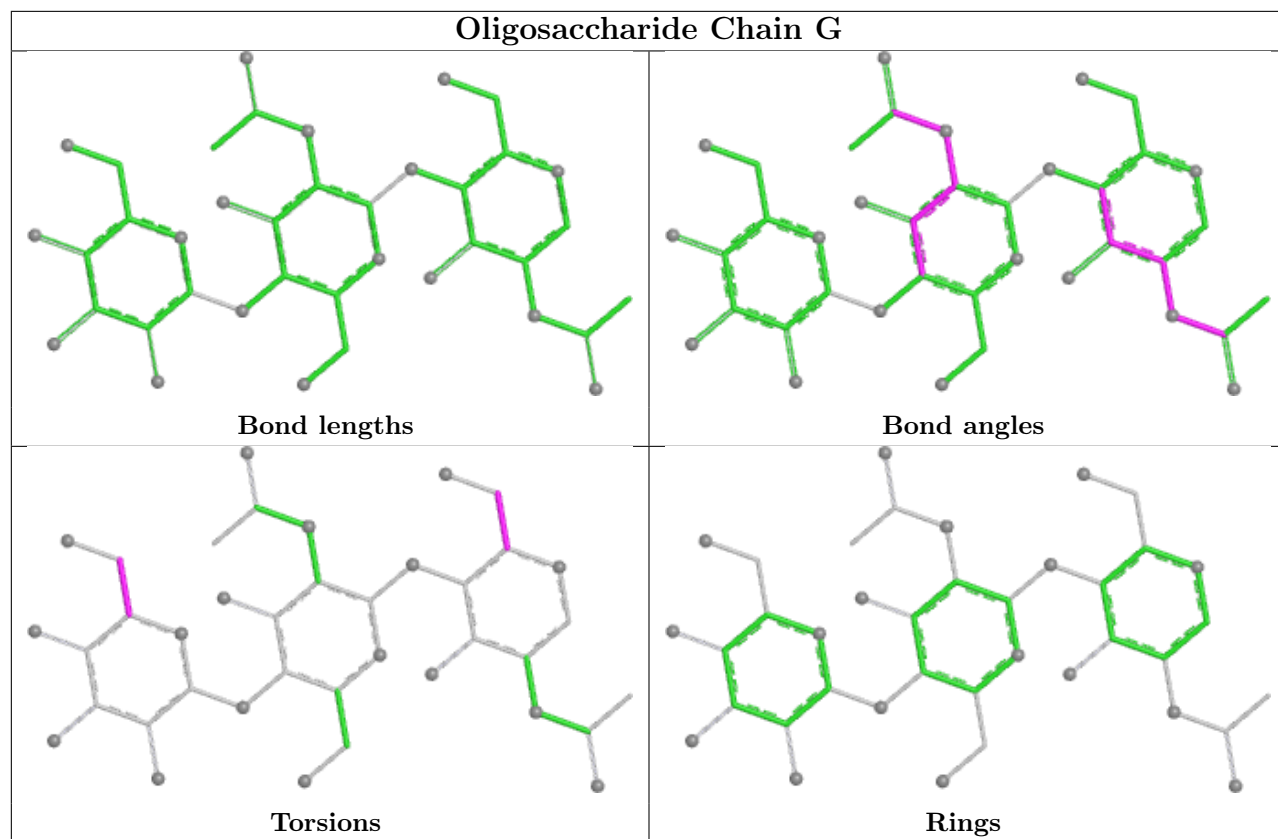
Mol	Chain	Res	Type	Atoms
4	U	2	NDG	C4-C5-C6-O6
4	K	1	NAG	C4-C5-C6-O6
3	T	1	NAG	C4-C5-C6-O6
3	T	1	NAG	O5-C5-C6-O6
3	J	1	NAG	C4-C5-C6-O6
3	J	2	NAG	O5-C5-C6-O6
5	N	2	NDG	C1-C2-N2-C7

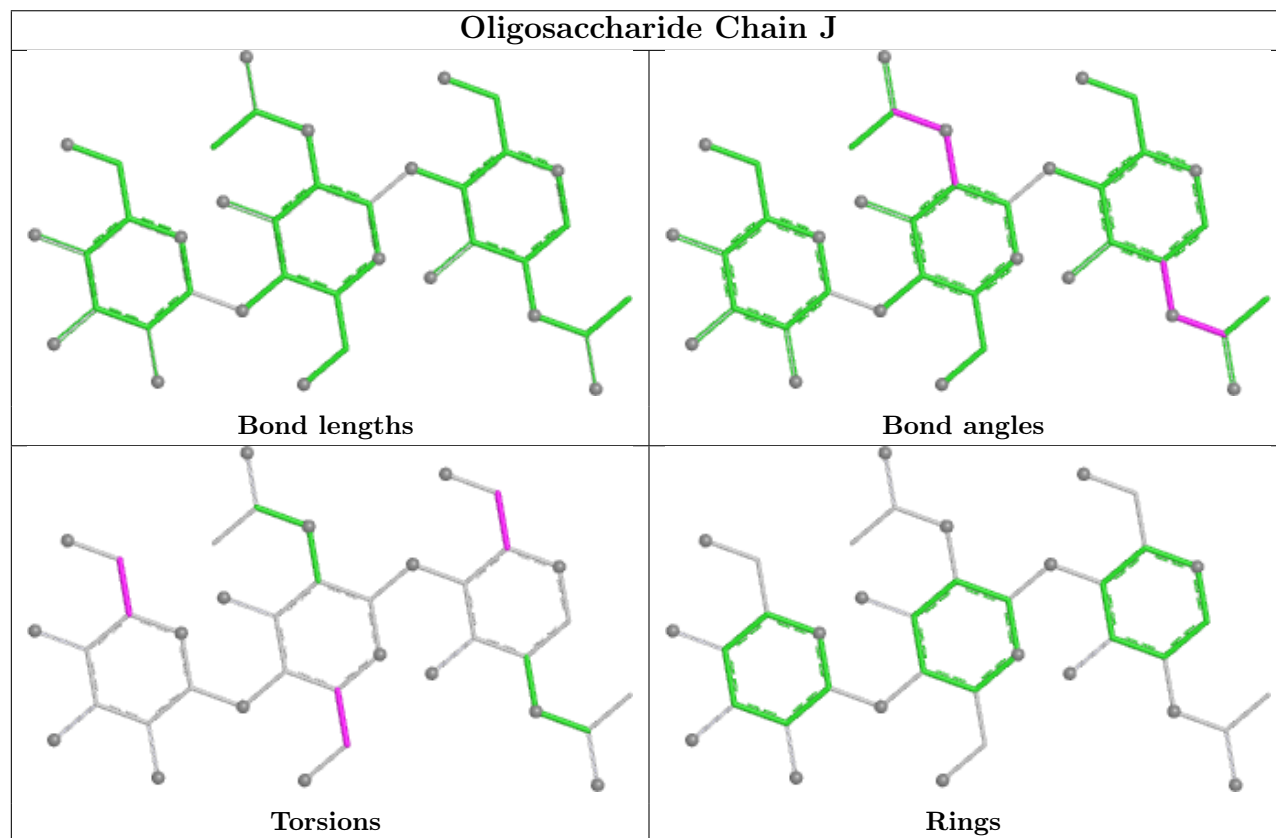
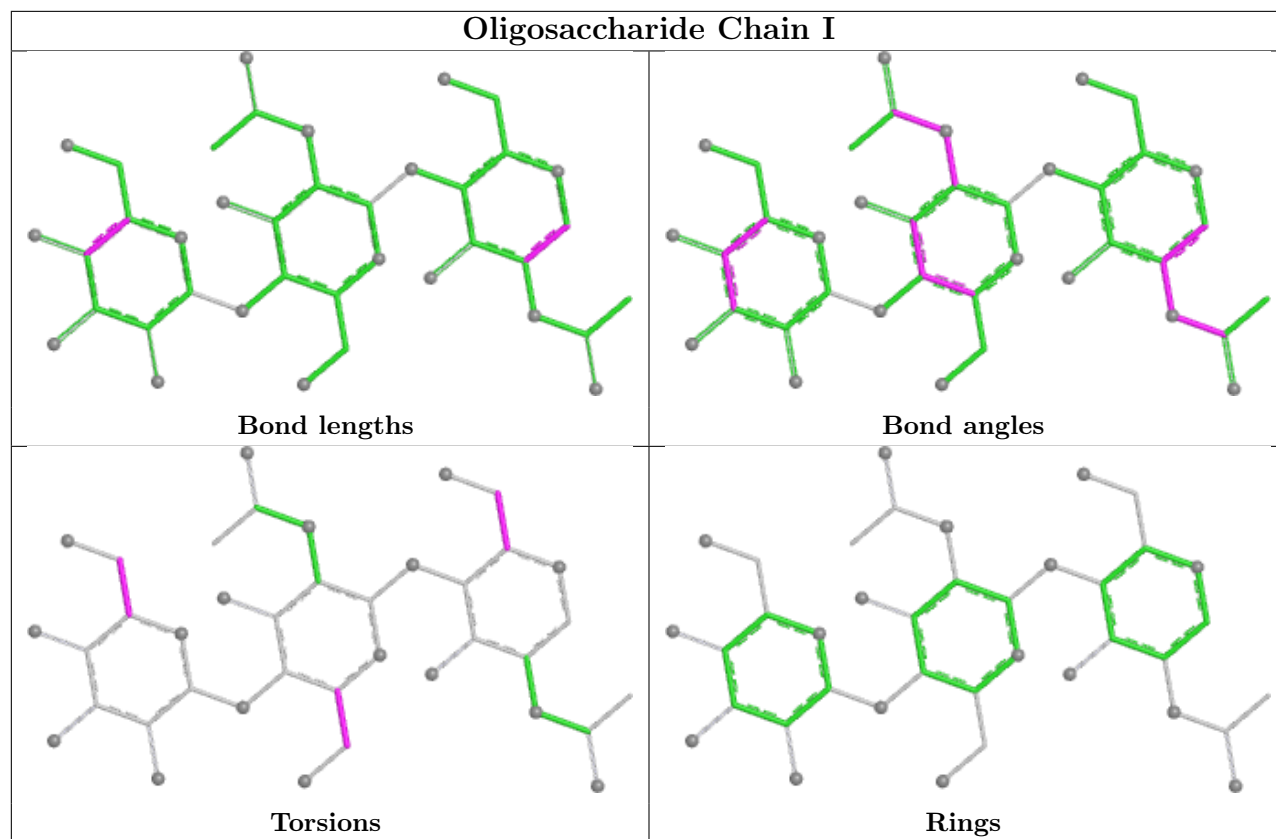
There are no ring outliers.

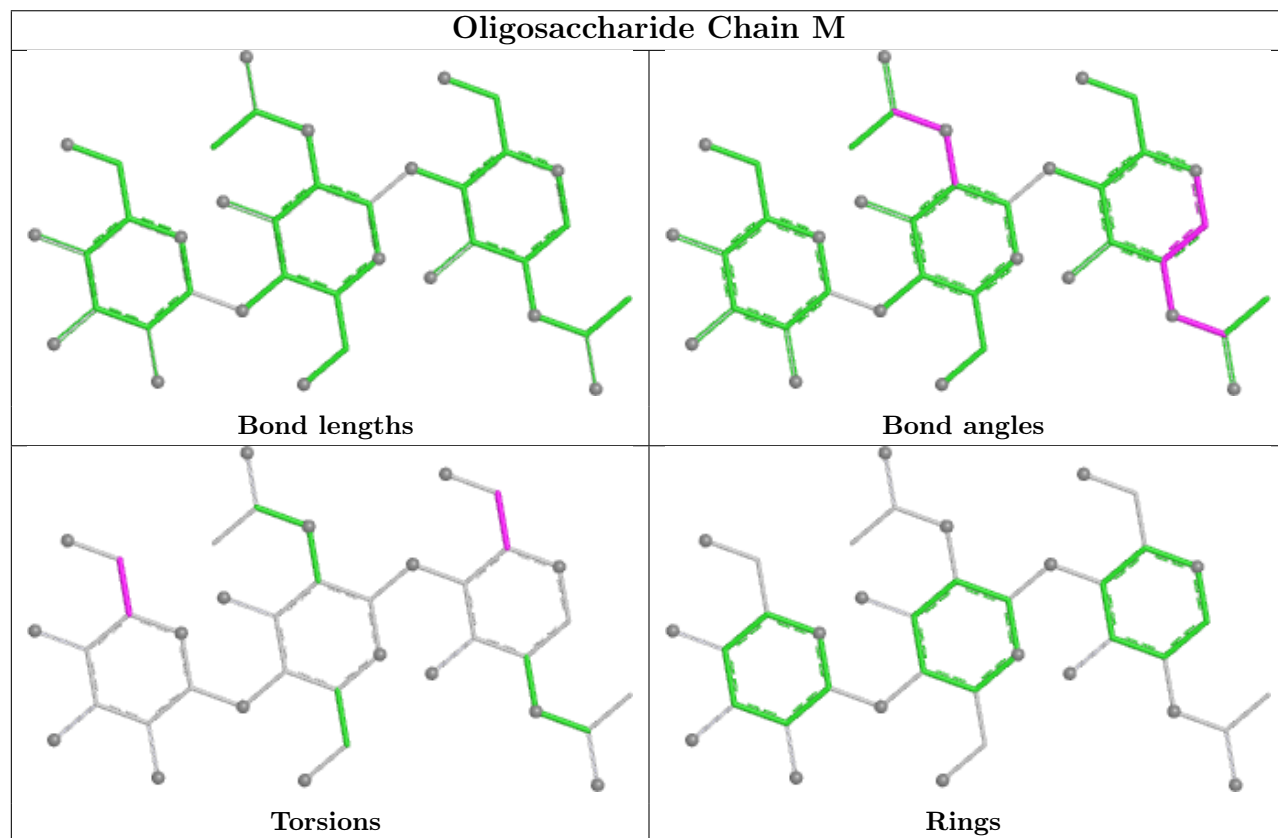
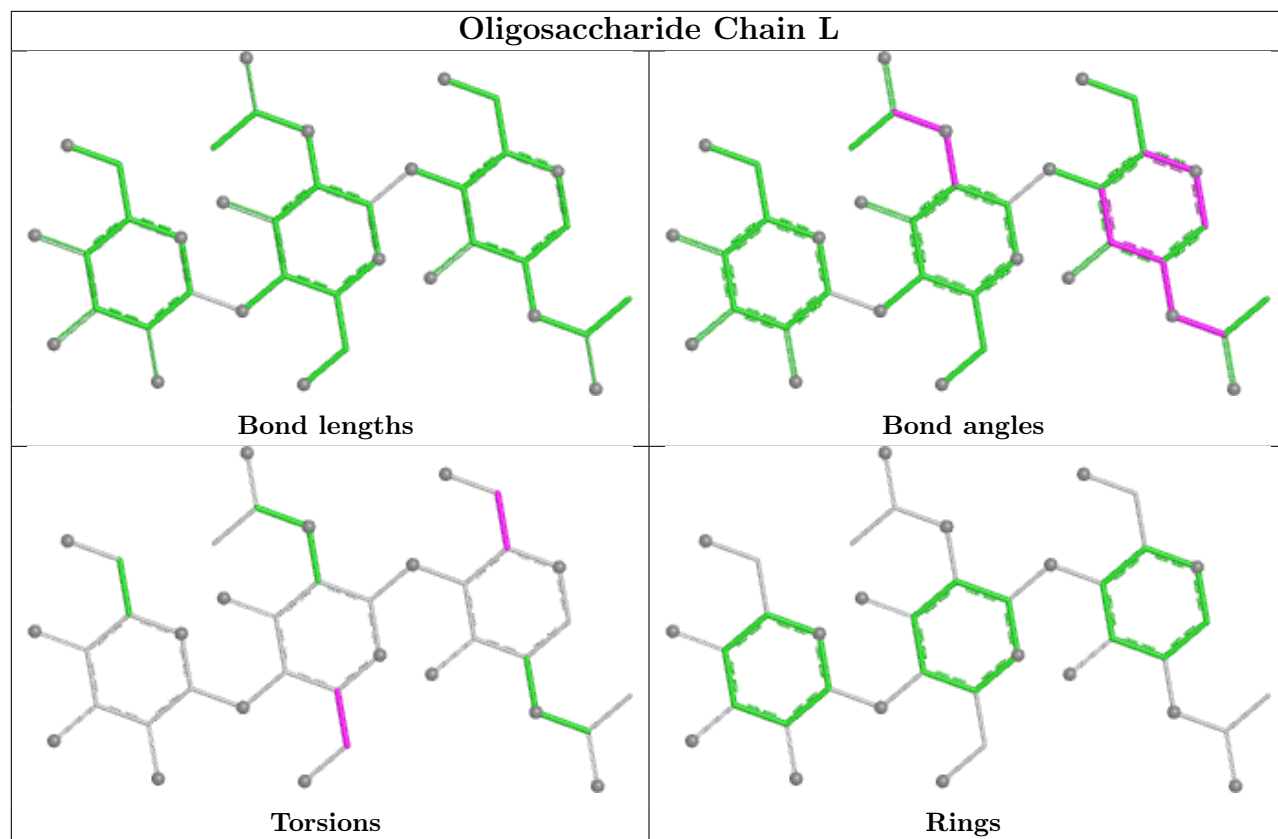
18 monomers are involved in 38 short contacts:

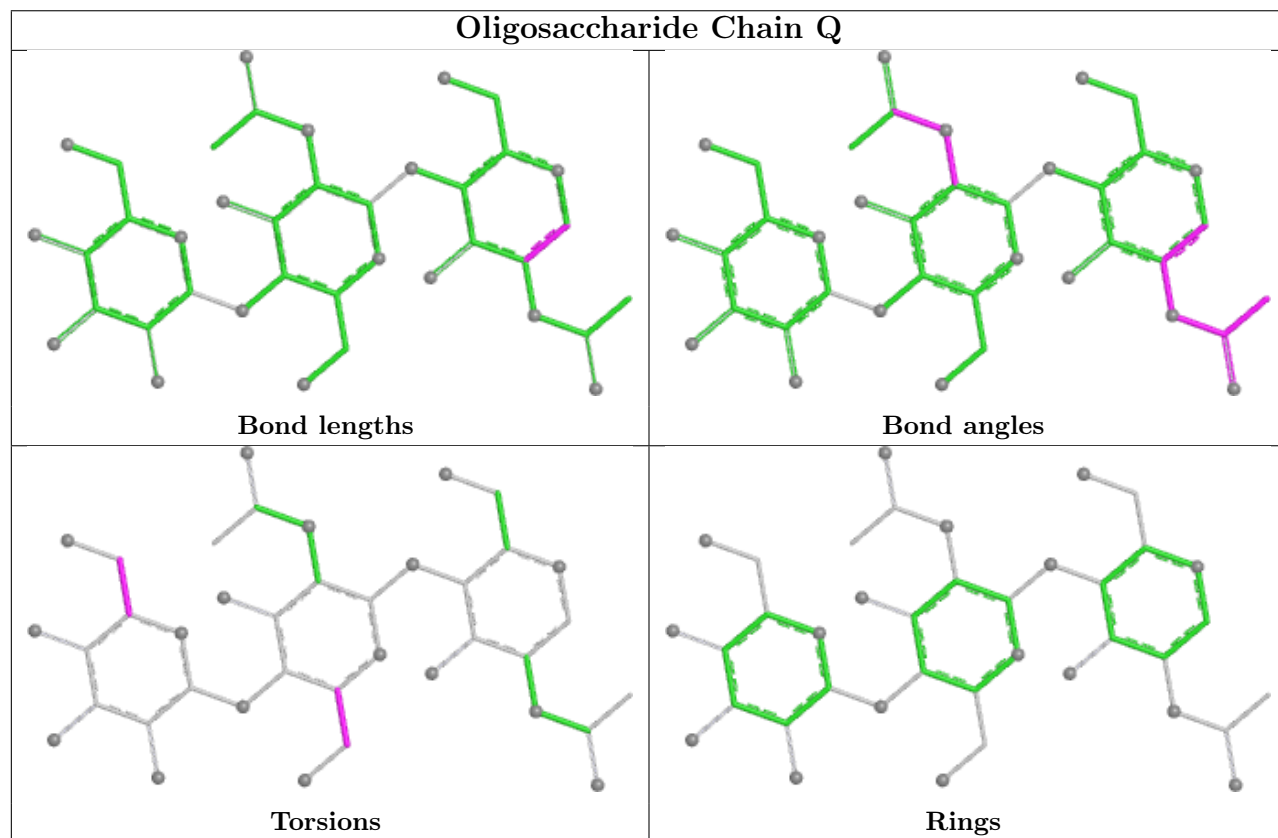
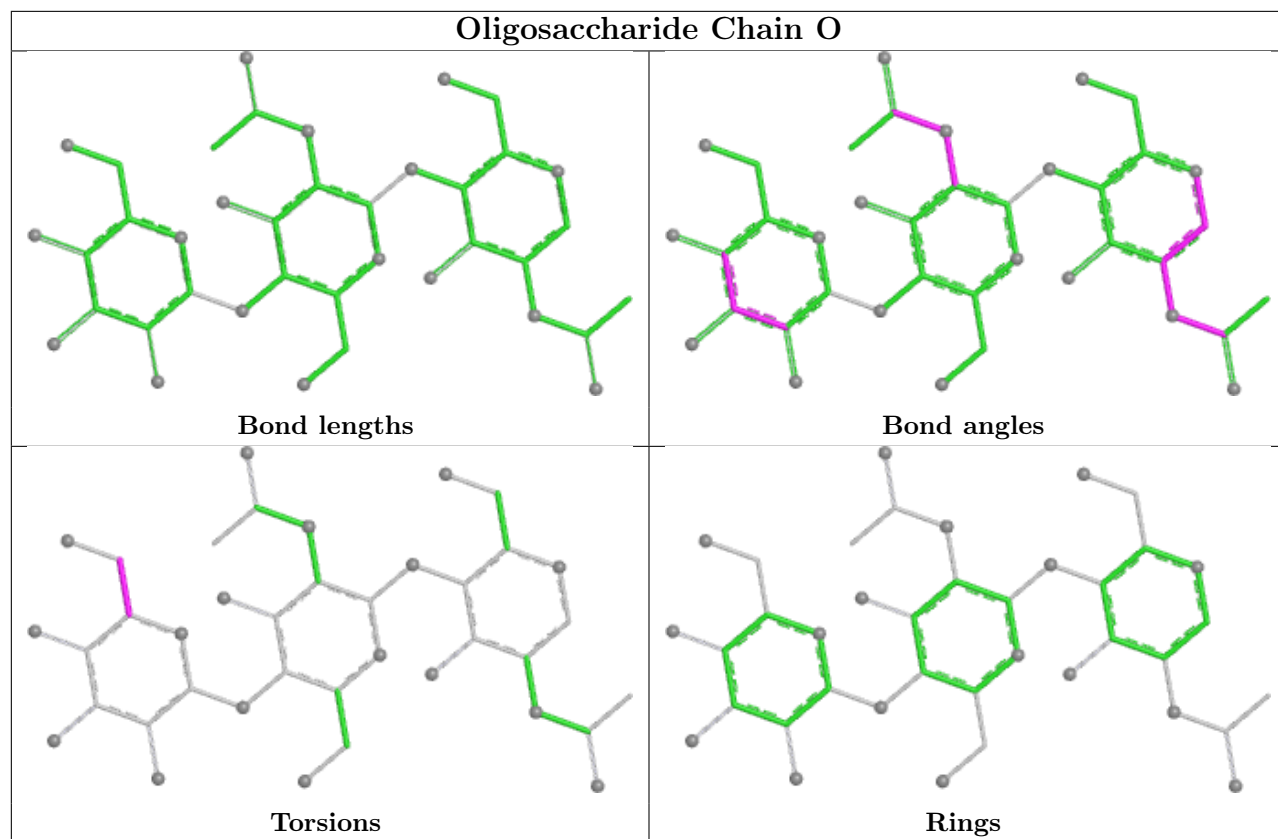
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	U	3	MAN	1	0
3	Q	2	NAG	6	0
4	K	3	MAN	6	0
3	S	2	NAG	1	0
3	L	2	NAG	1	0
3	G	2	NAG	1	0
4	P	3	MAN	1	0
3	T	1	NAG	2	0
3	L	1	NAG	2	0
3	G	1	NAG	2	0
3	T	2	NAG	2	0
4	K	2	NDG	10	0
3	R	2	NAG	1	0
4	P	2	NDG	4	0
4	U	2	NDG	8	0
4	P	1	NAG	1	0
4	U	1	NAG	3	0
3	R	1	NAG	1	0

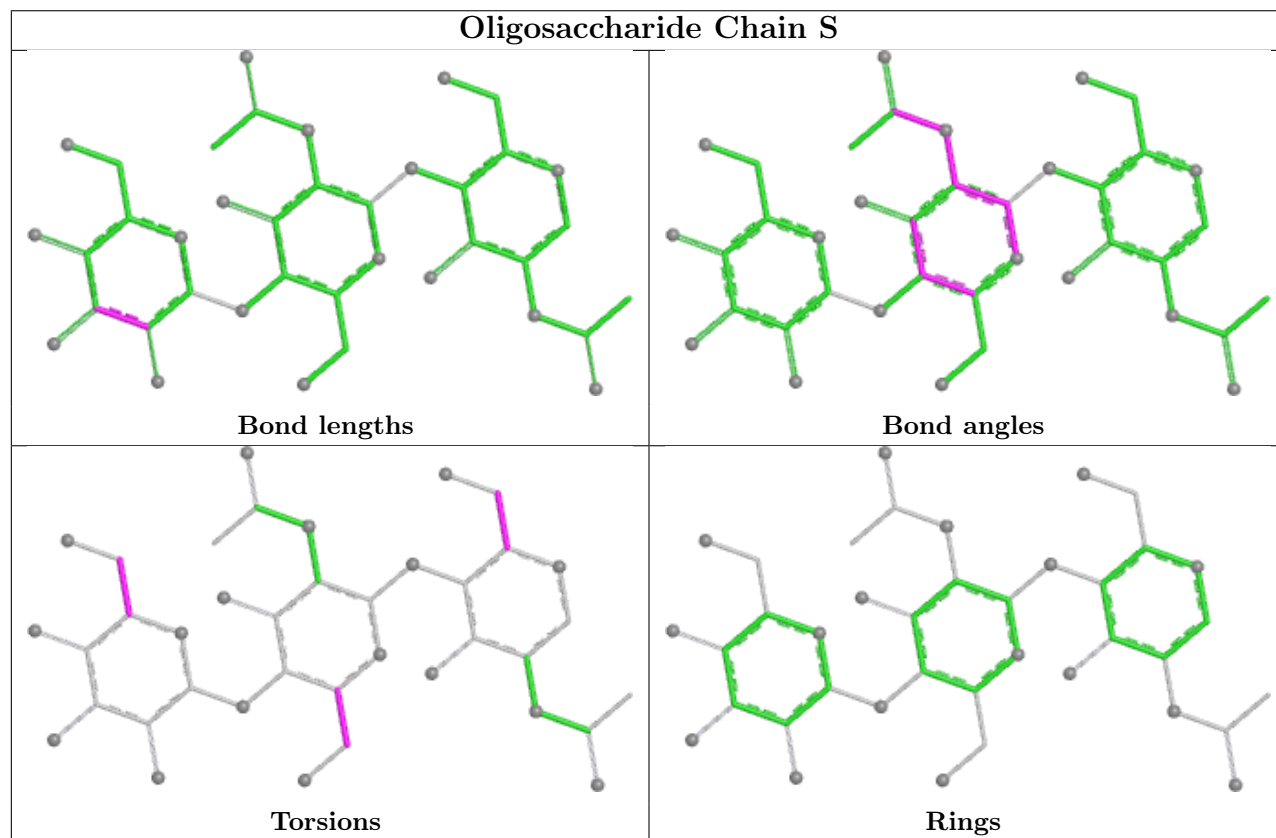
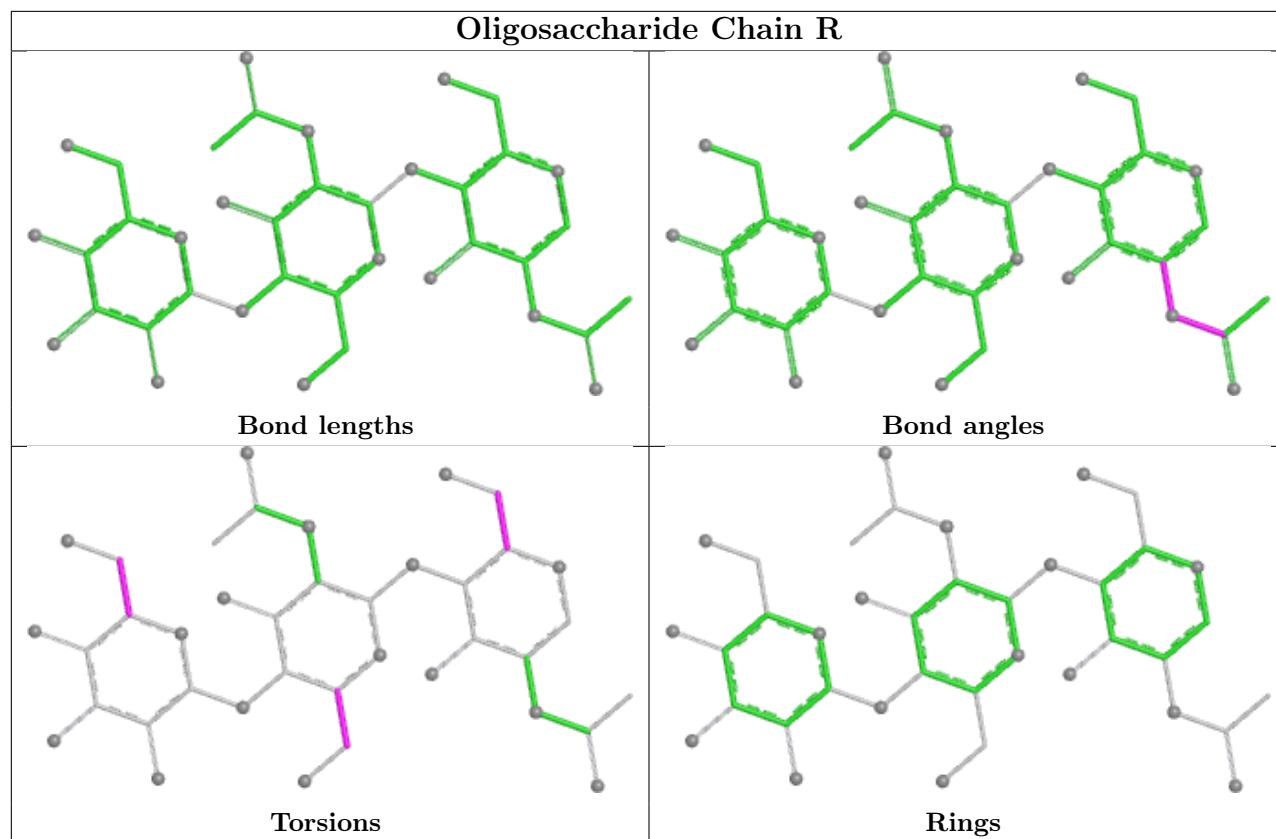
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

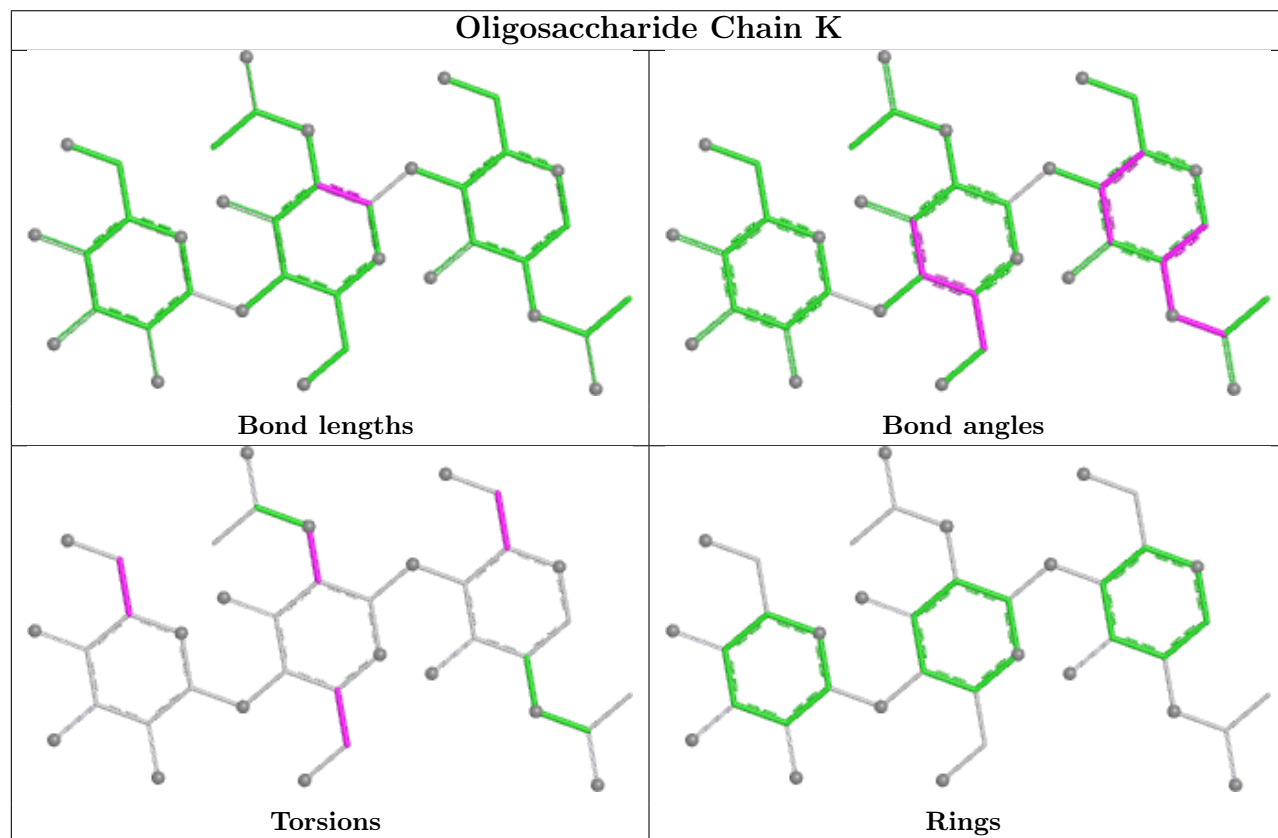
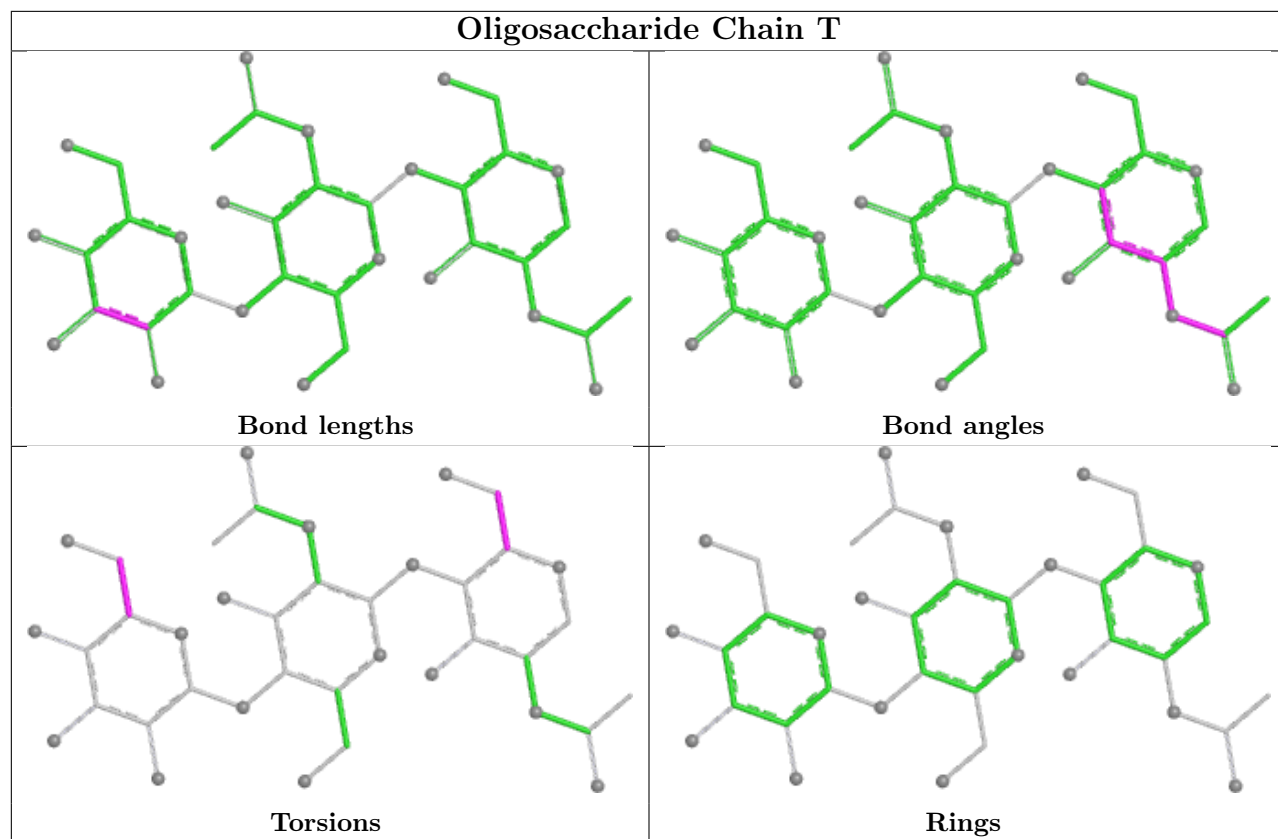


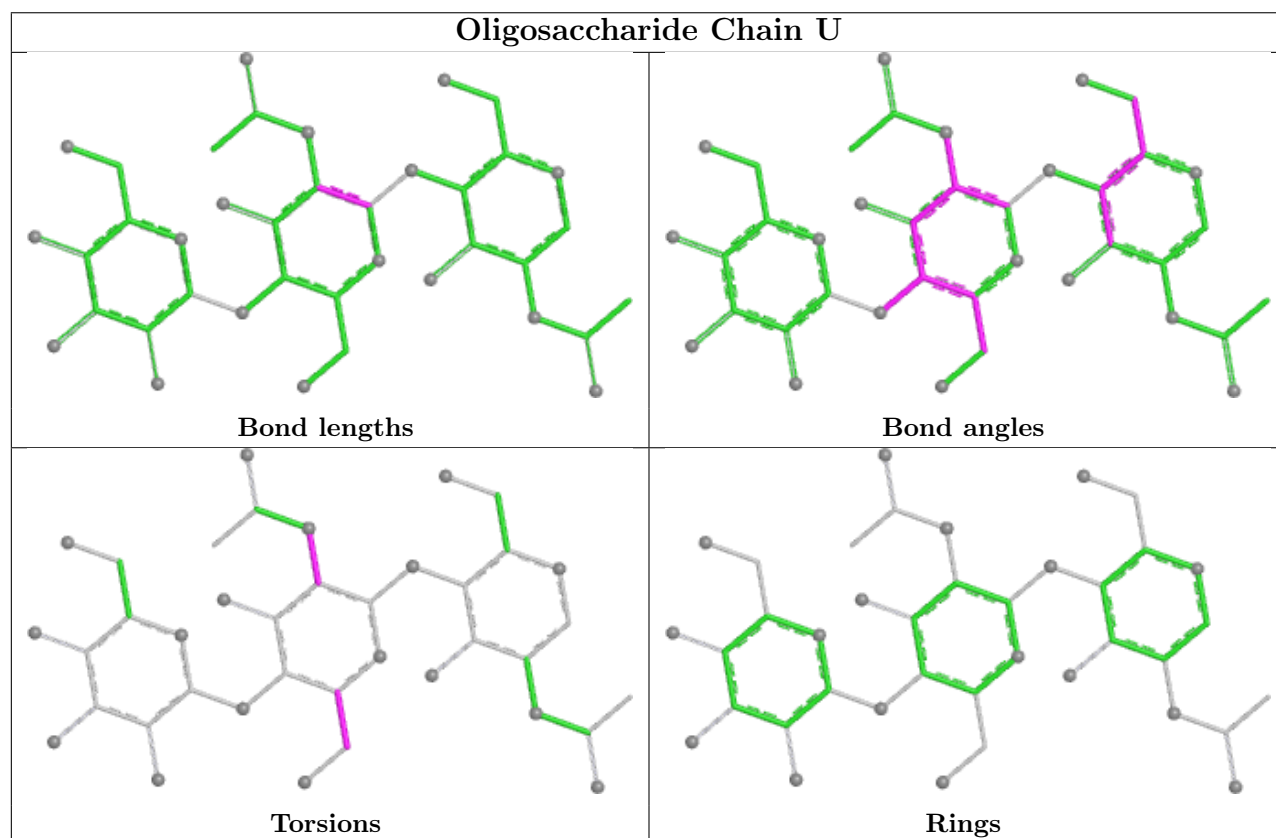
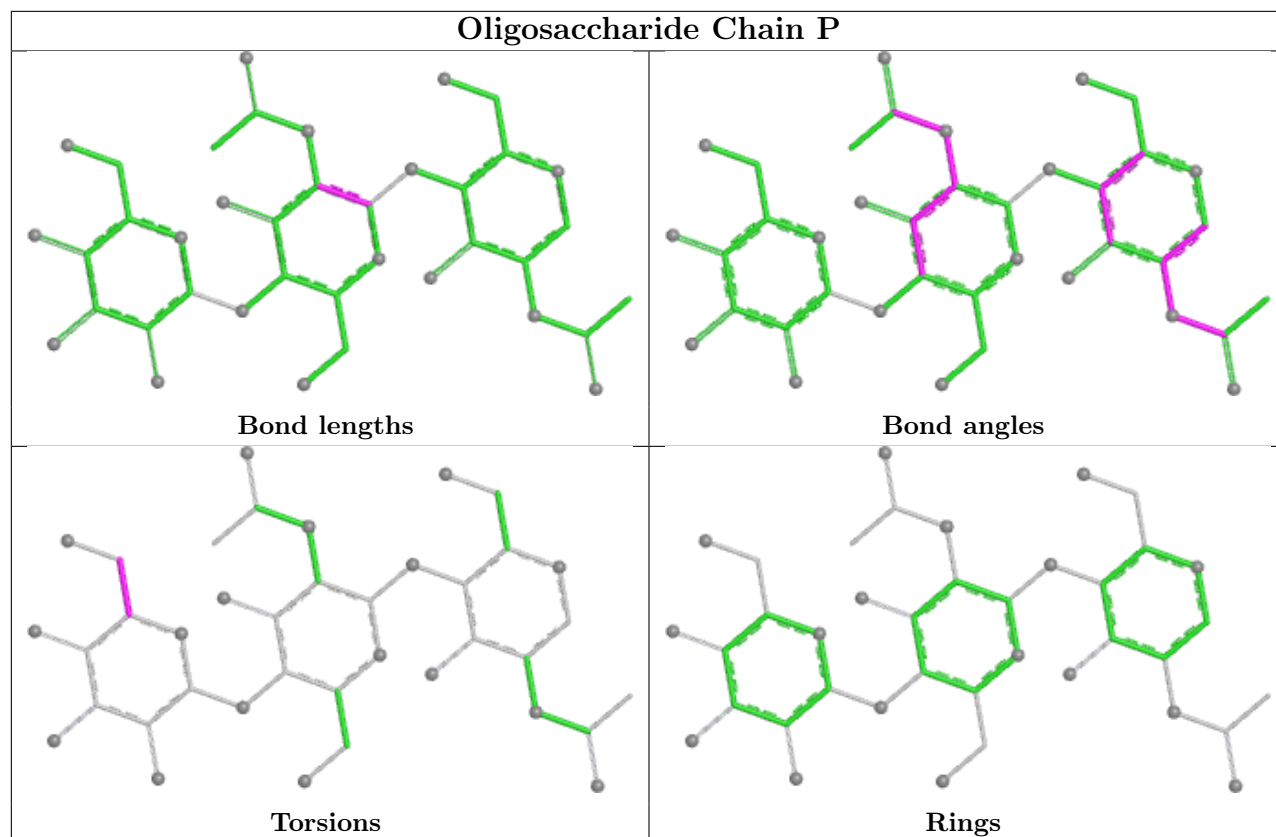


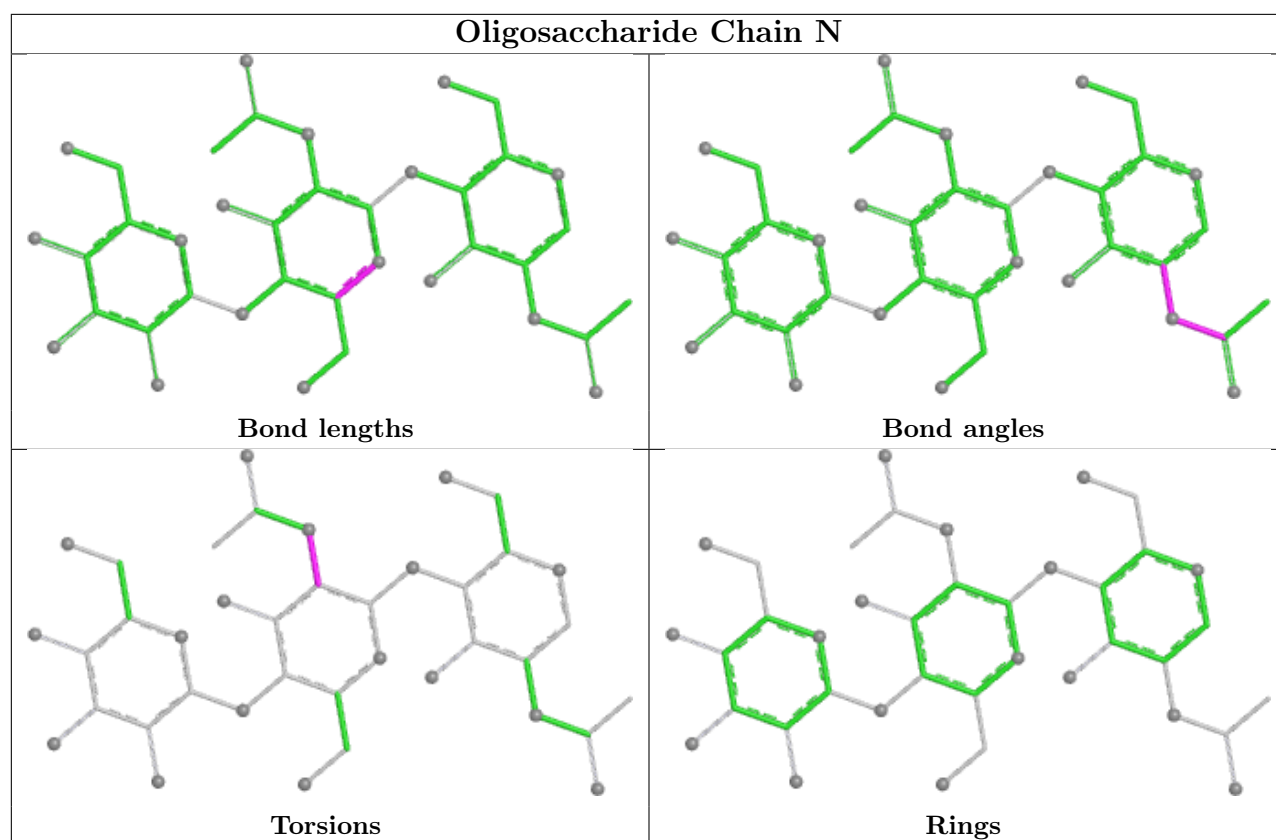












5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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.