



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 15, 2024 – 04:17 PM EST

PDB ID : 1YPZ
Title : Immune receptor
Authors : Adams, E.J.; Garcia, K.C.
Deposited on : 2005-01-31
Resolution : 3.40 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

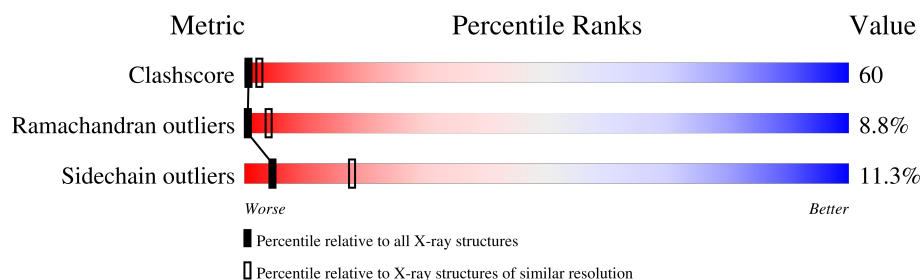
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 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	180529	1172 (3.46-3.34)
Ramachandran outliers	177936	1172 (3.46-3.34)
Sidechain outliers	177891	1172 (3.46-3.34)

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	260	27% 58% 15%
1	C	260	22% 68% 9% .
2	B	102	37% 53% 10%
2	D	102	24% 63% 13% .
3	E	207	31% 57% 11%
3	G	207	42% 47% 10% .
4	F	230	28% 55% 16% .
4	H	230	40% 49% 10% .

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Mol	Chain	Length	Quality of chain
5	I	3	 33%67%
5	L	3	 67%33%
6	J	2	 100%
6	K	2	 50%50%
7	M	3	 67%33%

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
5	NAG	I	1	X	-	-	-
5	NAG	L	1	X	-	X	-
6	NAG	J	1	X	-	X	-
6	NAG	K	1	-	-	X	-
7	NAG	M	1	X	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 12984 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 H2-T22 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	260	Total	C	N	O	S	0	0	0
			2106	1330	363	402	11			
1	C	260	Total	C	N	O	S	0	0	0
			2106	1330	363	402	11			

- Molecule 2 is a protein called Beta-2-microglobulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	102	Total	C	N	O	S	0	0	0
			849	540	143	163	3			
2	D	102	Total	C	N	O	S	0	0	0
			849	540	143	163	3			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-1	ASP	-	cloning artifact	UNP P61769
B	0	PRO	-	cloning artifact	UNP P61769
D	-1	ASP	-	cloning artifact	UNP P61769
D	0	PRO	-	cloning artifact	UNP P61769

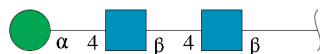
- Molecule 3 is a protein called T cell receptor delta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	207	Total	C	N	O	S	0	0	0
			1603	1000	276	321	6			
3	G	207	Total	C	N	O	S	281	0	0
			1592	992	274	321	5			

- Molecule 4 is a protein called T-cell receptor gamma chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	230	Total	C	N	O	S	0	0	0
			1852	1187	305	353	7			
4	H	230	Total	C	N	O	S	371	0	0
			1844	1181	303	353	7			

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



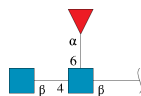
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	I	3	Total	C	N	O	0	0	0
			42	22	2	18			
5	L	3	Total	C	N	O	0	0	0
			42	22	2	18			

- Molecule 6 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	J	2	Total	C	N	O	0	0	0
			30	16	2	12			
6	K	2	Total	C	N	O	0	0	0
			30	16	2	12			

- Molecule 7 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



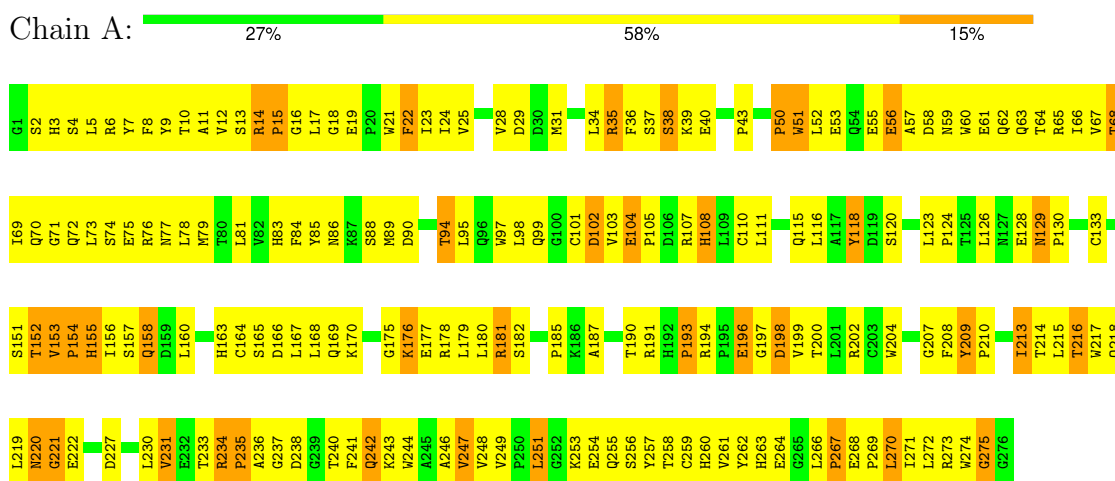
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	M	3	Total	C	N	O	0	0	0
			39	22	2	15			

3 Residue-property plots

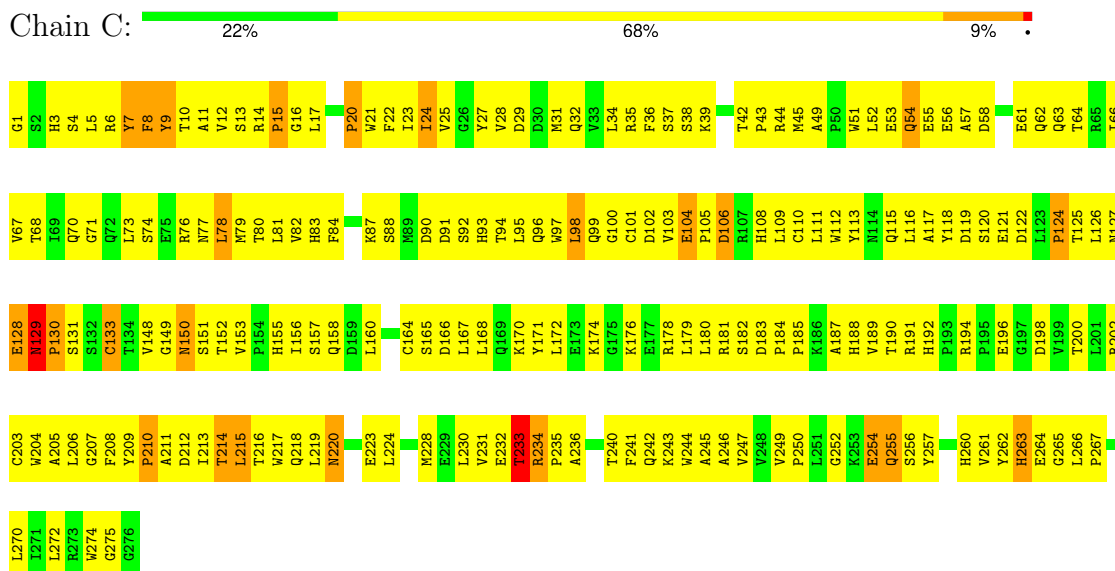
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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: H2-T22 protein

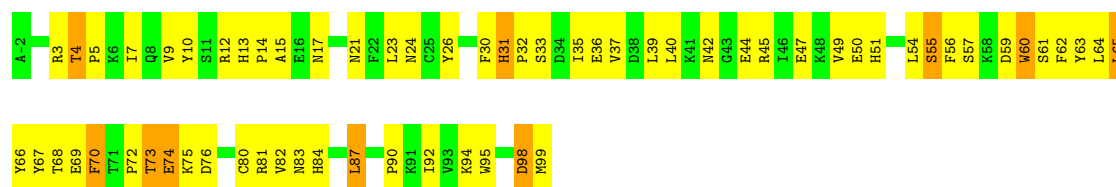


- Molecule 1: H2-T22 protein

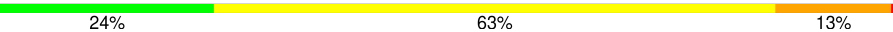


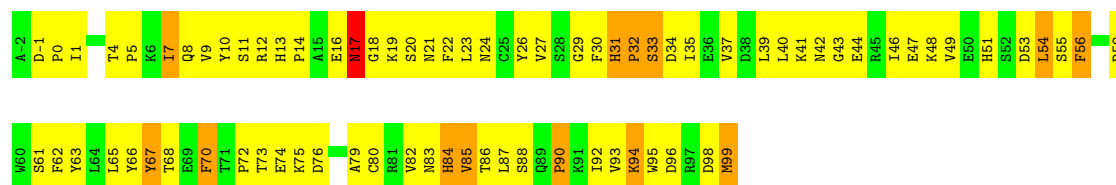
- Molecule 2: Beta-2-microglobulin

Chain B: 



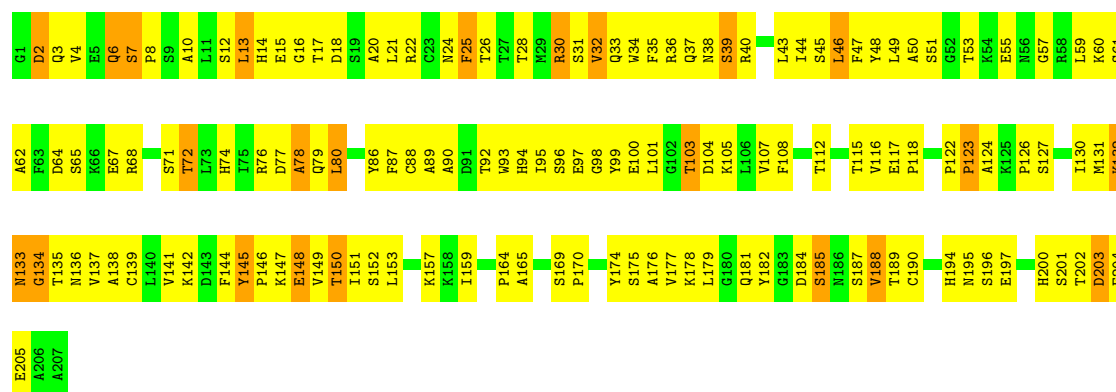
- Molecule 2: Beta-2-microglobulin

Chain D: 



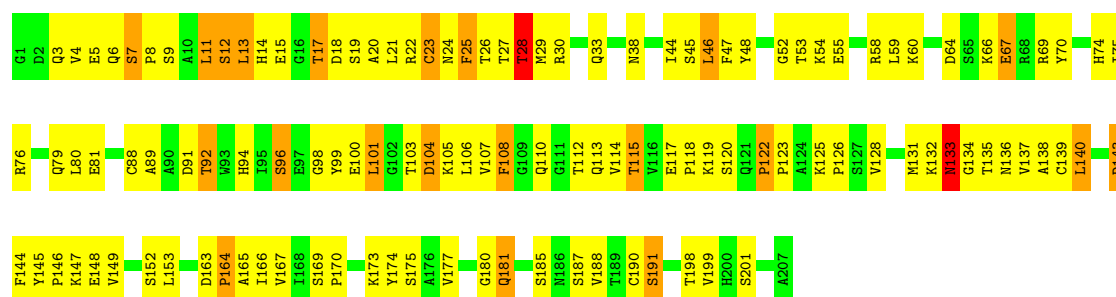
- Molecule 3: T cell receptor delta

Chain E: 

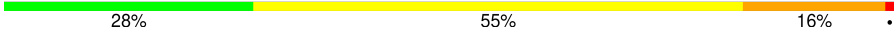


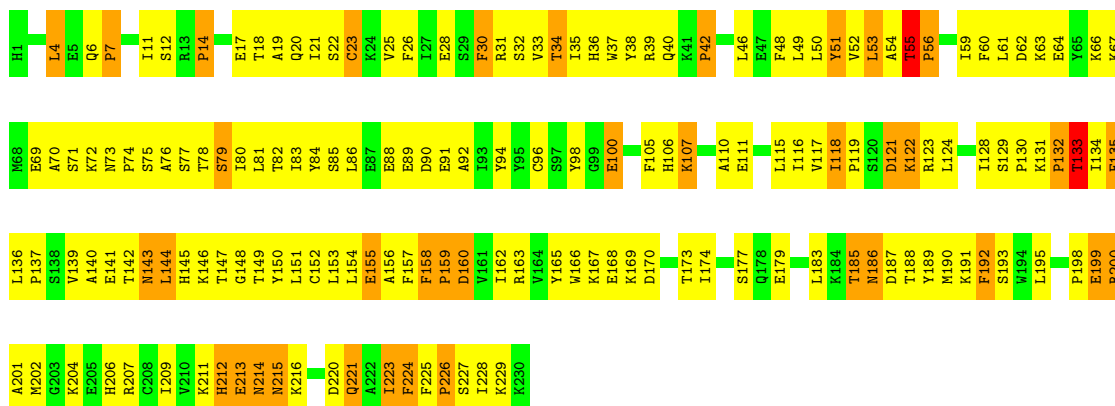
- Molecule 3: T cell receptor delta

Chain G: 



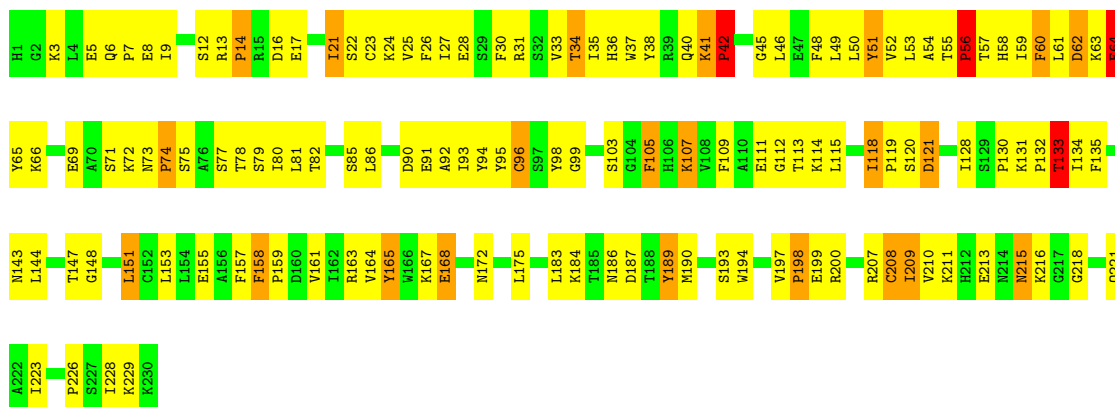
- Molecule 4: T-cell receptor gamma chain

Chain F:  28% 55% 16%



- Molecule 4: T-cell receptor gamma chain

Chain H:  40% 49% 10%



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

Chain I:  33% 67%



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

Chain L:  67% 33%



- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:  100%


NAG1
NAG2

- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:  50% 50%

NAG1
NAG2

- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:  67% 33%

NAG1
NAG2
FUC3

4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	110.53Å 113.05Å 167.97Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.40	Depositor
% Data completeness (in resolution range)	97.4 (20.00-3.40)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.264 , 0.330	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	12984	wwPDB-VP
Average B, all atoms (Å ²)	103.0	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: FUC, NAG, MAN

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	0.58	0/2166	0.89	2/2951 (0.1%)
1	C	0.48	0/2166	0.82	0/2951
2	B	0.46	0/873	0.81	0/1182
2	D	0.43	0/873	0.70	0/1182
3	E	0.55	0/1636	0.86	0/2212
3	G	0.50	0/1625	0.82	1/2201 (0.0%)
4	F	0.51	0/1898	0.84	0/2565
4	H	0.45	0/1889	0.82	0/2553
All	All	0.51	0/13126	0.83	3/17797 (0.0%)

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
2	D	0	1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	46	LEU	CA-CB-CG	-5.97	101.58	115.30
1	A	155	HIS	CB-CA-C	-5.69	99.03	110.40
1	A	154	PRO	CA-N-CD	-5.56	103.72	111.50

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	D	63	TYR	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	2106	0	2006	275	1
1	C	2106	0	2009	275	4
2	B	849	0	810	83	0
2	D	849	0	810	121	0
3	E	1603	0	1554	196	1
3	G	1592	0	1524	162	0
4	F	1852	0	1832	236	4
4	H	1844	0	1816	164	0
5	I	42	0	38	9	0
5	L	42	0	36	7	0
6	J	30	0	27	9	0
6	K	30	0	27	22	0
7	M	39	0	36	12	0
All	All	12984	0	12525	1441	5

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 60.

All (1441) 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)
3:G:24:ASN:HD21	7:M:1:NAG:C1	1.10	1.58
4:F:186:ASN:HD22	6:K:1:NAG:C1	0.99	1.57
3:E:133:ASN:HD21	5:I:1:NAG:C1	0.88	1.53
1:A:155:HIS:CD2	1:A:157:SER:N	1.88	1.41
4:F:186:ASN:CB	6:K:1:NAG:O1	1.67	1.38
1:A:219:LEU:O	1:A:221:GLY:N	1.58	1.32
3:E:7:SER:OG	3:E:8:PRO:HD2	1.24	1.31
3:E:133:ASN:ND2	5:I:1:NAG:H1	0.97	1.28
1:C:84:PHE:CE1	3:G:30:ARG:NH2	2.07	1.23
3:E:22:ARG:NH2	6:J:2:NAG:O7	1.72	1.21

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:24:ASN:ND2	7:M:1:NAG:H1	0.88	1.19
4:F:186:ASN:ND2	6:K:1:NAG:H1	1.43	1.16
1:C:228:MET:HE2	1:C:245:ALA:HB1	1.19	1.15
1:A:155:HIS:NE2	1:A:157:SER:CB	2.10	1.15
1:C:194:ARG:HB2	1:C:198:ASP:O	1.46	1.11
4:F:224:PHE:CE1	5:I:3:MAN:O2	2.03	1.11
4:F:186:ASN:ND2	6:K:1:NAG:O5	1.71	1.10
4:H:158:PHE:H	4:H:159:PRO:HD3	1.17	1.09
3:G:58:ARG:HH22	3:G:81:GLU:HG3	0.95	1.09
4:F:40:GLN:O	4:F:92:ALA:HB1	1.52	1.08
4:H:134:ILE:N	5:L:1:NAG:O6	1.86	1.08
4:H:40:GLN:HB2	4:H:46:LEU:HD12	1.32	1.08
4:F:186:ASN:HB2	6:K:1:NAG:O1	1.46	1.07
4:F:186:ASN:HB3	6:K:1:NAG:O1	1.38	1.07
1:C:81:LEU:HD21	3:G:101:LEU:HD12	1.34	1.07
4:F:6:GLN:HE21	4:F:110:ALA:HB3	1.19	1.06
4:F:50:LEU:HD21	4:F:61:LEU:HG	1.38	1.06
1:A:155:HIS:HE2	1:A:157:SER:CB	1.67	1.05
3:E:7:SER:OG	3:E:8:PRO:CD	2.02	1.05
1:C:129:ASN:HB3	1:C:130:PRO:CD	1.86	1.05
4:F:186:ASN:CB	6:K:1:NAG:C1	2.33	1.05
4:F:186:ASN:HB2	6:K:1:NAG:C1	1.86	1.05
3:E:126:PRO:HG3	3:E:144:PHE:HB3	1.36	1.04
3:E:24:ASN:ND2	6:J:1:NAG:N2	2.06	1.04
3:G:11:LEU:HD21	3:G:13:LEU:HD21	1.35	1.04
4:F:128:ILE:HG21	4:F:158:PHE:HB2	1.36	1.02
3:E:132:LYS:HE2	3:E:132:LYS:H	1.23	1.02
4:H:52:VAL:HG22	4:H:71:SER:HB2	1.40	1.01
3:E:24:ASN:ND2	6:J:1:NAG:C2	2.24	1.01
1:A:155:HIS:CD2	1:A:157:SER:H	1.74	1.00
1:C:228:MET:CE	1:C:245:ALA:HB1	1.92	1.00
1:C:49:ALA:HB3	1:C:52:LEU:HD12	1.38	1.00
1:A:155:HIS:CD2	1:A:157:SER:CB	2.44	0.99
1:C:80:THR:HB	4:H:103:SER:HB3	1.41	0.99
3:G:15:GLU:HB3	3:G:119:LYS:HG3	1.42	0.99
1:A:22:PHE:O	1:A:37:SER:HB2	1.62	0.98
1:A:155:HIS:CD2	1:A:157:SER:CA	2.47	0.98
1:A:31:MET:HG2	1:A:209:TYR:OH	1.63	0.97
4:F:224:PHE:HE1	5:I:3:MAN:O2	1.45	0.97
1:C:129:ASN:HB3	1:C:130:PRO:HD3	1.42	0.97
4:F:185:THR:HG23	6:K:1:NAG:H82	1.46	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:58:ARG:NH2	3:G:81:GLU:HG3	1.78	0.97
4:H:134:ILE:CA	5:L:1:NAG:O6	2.12	0.97
1:A:129:ASN:HB2	1:A:130:PRO:HD3	1.47	0.94
4:F:186:ASN:CG	6:K:1:NAG:C1	2.34	0.94
1:A:266:LEU:HD22	1:A:270:LEU:HD13	1.48	0.94
1:C:96:GLN:NE2	2:D:31:HIS:NE2	2.15	0.94
1:C:194:ARG:CB	1:C:198:ASP:O	2.14	0.94
4:F:207:ARG:HG2	4:F:224:PHE:HA	1.49	0.94
1:A:155:HIS:HD2	1:A:157:SER:N	1.44	0.93
1:A:218:GLN:HB2	1:A:222:GLU:O	1.69	0.93
3:G:58:ARG:NH1	3:G:79:GLN:HB2	1.84	0.92
1:C:32:GLN:HE22	2:D:53:ASP:CG	1.72	0.92
3:G:24:ASN:ND2	7:M:1:NAG:C2	2.32	0.92
4:H:17:GLU:O	4:H:86:LEU:HG	1.68	0.92
4:H:52:VAL:CG2	4:H:71:SER:HB2	2.01	0.91
3:G:3:GLN:HE21	3:G:26:THR:H	0.98	0.91
1:C:99:GLN:NE2	1:C:160:LEU:HD23	1.86	0.91
3:G:4:VAL:HG13	3:G:25:PHE:HD2	1.34	0.91
3:G:24:ASN:HD21	7:M:1:NAG:C2	1.83	0.91
3:G:24:ASN:HD22	7:M:1:NAG:H1	1.32	0.91
1:A:155:HIS:CD2	1:A:157:SER:HB3	2.06	0.91
4:F:185:THR:HG23	6:K:1:NAG:C8	2.02	0.89
3:E:37:GLN:HB3	3:E:43:LEU:HD23	1.51	0.89
3:G:166:ILE:HG23	3:G:175:SER:O	1.72	0.89
4:H:134:ILE:N	5:L:1:NAG:C6	2.36	0.89
4:H:34:THR:HA	4:H:52:VAL:O	1.72	0.88
1:C:98:LEU:HD12	1:C:99:GLN:N	1.86	0.88
1:C:202:ARG:HH11	1:C:202:ARG:HB2	1.38	0.88
4:F:186:ASN:CG	6:K:1:NAG:H1	1.93	0.88
4:H:12:SER:HB2	4:H:118:ILE:HD11	1.53	0.88
4:F:91:GLU:HG3	4:F:115:LEU:O	1.73	0.87
1:A:103:VAL:HG12	1:A:105:PRO:HD3	1.55	0.87
1:A:84:PHE:CZ	3:E:30:ARG:NE	2.43	0.87
1:C:84:PHE:CD1	3:G:30:ARG:NH2	2.43	0.87
1:C:194:ARG:HD2	1:C:198:ASP:HB2	1.57	0.87
2:B:40:LEU:HA	2:B:44:GLU:O	1.75	0.87
4:H:30:PHE:O	4:H:54:ALA:HB1	1.74	0.87
1:A:51:TRP:CE3	1:A:51:TRP:O	2.27	0.87
1:A:219:LEU:O	1:A:220:ASN:C	2.13	0.87
3:G:4:VAL:HG13	3:G:25:PHE:CD2	2.09	0.86
1:C:81:LEU:CD2	3:G:101:LEU:HD12	2.04	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:9:TYR:OH	1:C:74:SER:HB2	1.76	0.86
4:H:25:VAL:HG12	4:H:27:ILE:H	1.39	0.86
2:B:83:ASN:ND2	2:B:90:PRO:HG3	1.90	0.86
4:F:129:SER:HB2	4:F:215:ASN:HA	1.56	0.86
1:C:32:GLN:NE2	2:D:53:ASP:OD2	2.09	0.85
2:D:86:THR:HG22	2:D:87:LEU:H	1.38	0.85
3:G:3:GLN:HE21	3:G:26:THR:N	1.72	0.85
4:H:134:ILE:H	5:L:1:NAG:C6	1.88	0.85
1:A:157:SER:O	1:A:158:GLN:CD	2.15	0.85
1:C:31:MET:HB2	1:C:209:TYR:OH	1.76	0.85
1:C:189:VAL:HG12	1:C:190:THR:N	1.91	0.85
1:C:24:ILE:HD12	1:C:67:VAL:HG13	1.58	0.85
3:G:58:ARG:HH22	3:G:81:GLU:CG	1.86	0.85
4:F:156:ALA:HA	4:F:188:THR:HG21	1.57	0.84
1:A:124:PRO:HB3	3:E:28:THR:HG22	1.58	0.84
1:C:103:VAL:HG21	1:C:168:LEU:HD23	1.59	0.84
1:C:111:LEU:HD12	1:C:111:LEU:N	1.93	0.84
3:E:53:THR:HB	3:E:62:ALA:HB2	1.60	0.84
3:E:126:PRO:HG3	3:E:144:PHE:CB	2.07	0.84
4:F:186:ASN:ND2	6:K:1:NAG:C5	2.41	0.83
3:E:24:ASN:ND2	6:J:1:NAG:O1	2.09	0.83
1:C:234:ARG:HG2	2:D:8:GLN:OE1	1.79	0.83
2:D:59:ASP:OD1	2:D:61:SER:HB2	1.79	0.83
1:A:155:HIS:NE2	1:A:157:SER:OG	1.66	0.83
4:H:158:PHE:H	4:H:159:PRO:CD	1.92	0.83
2:D:37:VAL:HB	2:D:66:TYR:CZ	2.14	0.83
4:H:93:ILE:HG12	4:H:114:LYS:HB2	1.62	0.82
2:B:31:HIS:HB3	2:B:32:PRO:HD3	1.62	0.82
3:G:11:LEU:C	3:G:11:LEU:HD23	2.00	0.82
4:H:52:VAL:HG22	4:H:71:SER:CB	2.10	0.82
2:B:84:HIS:H	2:B:87:LEU:CD2	1.92	0.81
3:G:46:LEU:HD22	3:G:59:LEU:HD12	1.60	0.81
3:E:24:ASN:OD1	3:E:24:ASN:O	1.97	0.81
2:B:84:HIS:H	2:B:87:LEU:HD21	1.45	0.81
1:A:155:HIS:CE1	1:A:157:SER:HG	1.98	0.81
4:F:224:PHE:CZ	5:I:3:MAN:O2	2.33	0.81
3:G:11:LEU:HD21	3:G:13:LEU:CD2	2.10	0.81
1:C:31:MET:HE3	1:C:31:MET:HA	1.62	0.81
2:D:17:ASN:N	2:D:17:ASN:HD22	1.79	0.81
3:E:78:ALA:O	3:E:79:GLN:HG2	1.81	0.81
3:E:164:PRO:HG3	3:E:178:LYS:HD2	1.62	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:159:PRO:HD2	4:F:212:HIS:NE2	1.94	0.81
1:C:78:LEU:O	1:C:82:VAL:HG23	1.81	0.80
2:D:31:HIS:HB3	2:D:32:PRO:HD3	1.61	0.80
1:C:23:ILE:HG22	1:C:24:ILE:H	1.46	0.80
1:C:178:ARG:O	1:C:179:LEU:HD23	1.81	0.80
4:F:152:CYS:HB2	4:F:166:TRP:CZ2	2.16	0.80
1:C:84:PHE:CE1	3:G:30:ARG:CZ	2.65	0.80
1:A:155:HIS:NE2	1:A:157:SER:N	2.29	0.80
4:H:134:ILE:O	5:L:1:NAG:O5	1.99	0.80
1:A:24:ILE:HD12	1:A:67:VAL:HG13	1.62	0.80
3:E:7:SER:CB	3:E:8:PRO:CD	2.60	0.80
3:G:7:SER:HB2	3:G:8:PRO:HD3	1.64	0.80
1:A:155:HIS:HD2	1:A:157:SER:CA	1.92	0.80
3:E:15:GLU:OE1	3:E:118:PRO:HA	1.82	0.79
1:A:234:ARG:HG3	2:B:10:TYR:CZ	2.17	0.79
4:F:153:LEU:HD12	4:F:154:LEU:N	1.96	0.79
3:E:169:SER:OG	3:E:175:SER:HB2	1.82	0.79
4:H:40:GLN:HB2	4:H:46:LEU:CD1	2.12	0.79
3:G:3:GLN:NE2	3:G:26:THR:H	1.78	0.79
1:A:77:ASN:OD1	3:E:101:LEU:HB2	1.83	0.79
1:A:153:VAL:HB	1:A:154:PRO:CD	2.13	0.79
3:E:145:TYR:HB3	3:E:146:PRO:HD3	1.65	0.79
4:F:186:ASN:HD22	6:K:1:NAG:C5	1.94	0.79
1:C:81:LEU:HD21	3:G:101:LEU:CD1	2.13	0.78
2:D:20:SER:O	2:D:21:ASN:CG	2.21	0.78
3:G:30:ARG:HG2	3:G:91:ASP:O	1.83	0.78
4:F:130:PRO:HD2	4:F:215:ASN:HB2	1.65	0.78
1:C:97:TRP:HD1	1:C:98:LEU:N	1.79	0.78
2:D:23:LEU:O	2:D:67:TYR:HA	1.84	0.78
3:E:26:THR:HG22	3:E:26:THR:O	1.81	0.78
3:G:144:PHE:O	3:G:173:LYS:HB3	1.84	0.78
4:H:93:ILE:HA	4:H:114:LYS:HA	1.66	0.78
4:H:158:PHE:N	4:H:159:PRO:HD3	1.95	0.78
2:D:5:PRO:HB3	2:D:30:PHE:HB3	1.66	0.78
1:C:87:LYS:HB3	1:C:93:HIS:HE1	1.49	0.78
1:C:23:ILE:HG22	1:C:24:ILE:N	1.99	0.78
2:D:20:SER:O	2:D:21:ASN:OD1	2.02	0.78
2:D:23:LEU:HB3	2:D:68:THR:HG22	1.63	0.78
3:G:3:GLN:HG3	3:G:3:GLN:O	1.83	0.77
1:A:259:CYS:HB3	1:A:272:LEU:HB2	1.64	0.77
4:H:36:HIS:HA	4:H:50:LEU:O	1.83	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:19:LYS:O	2:D:72:PRO:HD2	1.84	0.77
4:F:12:SER:HA	4:F:116:ILE:O	1.84	0.77
2:D:54:LEU:HD11	2:D:62:PHE:HD2	1.50	0.77
3:G:148:GLU:O	3:G:149:VAL:HG23	1.83	0.77
4:F:6:GLN:NE2	4:F:110:ALA:HB3	1.97	0.76
4:F:25:VAL:HG23	4:F:78:THR:HA	1.66	0.76
3:E:108:PHE:CD1	4:F:46:LEU:HB2	2.19	0.76
2:D:17:ASN:HA	2:D:72:PRO:HB2	1.68	0.76
1:C:209:TYR:O	1:C:211:ALA:N	2.19	0.76
4:H:92:ALA:O	4:H:94:TYR:CE1	2.39	0.76
4:F:25:VAL:HG21	4:F:35:ILE:HD11	1.66	0.76
2:D:80:CYS:O	2:D:92:ILE:HA	1.86	0.76
4:F:188:THR:HG22	4:F:189:TYR:H	1.50	0.76
1:C:176:LYS:HB3	1:C:180:LEU:HD12	1.67	0.75
1:A:5:LEU:HD12	1:A:6:ARG:N	2.02	0.75
4:F:62:ASP:HA	4:F:67:LYS:HA	1.68	0.75
2:B:70:PHE:CZ	2:B:72:PRO:HG3	2.22	0.75
3:E:7:SER:CB	3:E:8:PRO:HD2	2.15	0.75
4:F:152:CYS:HB2	4:F:166:TRP:HZ2	1.51	0.75
1:C:103:VAL:CG2	1:C:168:LEU:HD23	2.17	0.75
1:A:266:LEU:HD12	1:A:266:LEU:O	1.87	0.75
4:F:69:GLU:OE1	4:F:81:LEU:HD21	1.87	0.75
4:H:74:PRO:HD2	4:H:78:THR:O	1.87	0.75
4:H:107:LYS:HG3	4:H:109:PHE:CE1	2.22	0.75
2:D:23:LEU:HD23	2:D:39:LEU:HD13	1.67	0.74
1:A:238:ASP:OD1	1:A:240:THR:HG23	1.86	0.74
2:B:17:ASN:HA	2:B:72:PRO:O	1.87	0.74
1:A:155:HIS:CD2	1:A:156:ILE:C	2.60	0.74
1:A:202:ARG:HD3	1:A:204:TRP:CZ2	2.22	0.74
1:A:209:TYR:HB3	1:A:210:PRO:HD3	1.69	0.74
3:G:131:MET:CB	3:G:140:LEU:HD21	2.18	0.74
1:A:194:ARG:HG2	1:A:198:ASP:O	1.87	0.74
3:E:53:THR:HB	3:E:62:ALA:CB	2.18	0.74
4:H:210:VAL:HG12	4:H:211:LYS:H	1.53	0.74
4:F:128:ILE:CG2	4:F:158:PHE:HB2	2.15	0.74
4:F:168:GLU:HG2	4:F:170:ASP:OD1	1.87	0.74
1:A:208:PHE:CZ	1:A:213:ILE:HD12	2.23	0.74
2:B:23:LEU:HD23	2:B:39:LEU:HD13	1.69	0.74
3:E:33:GLN:HE22	4:F:107:LYS:HB2	1.52	0.74
1:C:182:SER:O	1:C:184:PRO:HD3	1.87	0.73
7:M:1:NAG:H83	7:M:1:NAG:O1	1.87	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:133:ASN:HD22	5:I:1:NAG:H1	1.47	0.73
3:E:185:SER:O	3:E:188:VAL:HG23	1.87	0.73
4:F:147:THR:HG22	4:F:148:GLY:N	2.02	0.73
4:F:165:TYR:HE1	4:F:167:LYS:HD2	1.52	0.73
3:G:7:SER:CB	3:G:8:PRO:CD	2.67	0.73
4:F:33:VAL:HG12	4:F:34:THR:H	1.52	0.73
1:C:17:LEU:O	1:C:17:LEU:HD23	1.88	0.73
3:E:133:ASN:ND2	5:I:1:NAG:O1	2.21	0.73
4:H:37:TRP:CE3	4:H:81:LEU:HD22	2.23	0.73
4:H:41:LYS:HB3	4:H:42:PRO:HD2	1.71	0.73
1:C:80:THR:CB	4:H:103:SER:HB3	2.17	0.73
1:A:153:VAL:HB	1:A:154:PRO:HD2	1.69	0.73
3:E:53:THR:CB	3:E:62:ALA:HB2	2.18	0.72
4:F:33:VAL:HG12	4:F:34:THR:N	2.04	0.72
3:G:5:GLU:O	3:G:23:CYS:HA	1.89	0.72
4:H:210:VAL:HG12	4:H:211:LYS:N	2.02	0.72
1:C:115:GLN:C	1:C:116:LEU:HD12	2.10	0.72
3:E:34:TRP:CZ3	3:E:88:CYS:HB3	2.24	0.72
1:C:183:ASP:O	1:C:208:PHE:HA	1.89	0.72
1:C:189:VAL:CG1	1:C:190:THR:N	2.52	0.72
4:F:162:ILE:O	4:F:163:ARG:HD3	1.90	0.72
3:G:38:ASN:ND2	3:G:44:ILE:HD11	2.04	0.72
1:C:202:ARG:HB2	1:C:202:ARG:NH1	2.04	0.72
4:H:33:VAL:HB	4:H:54:ALA:HB2	1.70	0.72
1:A:155:HIS:NE2	1:A:157:SER:HB3	2.01	0.72
1:C:249:VAL:HG13	1:C:250:PRO:HD2	1.71	0.72
1:C:5:LEU:O	1:C:6:ARG:HD3	1.89	0.72
1:C:13:SER:HB3	1:C:93:HIS:H	1.55	0.72
4:H:33:VAL:HB	4:H:54:ALA:CB	2.20	0.72
1:C:185:PRO:HD2	1:C:266:LEU:HD11	1.70	0.72
3:E:124:ALA:HB3	3:E:145:TYR:H	1.55	0.72
2:B:55:SER:HB3	2:B:63:TYR:CZ	2.25	0.72
2:D:54:LEU:HD11	2:D:62:PHE:CD2	2.25	0.72
1:A:39:LYS:O	1:A:40:GLU:HG3	1.89	0.71
1:A:215:LEU:CD2	1:A:261:VAL:HG13	2.20	0.71
3:E:61:SER:HB2	3:E:72:THR:O	1.88	0.71
4:F:213:GLU:O	4:F:215:ASN:N	2.23	0.71
4:H:167:LYS:HE2	4:H:209:ILE:CD1	2.20	0.71
4:H:158:PHE:N	4:H:159:PRO:CD	2.49	0.71
3:E:7:SER:HB3	3:E:22:ARG:HB2	1.72	0.71
1:C:129:ASN:CB	1:C:130:PRO:HD3	2.18	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:147:LYS:HG3	3:G:174:TYR:HE2	1.55	0.71
4:H:134:ILE:N	5:L:1:NAG:H62	2.05	0.71
1:A:251:LEU:HD23	1:A:251:LEU:H	1.54	0.71
4:F:132:PRO:O	4:F:133:THR:OG1	2.09	0.71
4:H:22:SER:HB3	4:H:80:ILE:HG12	1.71	0.71
4:H:41:LYS:HB3	4:H:42:PRO:CD	2.19	0.71
3:E:138:ALA:HB2	3:E:179:LEU:HD23	1.71	0.71
4:F:4:LEU:HD22	4:F:98:TYR:HD2	1.53	0.71
4:F:6:GLN:HE21	4:F:110:ALA:CB	2.02	0.71
1:C:98:LEU:HD12	1:C:98:LEU:C	2.10	0.71
3:E:179:LEU:HD13	4:F:153:LEU:HD22	1.73	0.71
1:A:50:PRO:O	1:A:52:LEU:N	2.24	0.70
1:A:208:PHE:CE2	1:A:213:ILE:HD12	2.25	0.70
2:B:17:ASN:HB2	2:B:73:THR:HA	1.72	0.70
1:C:31:MET:HA	1:C:31:MET:CE	2.21	0.70
1:C:99:GLN:HA	1:C:113:TYR:O	1.92	0.70
1:C:189:VAL:HB	1:C:274:TRP:CB	2.22	0.70
3:E:48:TYR:O	3:E:49:LEU:HD23	1.91	0.70
3:G:24:ASN:HD22	7:M:1:NAG:C1	1.89	0.70
3:G:139:CYS:O	3:G:140:LEU:HD23	1.91	0.70
1:C:184:PRO:HB3	1:C:266:LEU:CD2	2.21	0.70
2:D:41:LYS:HB2	2:D:46:ILE:HD11	1.73	0.70
4:F:228:ILE:HG22	4:F:229:LYS:N	2.06	0.70
3:E:132:LYS:H	3:E:132:LYS:CE	2.02	0.70
3:G:7:SER:HB2	3:G:8:PRO:CD	2.22	0.70
1:C:124:PRO:O	3:G:92:THR:HG23	1.91	0.70
1:C:34:LEU:HD23	1:C:35:ARG:N	2.05	0.70
1:A:81:LEU:HB3	1:A:118:TYR:CE1	2.27	0.70
1:A:31:MET:HG2	1:A:209:TYR:HH	1.55	0.70
4:F:131:LYS:HD2	4:F:156:ALA:HB3	1.73	0.70
4:F:55:THR:HG22	4:F:56:PRO:HD3	1.72	0.69
3:G:48:TYR:CE1	4:H:105:PHE:O	2.44	0.69
1:C:203:CYS:HB2	1:C:217:TRP:CZ2	2.28	0.69
3:G:58:ARG:HH12	3:G:79:GLN:HB2	1.57	0.69
1:A:155:HIS:HD2	1:A:156:ILE:C	1.95	0.69
1:C:66:ILE:HD13	1:C:160:LEU:HB2	1.72	0.69
4:H:62:ASP:HA	4:H:66:LYS:O	1.92	0.69
1:A:129:ASN:CB	1:A:130:PRO:HD3	2.23	0.69
1:C:213:ILE:HG12	1:C:214:THR:N	2.07	0.69
1:A:61:GLU:HA	1:A:64:THR:OG1	1.92	0.69
1:A:160:LEU:HD12	1:A:160:LEU:O	1.93	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:209:TYR:O	1:A:210:PRO:C	2.31	0.69
2:B:42:ASN:HD21	2:B:76:ASP:HA	1.57	0.69
3:E:144:PHE:CE1	3:E:149:VAL:HG21	2.27	0.69
4:H:151:LEU:HD23	4:H:151:LEU:N	2.08	0.69
1:A:6:ARG:HB3	1:A:8:PHE:HE1	1.58	0.69
1:C:105:PRO:O	1:C:108:HIS:N	2.24	0.69
4:H:157:PHE:CD1	4:H:159:PRO:HD2	2.27	0.69
1:C:167:LEU:HD21	1:C:171:TYR:CE2	2.28	0.68
1:A:202:ARG:HA	1:A:246:ALA:HB2	1.75	0.68
4:H:131:LYS:H	4:H:155:GLU:H	1.39	0.68
1:C:211:ALA:HB2	1:C:241:PHE:CE1	2.29	0.68
1:C:49:ALA:HB1	1:C:51:TRP:NE1	2.07	0.68
1:C:184:PRO:HG3	1:C:265:GLY:O	1.94	0.68
3:E:126:PRO:CG	3:E:144:PHE:HB3	2.19	0.68
4:H:208:CYS:O	4:H:208:CYS:SG	2.51	0.68
1:A:51:TRP:O	1:A:51:TRP:HE3	1.74	0.68
1:C:97:TRP:CD1	1:C:98:LEU:N	2.62	0.68
1:A:81:LEU:HB3	1:A:118:TYR:HE1	1.59	0.68
3:E:96:SER:C	3:E:98:GLY:H	1.96	0.68
3:E:179:LEU:CD1	4:F:153:LEU:HD22	2.24	0.68
3:G:25:PHE:O	3:G:69:ARG:HB2	1.94	0.68
2:B:9:VAL:HG21	2:B:80:CYS:HB2	1.76	0.67
4:F:31:ARG:O	4:F:54:ALA:HB1	1.94	0.67
3:G:98:GLY:C	3:G:99:TYR:HD1	1.97	0.67
4:F:53:LEU:HD13	4:F:59:ILE:HD11	1.76	0.67
1:A:5:LEU:HD12	1:A:6:ARG:H	1.59	0.67
1:C:76:ARG:O	1:C:79:MET:HB2	1.94	0.67
3:E:184:ASP:HB2	3:E:187:SER:OG	1.93	0.67
4:F:52:VAL:HG22	4:F:71:SER:HB2	1.75	0.67
2:B:73:THR:O	2:B:75:LYS:N	2.27	0.67
3:E:14:HIS:HA	3:E:117:GLU:O	1.95	0.67
3:G:12:SER:HB2	3:G:115:THR:HB	1.77	0.67
4:H:3:LYS:HE3	4:H:98:TYR:OH	1.95	0.67
4:H:60:PHE:N	4:H:60:PHE:CD2	2.62	0.67
4:F:23:CYS:CB	4:F:96:CYS:SG	2.83	0.67
4:F:121:ASP:O	4:F:122:LYS:C	2.31	0.67
1:C:63:GLN:O	1:C:67:VAL:HG23	1.95	0.67
4:F:130:PRO:CD	4:F:215:ASN:HB2	2.25	0.67
1:A:14:ARG:HB2	1:A:15:PRO:CD	2.25	0.66
3:E:24:ASN:HD21	6:J:1:NAG:HN2	1.42	0.66
4:F:30:PHE:CZ	4:F:77:SER:HA	2.31	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:219:LEU:O	1:A:221:GLY:CA	2.42	0.66
1:C:21:TRP:CH2	1:C:23:ILE:HD11	2.30	0.66
1:C:52:LEU:HD23	1:C:174:LYS:C	2.15	0.66
2:D:17:ASN:OD1	2:D:74:GLU:HB2	1.96	0.66
4:F:185:THR:CG2	6:K:1:NAG:H82	2.24	0.66
3:G:3:GLN:NE2	3:G:27:THR:H	1.92	0.66
3:G:19:SER:O	3:G:75:ILE:N	2.23	0.66
1:C:150:ASN:HB3	1:C:153:VAL:HG21	1.76	0.66
1:C:45:MET:CE	1:C:54:GLN:HE22	2.09	0.66
1:A:23:ILE:HG22	1:A:24:ILE:N	2.10	0.65
4:F:51:TYR:O	4:F:59:ILE:HD12	1.96	0.65
4:F:32:SER:HA	4:F:54:ALA:HB1	1.78	0.65
1:C:254:GLU:O	1:C:256:SER:N	2.29	0.65
4:F:179:GLU:HA	4:F:193:SER:HA	1.77	0.65
3:G:96:SER:OG	3:G:100:GLU:N	2.30	0.65
4:H:63:LYS:O	4:H:63:LYS:HG3	1.96	0.65
1:A:11:ALA:O	1:A:94:THR:HA	1.96	0.65
2:D:16:GLU:O	2:D:16:GLU:HG3	1.95	0.65
1:A:57:ALA:C	1:A:59:ASN:H	1.98	0.65
1:C:185:PRO:HD2	1:C:266:LEU:CG	2.27	0.65
1:A:6:ARG:NH1	1:A:102:ASP:OD1	2.30	0.65
1:C:170:LYS:HA	1:C:170:LYS:HE2	1.79	0.65
1:C:185:PRO:HD2	1:C:266:LEU:CD1	2.26	0.65
4:F:146:LYS:HG3	4:F:199:GLU:HG3	1.77	0.65
3:G:7:SER:OG	3:G:8:PRO:HD2	1.97	0.65
1:A:65:ARG:HH12	1:A:158:GLN:HG3	1.62	0.64
3:G:58:ARG:HB2	3:G:76:ARG:O	1.96	0.64
4:H:33:VAL:CG1	4:H:34:THR:N	2.59	0.64
1:C:191:ARG:HB3	1:C:274:TRP:HZ3	1.62	0.64
2:D:5:PRO:CB	2:D:30:PHE:HB3	2.27	0.64
4:H:107:LYS:HG3	4:H:109:PHE:HE1	1.59	0.64
1:C:8:PHE:CD1	1:C:8:PHE:N	2.65	0.64
1:C:191:ARG:H	1:C:274:TRP:HZ3	1.45	0.64
1:C:200:THR:HA	1:C:247:VAL:O	1.98	0.64
4:F:157:PHE:O	4:F:188:THR:HG22	1.96	0.64
4:H:35:ILE:O	4:H:51:TYR:HA	1.96	0.64
2:B:30:PHE:HE1	2:B:33:SER:HA	1.62	0.64
1:C:189:VAL:CG1	1:C:190:THR:H	2.09	0.64
1:A:101:CYS:HA	1:A:111:LEU:O	1.97	0.64
1:A:213:ILE:HG13	1:A:263:HIS:HD2	1.61	0.64
1:C:119:ASP:O	1:C:120:SER:HB3	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:52:VAL:HG22	4:F:71:SER:CB	2.28	0.64
4:F:147:THR:HG22	4:F:148:GLY:H	1.60	0.64
4:H:93:ILE:HG12	4:H:114:LYS:CB	2.27	0.64
1:A:190:THR:HA	1:A:274:TRP:HZ3	1.63	0.63
4:F:37:TRP:CD2	4:F:81:LEU:HD13	2.32	0.63
4:F:111:GLU:OE2	4:F:111:GLU:N	2.31	0.63
3:G:152:SER:O	3:G:153:LEU:HD23	1.98	0.63
1:C:167:LEU:O	1:C:167:LEU:HD23	1.98	0.63
2:D:79:ALA:HA	2:D:93:VAL:O	1.98	0.63
4:F:30:PHE:CZ	4:F:73:ASN:OD1	2.52	0.63
4:F:157:PHE:CE1	4:F:189:TYR:HB2	2.34	0.63
1:A:110:CYS:O	1:A:111:LEU:HD12	1.98	0.63
1:C:67:VAL:O	1:C:70:GLN:HB3	1.98	0.63
1:C:189:VAL:HB	1:C:274:TRP:HB3	1.80	0.63
3:E:18:ASP:OD1	3:E:76:ARG:HA	1.98	0.63
1:C:8:PHE:HD2	2:D:56:PHE:CD1	2.17	0.63
4:F:28:GLU:C	4:F:30:PHE:H	2.01	0.63
2:B:70:PHE:CE2	2:B:72:PRO:HG3	2.34	0.63
3:G:17:THR:HG22	3:G:18:ASP:H	1.64	0.63
1:A:103:VAL:HG12	1:A:104:GLU:N	2.14	0.63
1:A:24:ILE:HG22	1:A:24:ILE:O	1.97	0.63
1:C:208:PHE:CE2	1:C:241:PHE:O	2.52	0.63
4:F:134:ILE:HG23	4:F:225:PHE:CE2	2.34	0.63
1:A:14:ARG:CB	1:A:15:PRO:CD	2.76	0.62
1:A:66:ILE:HD13	1:A:160:LEU:HB2	1.81	0.62
1:C:111:LEU:N	1:C:111:LEU:CD1	2.61	0.62
3:E:30:ARG:HG3	3:E:31:SER:N	2.13	0.62
1:A:24:ILE:HD12	1:A:67:VAL:CG1	2.29	0.62
2:D:17:ASN:HB2	2:D:73:THR:HA	1.80	0.62
3:E:46:LEU:HD22	3:E:59:LEU:CD1	2.29	0.62
3:G:89:ALA:HA	3:G:107:VAL:O	1.98	0.62
4:H:51:TYR:O	4:H:59:ILE:HD12	1.99	0.62
4:H:153:LEU:HD23	4:H:153:LEU:C	2.20	0.62
1:C:261:VAL:HG12	1:C:261:VAL:O	1.99	0.62
4:F:186:ASN:HB2	6:K:1:NAG:H1	1.80	0.62
1:C:191:ARG:N	1:C:274:TRP:CZ3	2.68	0.62
3:G:6:GLN:HA	3:G:23:CYS:HB2	1.80	0.62
1:C:249:VAL:CG1	1:C:250:PRO:HD2	2.29	0.62
3:G:67:GLU:OE1	3:G:69:ARG:NE	2.32	0.62
4:H:56:PRO:HD3	4:H:73:ASN:HB3	1.80	0.62
2:B:57:SER:O	2:B:60:TRP:N	2.33	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:88:GLU:C	4:F:90:ASP:H	2.02	0.62
1:A:234:ARG:NH1	1:A:242:GLN:OE1	2.33	0.62
3:G:98:GLY:C	3:G:99:TYR:CD1	2.73	0.62
2:B:17:ASN:CB	2:B:73:THR:HA	2.30	0.62
2:D:70:PHE:CZ	2:D:72:PRO:HG3	2.34	0.62
3:E:30:ARG:NH2	3:E:103:THR:HG21	2.15	0.61
3:G:26:THR:HA	3:G:69:ARG:HB2	1.82	0.61
1:C:230:LEU:HD21	1:C:245:ALA:HB2	1.82	0.61
3:E:17:THR:HG22	3:E:18:ASP:N	2.15	0.61
3:G:139:CYS:C	3:G:140:LEU:HD23	2.21	0.61
2:D:5:PRO:CA	2:D:30:PHE:HB3	2.31	0.61
2:B:3:ARG:O	2:B:30:PHE:HA	1.99	0.61
2:D:59:ASP:OD1	2:D:61:SER:CB	2.49	0.61
4:F:88:GLU:O	4:F:90:ASP:N	2.29	0.61
4:F:153:LEU:HD12	4:F:153:LEU:C	2.20	0.61
3:E:94:HIS:C	3:E:95:ILE:HG13	2.21	0.61
1:A:234:ARG:NH1	2:B:10:TYR:CG	2.69	0.61
1:C:249:VAL:HG22	1:C:257:TYR:CE2	2.36	0.61
3:E:134:GLY:O	3:E:135:THR:HB	2.00	0.61
4:F:14:PRO:HB2	4:F:17:GLU:HG3	1.82	0.61
4:F:158:PHE:O	4:F:160:ASP:N	2.34	0.61
3:G:8:PRO:O	3:G:112:THR:OG1	2.11	0.61
4:F:25:VAL:HG21	4:F:35:ILE:CD1	2.29	0.61
3:G:106:LEU:HD22	4:H:107:LYS:HE2	1.83	0.61
2:D:84:HIS:O	2:D:86:THR:N	2.34	0.61
3:G:25:PHE:O	3:G:69:ARG:O	2.18	0.61
2:D:41:LYS:HG2	2:D:42:ASN:ND2	2.16	0.61
1:C:73:LEU:HD12	3:G:99:TYR:HB2	1.81	0.60
4:H:132:PRO:HG2	4:H:221:GLN:HE22	1.65	0.60
1:A:128:GLU:O	1:A:129:ASN:C	2.39	0.60
1:C:24:ILE:HG22	1:C:24:ILE:O	2.00	0.60
1:C:84:PHE:HE1	3:G:30:ARG:NH2	1.92	0.60
4:F:63:LYS:HG2	4:F:66:LYS:O	2.01	0.60
3:G:128:VAL:HG13	3:G:140:LEU:O	2.01	0.60
1:A:71:GLY:O	1:A:74:SER:HB3	2.01	0.60
2:B:9:VAL:CG2	2:B:80:CYS:HB2	2.30	0.60
4:F:192:PHE:HD1	4:F:192:PHE:H	1.49	0.60
3:G:143:ASP:HB3	3:G:173:LYS:HD2	1.83	0.60
1:A:219:LEU:HD21	1:A:257:TYR:CE2	2.35	0.60
1:C:189:VAL:HG12	1:C:190:THR:H	1.64	0.60
3:E:132:LYS:HE2	3:E:132:LYS:N	2.05	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:9:TYR:OH	1:A:74:SER:CB	2.49	0.60
1:A:34:LEU:CD1	1:A:63:GLN:OE1	2.49	0.60
1:A:152:THR:HG22	1:A:153:VAL:H	1.66	0.60
4:F:211:LYS:HE2	4:F:220:ASP:OD1	2.02	0.60
3:G:137:VAL:N	3:G:180:GLY:O	2.30	0.60
4:H:105:PHE:CZ	4:H:107:LYS:NZ	2.68	0.60
1:A:215:LEU:HD22	1:A:261:VAL:HG22	1.83	0.60
4:F:139:VAL:O	4:F:143:ASN:HB2	2.01	0.60
4:F:6:GLN:HG2	4:F:23:CYS:HB2	1.83	0.60
1:A:235:PRO:HG2	2:B:65:LEU:HD13	1.83	0.60
1:C:80:THR:HB	4:H:103:SER:CB	2.24	0.60
4:F:149:THR:HA	4:F:195:LEU:O	2.02	0.60
4:F:169:LYS:CG	4:F:207:ARG:HB2	2.32	0.60
7:M:1:NAG:H83	7:M:1:NAG:H3	1.84	0.60
3:E:133:ASN:O	3:E:136:ASN:HB2	2.02	0.60
1:A:22:PHE:HZ	1:A:36:PHE:HE2	1.48	0.59
1:A:58:ASP:O	1:A:61:GLU:HG3	2.02	0.59
1:A:219:LEU:C	1:A:221:GLY:N	2.49	0.59
4:F:51:TYR:H	4:F:51:TYR:HD2	1.48	0.59
1:A:6:ARG:HB3	1:A:8:PHE:CE1	2.36	0.59
1:A:9:TYR:HB3	1:A:97:TRP:HB3	1.84	0.59
1:A:263:HIS:ND1	1:A:264:GLU:N	2.50	0.59
1:C:4:SER:O	1:C:28:VAL:HG13	2.01	0.59
3:G:94:HIS:HB2	3:G:104:ASP:N	2.17	0.59
1:A:69:ILE:O	1:A:72:GLN:N	2.35	0.59
1:A:129:ASN:HB2	1:A:130:PRO:CD	2.27	0.59
3:E:35:PHE:CD1	3:E:108:PHE:HE2	2.20	0.59
1:A:9:TYR:OH	1:A:74:SER:HB2	2.02	0.59
1:A:187:ALA:HB1	1:A:272:LEU:HD11	1.83	0.59
1:C:129:ASN:CB	1:C:130:PRO:CD	2.68	0.59
1:C:160:LEU:O	1:C:160:LEU:HD12	2.02	0.59
4:F:156:ALA:CA	4:F:188:THR:HG21	2.31	0.59
4:F:158:PHE:O	4:F:159:PRO:C	2.40	0.59
3:G:3:GLN:NE2	3:G:27:THR:N	2.51	0.59
3:G:6:GLN:NE2	3:G:88:CYS:H	1.99	0.59
3:G:15:GLU:HB2	3:G:118:PRO:HA	1.84	0.59
1:A:24:ILE:CD1	1:A:67:VAL:HG13	2.32	0.59
1:A:28:VAL:HG11	1:A:179:LEU:HD13	1.84	0.59
1:A:230:LEU:HD22	1:A:243:LYS:HE3	1.84	0.59
3:E:195:ASN:O	3:E:196:SER:OG	2.16	0.59
4:F:150:TYR:HB3	4:F:225:PHE:CE2	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:3:GLN:O	3:G:3:GLN:CG	2.48	0.59
4:H:55:THR:O	4:H:57:THR:N	2.36	0.59
4:H:168:GLU:HG3	4:H:175:LEU:CD1	2.32	0.59
2:D:31:HIS:O	2:D:32:PRO:C	2.39	0.59
3:E:26:THR:O	3:E:26:THR:CG2	2.51	0.59
3:E:164:PRO:HG3	3:E:178:LYS:CD	2.32	0.59
4:F:192:PHE:HD1	4:F:192:PHE:N	2.00	0.59
7:M:1:NAG:O1	7:M:1:NAG:C8	2.51	0.59
3:E:46:LEU:HD22	3:E:59:LEU:HD12	1.84	0.59
1:A:175:GLY:O	1:A:177:GLU:N	2.36	0.59
1:A:202:ARG:HD2	2:B:98:ASP:OD1	2.01	0.59
4:H:168:GLU:HG3	4:H:175:LEU:HD11	1.84	0.59
1:A:266:LEU:CD2	1:A:270:LEU:HD13	2.26	0.59
1:C:228:MET:CE	1:C:245:ALA:CB	2.76	0.59
1:A:73:LEU:HD12	3:E:99:TYR:C	2.23	0.59
1:A:234:ARG:HG3	2:B:10:TYR:CE2	2.38	0.59
3:E:137:VAL:HG21	3:E:188:VAL:HG21	1.84	0.59
4:F:137:PRO:HD3	4:F:150:TYR:CE2	2.37	0.59
4:F:192:PHE:N	4:F:192:PHE:CD1	2.70	0.59
1:A:62:GLN:O	1:A:66:ILE:HG13	2.03	0.58
3:E:12:SER:O	3:E:13:LEU:HD23	2.02	0.58
4:H:41:LYS:HD3	4:H:92:ALA:HB2	1.84	0.58
1:A:202:ARG:HG2	1:A:204:TRP:NE1	2.18	0.58
4:F:186:ASN:CB	6:K:1:NAG:H1	2.23	0.58
1:A:178:ARG:O	1:A:181:ARG:HD2	2.03	0.58
2:B:65:LEU:O	2:B:65:LEU:HD23	2.04	0.58
1:A:153:VAL:CB	1:A:154:PRO:CD	2.80	0.58
1:C:189:VAL:HB	1:C:274:TRP:HB2	1.85	0.58
4:H:37:TRP:CD2	4:H:81:LEU:HD13	2.38	0.58
3:G:26:THR:HG23	3:G:69:ARG:HH11	1.69	0.58
2:D:96:ASP:OD2	2:D:98:ASP:HB2	2.04	0.58
3:G:110:GLN:CD	3:G:110:GLN:H	2.07	0.58
4:H:120:SER:O	4:H:121:ASP:HB2	2.04	0.58
1:A:3:HIS:CE1	1:A:180:LEU:HD21	2.39	0.58
3:E:133:ASN:O	3:E:134:GLY:C	2.42	0.58
3:G:11:LEU:CD2	3:G:13:LEU:HD21	2.23	0.58
4:H:215:ASN:OD1	4:H:215:ASN:O	2.22	0.58
1:A:163:HIS:O	1:A:164:CYS:C	2.40	0.58
4:F:204:LYS:O	4:F:227:SER:HB3	2.04	0.58
1:A:63:GLN:NE2	1:A:167:LEU:HD22	2.18	0.57
4:H:6:GLN:HG2	4:H:23:CYS:CB	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:M:2:NAG:H82	7:M:2:NAG:H3	1.85	0.57
4:H:167:LYS:HE2	4:H:209:ILE:HD11	1.85	0.57
4:H:210:VAL:CG1	4:H:211:LYS:H	2.17	0.57
1:A:21:TRP:CZ2	1:A:23:ILE:HG13	2.38	0.57
2:D:26:TYR:HB2	2:D:65:LEU:HD13	1.86	0.57
3:E:34:TRP:CE3	3:E:88:CYS:HB3	2.39	0.57
1:A:71:GLY:O	1:A:74:SER:CB	2.52	0.57
4:F:165:TYR:CE1	4:F:167:LYS:HD2	2.37	0.57
4:F:228:ILE:HG22	4:F:229:LYS:H	1.69	0.57
4:H:22:SER:CB	4:H:80:ILE:HG12	2.33	0.57
4:H:33:VAL:CB	4:H:54:ALA:HB2	2.32	0.57
3:G:6:GLN:NE2	3:G:88:CYS:N	2.52	0.57
3:G:24:ASN:ND2	7:M:1:NAG:N2	2.51	0.57
4:H:53:LEU:O	4:H:53:LEU:HG	2.05	0.57
1:A:12:VAL:HG12	1:A:13:SER:N	2.20	0.57
1:C:81:LEU:HB3	1:C:118:TYR:CE1	2.40	0.57
1:C:233:THR:HB	1:C:243:LYS:HD2	1.87	0.57
2:D:22:PHE:HA	2:D:68:THR:O	2.04	0.57
1:A:253:LYS:O	1:A:255:GLN:N	2.38	0.57
4:H:99:GLY:HA3	4:H:105:PHE:CD2	2.40	0.57
3:G:33:GLN:NE2	3:G:47:PHE:O	2.38	0.57
3:G:66:LYS:O	3:G:67:GLU:HG3	2.05	0.57
1:A:234:ARG:HD3	1:A:242:GLN:OE1	2.05	0.56
1:C:5:LEU:HD13	1:C:28:VAL:HG22	1.87	0.56
3:E:24:ASN:CG	6:J:1:NAG:C1	2.65	0.56
3:E:96:SER:O	3:E:98:GLY:N	2.38	0.56
3:E:12:SER:C	3:E:13:LEU:HD23	2.26	0.56
3:E:36:ARG:HB2	3:E:46:LEU:HD11	1.86	0.56
4:H:46:LEU:HD11	4:H:95:TYR:CE1	2.40	0.56
1:C:249:VAL:HG13	1:C:257:TYR:CZ	2.39	0.56
2:D:-1:ASP:HB2	2:D:0:PRO:HD3	1.87	0.56
2:D:31:HIS:HB3	2:D:32:PRO:CD	2.32	0.56
3:E:153:LEU:HD12	3:E:182:TYR:OH	2.04	0.56
4:F:206:HIS:O	4:F:225:PHE:HB2	2.06	0.56
3:G:132:LYS:HA	4:H:135:PHE:HE2	1.69	0.56
4:H:75:SER:C	4:H:77:SER:H	2.08	0.56
3:E:146:PRO:HD2	3:E:194:HIS:CE1	2.39	0.56
3:G:33:GLN:OE1	3:G:48:TYR:CD1	2.59	0.56
1:C:209:TYR:HB3	1:C:210:PRO:HD3	1.88	0.56
4:H:56:PRO:C	4:H:58:HIS:H	2.07	0.56
4:H:165:TYR:CE1	4:H:209:ILE:HD12	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:GLN:C	1:A:116:LEU:HD12	2.26	0.56
3:E:6:GLN:HE22	3:E:87:PHE:HA	1.69	0.56
3:E:80:LEU:HD23	3:E:116:VAL:O	2.05	0.56
3:E:201:SER:OG	3:E:202:THR:N	2.38	0.56
4:F:128:ILE:HG22	4:F:158:PHE:N	2.21	0.56
4:H:37:TRP:CG	4:H:81:LEU:HD13	2.40	0.56
1:C:12:VAL:HG12	1:C:13:SER:N	2.19	0.56
2:D:11:SER:HB3	2:D:95:TRP:CZ2	2.40	0.56
3:E:134:GLY:O	3:E:135:THR:CB	2.54	0.56
3:E:189:THR:HG23	3:E:201:SER:OG	2.06	0.56
4:F:158:PHE:HB3	4:F:159:PRO:HD3	1.88	0.56
3:E:14:HIS:NE2	3:G:9:SER:OG	2.39	0.56
4:F:23:CYS:HB3	4:F:96:CYS:SG	2.46	0.56
4:H:57:THR:HB	4:H:59:ILE:HG13	1.87	0.56
1:A:74:SER:O	1:A:78:LEU:HB2	2.06	0.56
2:B:23:LEU:CD2	2:B:39:LEU:HD22	2.36	0.56
1:C:191:ARG:HD2	1:C:275:GLY:O	2.06	0.56
1:C:203:CYS:SG	1:C:272:LEU:HD12	2.46	0.56
3:E:3:GLN:CB	3:E:26:THR:HB	2.36	0.56
4:H:60:PHE:N	4:H:60:PHE:HD2	2.03	0.56
1:A:236:ALA:HB2	1:A:242:GLN:HE21	1.70	0.56
2:D:84:HIS:CG	2:D:85:VAL:N	2.74	0.56
1:C:32:GLN:NE2	2:D:53:ASP:CG	2.54	0.55
2:D:24:ASN:ND2	2:D:67:TYR:CB	2.69	0.55
3:G:133:ASN:C	3:G:133:ASN:OD1	2.44	0.55
4:H:134:ILE:HD11	4:H:223:ILE:CG2	2.36	0.55
1:C:105:PRO:O	1:C:106:ASP:C	2.44	0.55
3:E:130:ILE:HD11	3:E:201:SER:OG	2.06	0.55
3:G:3:GLN:O	3:G:25:PHE:HB3	2.06	0.55
1:C:34:LEU:HD23	1:C:34:LEU:C	2.27	0.55
2:D:74:GLU:HG2	2:D:74:GLU:O	2.06	0.55
3:E:108:PHE:CE1	4:F:46:LEU:HB2	2.41	0.55
1:A:202:ARG:HB2	1:A:202:ARG:CZ	2.37	0.55
1:C:184:PRO:HB3	1:C:266:LEU:HD23	1.86	0.55
2:D:79:ALA:HB2	2:D:94:LYS:HA	1.88	0.55
3:E:55:GLU:HB2	3:E:60:LYS:HG2	1.88	0.55
4:H:56:PRO:C	4:H:58:HIS:N	2.60	0.55
1:C:194:ARG:CD	1:C:198:ASP:HB2	2.33	0.55
4:F:146:LYS:CG	4:F:199:GLU:HG3	2.36	0.55
4:F:121:ASP:O	4:F:123:ARG:N	2.40	0.55
4:F:212:HIS:O	4:F:215:ASN:HB3	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:213:GLU:HG2	4:F:214:ASN:N	2.21	0.55
1:A:116:LEU:HD12	1:A:116:LEU:N	2.22	0.55
1:A:163:HIS:O	1:A:166:ASP:N	2.40	0.55
2:B:50:GLU:HB2	2:B:67:TYR:CZ	2.42	0.55
1:C:49:ALA:HB1	1:C:51:TRP:CD1	2.42	0.55
1:C:254:GLU:C	1:C:256:SER:H	2.10	0.55
1:C:266:LEU:CD1	1:C:270:LEU:HD22	2.36	0.55
3:G:30:ARG:NH1	3:G:91:ASP:OD2	2.40	0.55
3:G:53:THR:HG22	3:G:54:LYS:N	2.21	0.55
1:A:97:TRP:HD1	1:A:98:LEU:N	2.05	0.55
2:B:36:GLU:O	2:B:82:VAL:HA	2.07	0.55
4:H:51:TYR:O	4:H:51:TYR:CD2	2.60	0.55
1:A:215:LEU:HD23	1:A:261:VAL:HG13	1.88	0.55
1:C:6:ARG:HD3	1:C:100:GLY:HA3	1.89	0.55
2:D:17:ASN:N	2:D:17:ASN:ND2	2.49	0.55
4:F:55:THR:HB	4:F:56:PRO:HD2	1.89	0.55
1:C:13:SER:HB3	1:C:93:HIS:N	2.22	0.55
2:D:54:LEU:HD12	2:D:55:SER:N	2.21	0.55
2:B:84:HIS:H	2:B:87:LEU:HD22	1.71	0.54
1:A:22:PHE:CD1	1:A:22:PHE:C	2.81	0.54
1:A:249:VAL:HG13	1:A:257:TYR:CE1	2.43	0.54
4:F:157:PHE:CE1	4:F:189:TYR:CB	2.90	0.54
2:D:9:VAL:HG21	2:D:93:VAL:HB	1.88	0.54
4:F:159:PRO:HD3	4:F:214:ASN:HD22	1.71	0.54
4:H:165:TYR:CD1	4:H:165:TYR:C	2.80	0.54
2:D:73:THR:HB	2:D:76:ASP:OD2	2.07	0.54
1:C:1:GLY:O	1:C:3:HIS:CE1	2.60	0.54
1:C:13:SER:N	1:C:93:HIS:O	2.34	0.54
3:E:144:PHE:O	3:E:174:TYR:HB2	2.08	0.54
3:E:148:GLU:H	3:E:148:GLU:CD	2.11	0.54
1:A:55:GLU:O	1:A:56:GLU:C	2.46	0.54
1:A:103:VAL:HG12	1:A:104:GLU:H	1.71	0.54
2:D:7:ILE:HG23	2:D:27:VAL:HG22	1.88	0.54
3:E:7:SER:HB3	3:E:22:ARG:O	2.07	0.54
3:E:20:ALA:HB2	3:E:74:HIS:CD2	2.42	0.54
3:E:96:SER:C	3:E:98:GLY:N	2.60	0.54
4:F:23:CYS:SG	4:F:96:CYS:CB	2.96	0.54
1:A:9:TYR:CD1	1:A:70:GLN:HG2	2.42	0.54
1:A:269:PRO:O	1:A:271:ILE:HD12	2.08	0.54
2:B:40:LEU:HD23	2:B:45:ARG:HA	1.90	0.54
1:C:99:GLN:HE21	1:C:160:LEU:HD23	1.69	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:204:TRP:CH2	2:D:99:MET:HA	2.43	0.54
1:C:264:GLU:C	1:C:266:LEU:H	2.10	0.54
2:D:54:LEU:HD12	2:D:54:LEU:C	2.26	0.54
4:F:134:ILE:HG23	4:F:225:PHE:CZ	2.43	0.54
1:A:36:PHE:CD2	1:A:36:PHE:C	2.81	0.54
4:H:111:GLU:N	4:H:111:GLU:OE1	2.41	0.54
2:B:26:TYR:HD1	2:B:65:LEU:HB2	1.73	0.54
1:C:9:TYR:C	1:C:9:TYR:CD2	2.81	0.54
1:C:104:GLU:OE1	1:C:109:LEU:HD12	2.07	0.54
1:C:266:LEU:HD11	1:C:270:LEU:HD22	1.90	0.54
2:D:23:LEU:HB3	2:D:68:THR:CG2	2.35	0.54
3:E:124:ALA:HB3	3:E:145:TYR:N	2.21	0.54
3:G:94:HIS:HB2	3:G:104:ASP:CA	2.37	0.54
1:C:8:PHE:N	1:C:8:PHE:HD1	2.05	0.53
2:D:12:ARG:HG2	2:D:13:HIS:CE1	2.43	0.53
4:F:169:LYS:HG3	4:F:207:ARG:HD2	1.89	0.53
4:H:132:PRO:CG	4:H:221:GLN:HE22	2.20	0.53
4:H:210:VAL:CG1	4:H:211:LYS:N	2.69	0.53
4:H:27:ILE:CD1	4:H:98:TYR:OH	2.55	0.53
4:H:51:TYR:CE2	4:H:59:ILE:HD13	2.43	0.53
1:C:52:LEU:HD23	1:C:174:LYS:O	2.06	0.53
3:E:89:ALA:HB2	3:E:108:PHE:CD2	2.43	0.53
4:H:134:ILE:HG22	4:H:135:PHE:N	2.23	0.53
1:A:187:ALA:CB	1:A:272:LEU:HD11	2.38	0.53
1:C:9:TYR:CD1	1:C:70:GLN:NE2	2.74	0.53
4:F:4:LEU:HD22	4:F:98:TYR:CD2	2.39	0.53
4:F:61:LEU:HD12	4:F:69:GLU:HG3	1.91	0.53
1:C:7:TYR:N	1:C:7:TYR:CD1	2.76	0.53
1:C:216:THR:HG22	1:C:260:HIS:HB2	1.89	0.53
3:G:11:LEU:C	3:G:11:LEU:CD2	2.74	0.53
1:C:92:SER:O	1:C:93:HIS:HD2	1.91	0.53
1:A:23:ILE:CG2	1:A:24:ILE:N	2.72	0.53
2:B:5:PRO:CA	2:B:30:PHE:HB3	2.39	0.53
1:C:68:THR:O	1:C:71:GLY:N	2.42	0.53
1:C:148:VAL:HG12	1:C:149:GLY:N	2.24	0.53
2:D:35:ILE:HG12	2:D:37:VAL:HG23	1.90	0.53
4:F:33:VAL:CG1	4:F:34:THR:H	2.21	0.53
4:H:64:GLU:O	4:H:65:TYR:HB2	2.08	0.53
3:E:13:LEU:HB3	3:E:17:THR:HG21	1.90	0.53
4:F:28:GLU:C	4:F:30:PHE:N	2.61	0.53
1:C:61:GLU:O	1:C:64:THR:N	2.40	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:185:PRO:HD2	1:C:266:LEU:HG	1.90	0.53
1:C:252:GLY:N	1:C:254:GLU:OE2	2.42	0.53
4:F:50:LEU:CD2	4:F:61:LEU:HG	2.24	0.53
4:H:133:THR:HG22	4:H:153:LEU:O	2.09	0.53
1:A:157:SER:O	1:A:158:GLN:CG	2.57	0.53
1:A:208:PHE:CE2	1:A:242:GLN:HA	2.44	0.53
1:C:216:THR:CG2	1:C:260:HIS:HB2	2.39	0.53
4:F:38:TYR:CD2	4:F:48:PHE:HA	2.43	0.53
4:F:169:LYS:HG2	4:F:207:ARG:HB2	1.91	0.53
4:H:92:ALA:O	4:H:94:TYR:HE1	1.92	0.53
1:A:110:CYS:C	1:A:111:LEU:HD12	2.30	0.52
1:A:217:TRP:CD1	1:A:247:VAL:HG22	2.44	0.52
1:C:190:THR:HB	1:C:192:HIS:HE1	1.74	0.52
1:C:260:HIS:HB3	1:C:262:TYR:CE1	2.44	0.52
2:D:98:ASP:CB	2:D:99:MET:SD	2.98	0.52
1:C:242:GLN:OE1	2:D:10:TYR:CE1	2.62	0.52
3:E:15:GLU:O	3:E:17:THR:N	2.41	0.52
4:F:153:LEU:HD11	4:F:155:GLU:HG2	1.90	0.52
2:B:21:ASN:O	2:B:70:PHE:O	2.28	0.52
1:C:12:VAL:O	1:C:20:PRO:HB3	2.10	0.52
1:C:110:CYS:C	1:C:111:LEU:HD12	2.30	0.52
4:F:55:THR:HG22	4:F:56:PRO:CD	2.38	0.52
4:F:185:THR:O	4:F:188:THR:N	2.42	0.52
1:A:166:ASP:O	1:A:169:GLN:HB3	2.10	0.52
1:A:216:THR:HG22	1:A:260:HIS:HB2	1.92	0.52
3:G:6:GLN:HE22	3:G:88:CYS:N	2.07	0.52
1:A:207:GLY:HA2	1:A:240:THR:HB	1.90	0.52
3:E:200:HIS:HB2	3:E:203:ASP:OD2	2.10	0.52
1:A:8:PHE:HB2	1:A:25:VAL:CG2	2.40	0.52
1:A:31:MET:HG3	1:A:179:LEU:HD23	1.90	0.52
1:C:204:TRP:HH2	2:D:99:MET:HA	1.75	0.52
3:E:145:TYR:CD2	3:E:146:PRO:N	2.77	0.52
4:F:30:PHE:CE2	4:F:77:SER:HA	2.45	0.52
4:F:190:MET:HG2	4:F:191:LYS:N	2.23	0.52
3:G:11:LEU:HD23	3:G:12:SER:N	2.24	0.52
3:G:106:LEU:HB3	4:H:38:TYR:OH	2.09	0.52
1:A:61:GLU:O	1:A:64:THR:N	2.43	0.52
2:D:9:VAL:CG2	2:D:93:VAL:HB	2.39	0.52
2:D:59:ASP:OD1	2:D:59:ASP:C	2.48	0.52
3:E:3:GLN:HB2	3:E:26:THR:HB	1.92	0.52
3:G:20:ALA:HA	3:G:74:HIS:HA	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:133:ASN:HD21	5:I:1:NAG:H1	0.36	0.52
3:G:24:ASN:HB3	3:G:70:TYR:HD1	1.73	0.52
4:H:8:GLU:OE2	4:H:213:GLU:HG3	2.09	0.52
4:H:28:GLU:C	4:H:30:PHE:N	2.61	0.52
3:E:20:ALA:CB	3:E:74:HIS:CD2	2.93	0.52
4:F:185:THR:HG23	6:K:1:NAG:C7	2.40	0.52
4:H:14:PRO:O	4:H:17:GLU:HB2	2.10	0.52
4:H:54:ALA:HA	4:H:73:ASN:HD22	1.75	0.52
1:A:204:TRP:CH2	2:B:98:ASP:O	2.63	0.51
1:C:187:ALA:CB	1:C:272:LEU:HD11	2.39	0.51
3:E:145:TYR:CB	3:E:146:PRO:HD3	2.39	0.51
4:F:185:THR:O	4:F:186:ASN:C	2.49	0.51
1:A:65:ARG:NH1	1:A:158:GLN:HG3	2.24	0.51
3:G:137:VAL:O	3:G:180:GLY:N	2.43	0.51
2:D:27:VAL:HG11	2:D:35:ILE:CD1	2.41	0.51
4:F:33:VAL:CG1	4:F:34:THR:N	2.73	0.51
4:F:79:SER:O	4:F:80:ILE:HG13	2.09	0.51
1:C:184:PRO:HB3	1:C:266:LEU:HD21	1.92	0.51
4:F:228:ILE:CG2	4:F:229:LYS:N	2.73	0.51
1:C:73:LEU:CD1	3:G:99:TYR:H	2.24	0.51
1:C:262:TYR:O	1:C:263:HIS:HB2	2.11	0.51
4:F:173:THR:HG22	4:F:174:ILE:N	2.25	0.51
3:G:14:HIS:HA	3:G:117:GLU:O	2.10	0.51
1:C:152:THR:HG22	1:C:152:THR:O	2.10	0.51
2:D:98:ASP:HB3	2:D:99:MET:SD	2.49	0.51
1:A:248:VAL:O	1:A:248:VAL:HG23	2.10	0.51
2:B:5:PRO:HB3	2:B:30:PHE:HB3	1.91	0.51
3:E:44:ILE:HG22	3:E:45:SER:N	2.26	0.51
2:B:7:ILE:HD13	2:B:82:VAL:HG21	1.92	0.51
2:B:23:LEU:HD23	2:B:39:LEU:HD22	1.92	0.51
1:C:217:TRP:HD1	1:C:228:MET:HE3	1.76	0.51
3:E:30:ARG:HG2	3:E:30:ARG:HH11	1.76	0.51
4:H:63:LYS:O	4:H:63:LYS:CG	2.59	0.51
2:D:16:GLU:O	2:D:17:ASN:C	2.47	0.51
2:D:86:THR:HG22	2:D:87:LEU:N	2.16	0.51
3:E:38:ASN:O	3:E:39:SER:C	2.49	0.51
3:E:133:ASN:HB3	3:E:136:ASN:HB2	1.93	0.51
4:H:12:SER:HB2	4:H:118:ILE:CD1	2.34	0.51
4:H:208:CYS:HB3	4:H:223:ILE:HB	1.91	0.51
1:C:63:GLN:O	1:C:66:ILE:HB	2.11	0.51
1:C:208:PHE:O	1:C:240:THR:HB	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:37:GLN:O	3:E:37:GLN:HG3	2.11	0.51
3:E:185:SER:C	3:E:188:VAL:HG23	2.30	0.51
4:H:36:HIS:ND1	4:H:51:TYR:HB3	2.25	0.51
1:A:105:PRO:C	1:A:108:HIS:H	2.15	0.50
2:B:5:PRO:HA	2:B:30:PHE:HB3	1.93	0.50
3:E:30:ARG:HH22	3:E:103:THR:HG21	1.76	0.50
4:F:38:TYR:HB2	4:F:46:LEU:HD12	1.92	0.50
3:G:3:GLN:O	3:G:4:VAL:HG22	2.12	0.50
1:A:199:VAL:O	1:A:249:VAL:N	2.38	0.50
1:C:215:LEU:HD12	1:C:245:ALA:HB2	1.93	0.50
3:G:92:THR:O	3:G:104:ASP:HB2	2.12	0.50
1:A:208:PHE:CE1	1:A:213:ILE:HD12	2.46	0.50
1:A:219:LEU:HD21	1:A:257:TYR:CD2	2.47	0.50
1:C:104:GLU:HB3	1:C:109:LEU:HD12	1.93	0.50
4:F:25:VAL:CG2	4:F:35:ILE:HD11	2.39	0.50
3:G:7:SER:OG	3:G:8:PRO:CD	2.57	0.50
1:C:126:LEU:HD21	3:G:105:LYS:HE2	1.94	0.50
4:F:86:LEU:HD22	4:F:117:VAL:CG2	2.41	0.50
4:H:63:LYS:O	4:H:64:GLU:HG3	2.11	0.50
1:A:22:PHE:O	1:A:37:SER:CB	2.48	0.50
4:F:52:VAL:HG22	4:F:71:SER:OG	2.11	0.50
3:G:21:LEU:CD2	3:G:112:THR:HG21	2.42	0.50
1:A:209:TYR:O	1:A:241:PHE:HD1	1.95	0.50
1:A:213:ILE:O	1:A:213:ILE:HG22	2.12	0.50
2:D:31:HIS:O	2:D:33:SER:N	2.45	0.50
2:D:35:ILE:HG23	2:D:35:ILE:O	2.12	0.50
3:E:185:SER:CA	3:E:188:VAL:HG23	2.42	0.50
4:F:162:ILE:HG22	4:F:163:ARG:N	2.27	0.50
3:G:27:THR:O	3:G:28:THR:C	2.50	0.50
1:C:133:CYS:O	1:C:133:CYS:SG	2.70	0.50
3:E:197:GLU:OE1	3:E:197:GLU:HA	2.12	0.50
1:A:7:TYR:OH	1:A:63:GLN:NE2	2.45	0.50
1:A:14:ARG:O	1:A:15:PRO:O	2.29	0.50
1:A:16:GLY:C	1:A:18:GLY:H	2.14	0.50
1:A:202:ARG:HA	1:A:246:ALA:CB	2.41	0.50
1:A:231:VAL:HG23	1:A:244:TRP:O	2.11	0.50
1:A:258:THR:HG22	1:A:273:ARG:CG	2.42	0.50
1:C:12:VAL:CG1	1:C:13:SER:N	2.75	0.50
1:C:9:TYR:CZ	1:C:11:ALA:HB2	2.47	0.49
4:F:52:VAL:HG11	4:F:73:ASN:HB2	1.93	0.49
4:H:63:LYS:C	4:H:64:GLU:HG3	2.31	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:209:ILE:HG22	4:H:209:ILE:O	2.12	0.49
1:A:3:HIS:NE2	1:A:180:LEU:HD21	2.27	0.49
1:A:157:SER:O	1:A:158:GLN:NE2	2.44	0.49
1:C:23:ILE:CG2	1:C:24:ILE:H	2.21	0.49
1:C:113:TYR:CE2	1:C:130:PRO:HG3	2.47	0.49
3:E:50:ALA:O	3:E:68:ARG:NH1	2.45	0.49
3:E:104:ASP:OD2	4:F:36:HIS:CE1	2.65	0.49
3:E:133:ASN:CG	5:I:1:NAG:C1	2.67	0.49
3:G:105:LYS:HD3	4:H:48:PHE:CD2	2.47	0.49
1:A:19:GLU:O	1:A:19:GLU:HG3	2.13	0.49
1:C:187:ALA:HB1	1:C:272:LEU:HD11	1.93	0.49
1:C:208:PHE:CE1	1:C:241:PHE:HB2	2.47	0.49
2:D:24:ASN:HD21	2:D:67:TYR:HB2	1.78	0.49
4:F:55:THR:O	4:F:56:PRO:O	2.30	0.49
4:F:136:LEU:HD21	4:F:226:PRO:HD2	1.94	0.49
2:B:51:HIS:HB3	2:B:66:TYR:CD2	2.47	0.49
1:C:71:GLY:O	1:C:74:SER:OG	2.24	0.49
2:D:11:SER:HB3	2:D:95:TRP:HZ2	1.77	0.49
3:E:24:ASN:HD21	6:J:1:NAG:C7	2.19	0.49
3:E:24:ASN:CB	6:J:1:NAG:C1	2.90	0.49
4:H:24:LYS:HA	4:H:78:THR:HB	1.93	0.49
2:B:70:PHE:HE2	2:B:95:TRP:CZ3	2.30	0.49
1:C:88:SER:C	1:C:90:ASP:H	2.15	0.49
1:C:116:LEU:HD12	1:C:116:LEU:N	2.28	0.49
2:D:84:HIS:ND1	2:D:84:HIS:C	2.66	0.49
4:F:25:VAL:C	4:F:26:PHE:HD1	2.15	0.49
1:A:88:SER:C	1:A:90:ASP:H	2.16	0.49
1:C:9:TYR:OH	1:C:11:ALA:HB2	2.12	0.49
1:C:96:GLN:HB3	2:D:56:PHE:CE2	2.48	0.49
2:D:67:TYR:N	2:D:67:TYR:CD1	2.79	0.49
3:E:76:ARG:O	3:E:77:ASP:C	2.51	0.49
3:E:204:PHE:O	3:E:205:GLU:C	2.51	0.49
4:F:186:ASN:CG	6:K:1:NAG:O1	2.37	0.49
3:G:138:ALA:HB1	3:G:177:VAL:CG1	2.43	0.49
4:H:33:VAL:HG12	4:H:34:THR:N	2.27	0.49
4:H:50:LEU:HD11	4:H:61:LEU:HB2	1.94	0.49
4:F:37:TRP:CG	4:F:81:LEU:HD13	2.48	0.49
4:H:8:GLU:HA	4:H:8:GLU:OE1	2.13	0.49
4:H:27:ILE:HG22	4:H:28:GLU:O	2.13	0.49
1:A:63:GLN:O	1:A:67:VAL:HG23	2.13	0.49
3:E:185:SER:HA	3:E:188:VAL:CG2	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:11:ILE:O	4:F:116:ILE:N	2.40	0.49
4:F:159:PRO:O	4:F:160:ASP:OD1	2.31	0.49
4:F:185:THR:CG2	6:K:1:NAG:C8	2.83	0.49
4:F:186:ASN:ND2	6:K:1:NAG:H5	2.28	0.49
1:A:9:TYR:CB	1:A:70:GLN:NE2	2.75	0.48
1:C:95:LEU:C	1:C:95:LEU:HD12	2.33	0.48
4:F:53:LEU:HD13	4:F:59:ILE:CD1	2.43	0.48
4:H:12:SER:CB	4:H:118:ILE:HD11	2.35	0.48
1:A:2:SER:O	1:A:3:HIS:ND1	2.46	0.48
1:A:35:ARG:CZ	1:A:40:GLU:OE2	2.62	0.48
1:A:73:LEU:CD1	3:E:98:GLY:O	2.60	0.48
1:A:128:GLU:O	1:A:130:PRO:N	2.46	0.48
1:A:202:ARG:HB2	1:A:202:ARG:NH1	2.27	0.48
1:A:213:ILE:O	1:A:213:ILE:CG2	2.59	0.48
1:A:262:TYR:CD1	1:A:262:TYR:N	2.81	0.48
1:C:128:GLU:HG3	1:C:129:ASN:N	2.27	0.48
4:F:86:LEU:HD22	4:F:117:VAL:HG21	1.96	0.48
4:H:130:PRO:O	4:H:132:PRO:HD3	2.13	0.48
1:A:83:HIS:C	1:A:85:TYR:N	2.64	0.48
1:A:263:HIS:CG	1:A:264:GLU:N	2.82	0.48
3:E:17:THR:HG22	3:E:18:ASP:H	1.76	0.48
3:E:32:VAL:HG22	3:E:90:ALA:HB2	1.95	0.48
4:H:27:ILE:HD13	4:H:98:TYR:OH	2.13	0.48
1:C:191:ARG:N	1:C:274:TRP:HZ3	2.10	0.48
3:E:7:SER:OG	3:E:8:PRO:N	2.44	0.48
1:A:71:GLY:O	1:A:74:SER:OG	2.30	0.48
1:A:208:PHE:CE1	1:A:213:ILE:HB	2.49	0.48
1:A:209:TYR:CG	1:A:210:PRO:N	2.80	0.48
3:E:169:SER:HB3	3:E:170:PRO:CD	2.44	0.48
3:G:98:GLY:O	3:G:99:TYR:CD1	2.66	0.48
3:G:126:PRO:HG3	3:G:144:PHE:CB	2.43	0.48
4:H:207:ARG:HA	4:H:223:ILE:O	2.13	0.48
1:A:14:ARG:HB2	1:A:15:PRO:HD2	1.95	0.48
1:A:218:GLN:OE1	1:A:260:HIS:CG	2.66	0.48
1:C:204:TRP:HZ2	2:D:98:ASP:O	1.97	0.48
3:E:15:GLU:C	3:E:17:THR:H	2.17	0.48
4:F:157:PHE:CG	4:F:162:ILE:HD11	2.49	0.48
4:H:107:LYS:CG	4:H:109:PHE:HE1	2.25	0.48
1:A:69:ILE:O	1:A:72:GLN:HB2	2.13	0.48
2:B:73:THR:OG1	2:B:76:ASP:OD2	2.25	0.48
1:C:213:ILE:HG12	1:C:214:THR:H	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:149:VAL:CG1	3:E:150:THR:N	2.75	0.48
4:F:128:ILE:HG21	4:F:158:PHE:CB	2.26	0.48
4:H:134:ILE:CG2	4:H:135:PHE:N	2.76	0.48
1:A:209:TYR:HB3	1:A:210:PRO:CD	2.40	0.48
2:B:7:ILE:HD13	2:B:82:VAL:CG2	2.44	0.48
2:D:79:ALA:CA	2:D:93:VAL:O	2.62	0.48
1:A:124:PRO:HB3	3:E:28:THR:CG2	2.39	0.48
4:F:37:TRP:CZ2	4:F:96:CYS:SG	3.07	0.48
1:A:258:THR:HG22	1:A:273:ARG:HG2	1.95	0.48
3:E:2:ASP:CG	3:E:2:ASP:O	2.52	0.48
3:G:15:GLU:HG2	3:G:119:LYS:HE3	1.95	0.48
4:H:73:ASN:OD1	4:H:73:ASN:O	2.32	0.48
4:H:99:GLY:HA3	4:H:105:PHE:HD2	1.79	0.48
2:B:24:ASN:HD21	2:B:67:TYR:HB2	1.78	0.47
4:F:146:LYS:HG2	4:F:199:GLU:OE1	2.14	0.47
4:F:199:GLU:O	4:F:201:ALA:N	2.47	0.47
4:H:209:ILE:HA	4:H:221:GLN:O	2.13	0.47
1:A:9:TYR:HB2	1:A:70:GLN:NE2	2.29	0.47
1:A:57:ALA:C	1:A:59:ASN:N	2.66	0.47
1:C:5:LEU:HD21	1:C:167:LEU:HD22	1.96	0.47
1:C:217:TRP:HE1	1:C:246:ALA:HA	1.79	0.47
3:E:55:GLU:O	3:E:55:GLU:HG3	2.14	0.47
4:F:145:HIS:O	4:F:146:LYS:HB3	2.14	0.47
4:F:147:THR:CG2	4:F:148:GLY:N	2.71	0.47
4:F:160:ASP:HB2	4:F:189:TYR:CG	2.48	0.47
3:G:144:PHE:CE2	3:G:175:SER:HA	2.49	0.47
1:A:34:LEU:HD12	1:A:63:GLN:OE1	2.13	0.47
1:A:83:HIS:C	1:A:85:TYR:H	2.16	0.47
1:C:92:SER:O	1:C:93:HIS:CD2	2.66	0.47
2:D:23:LEU:HD23	2:D:39:LEU:HD22	1.96	0.47
3:E:61:SER:CB	3:E:72:THR:O	2.59	0.47
4:F:23:CYS:SG	4:F:96:CYS:SG	3.12	0.47
4:F:51:TYR:CE2	4:F:59:ILE:HD13	2.49	0.47
4:F:147:THR:CG2	4:F:148:GLY:H	2.27	0.47
1:A:97:TRP:CE3	1:A:116:LEU:HD21	2.49	0.47
1:A:105:PRO:C	1:A:107:ARG:N	2.68	0.47
2:B:4:THR:OG1	2:B:5:PRO:HD2	2.14	0.47
2:D:18:GLY:N	2:D:72:PRO:O	2.47	0.47
3:E:135:THR:O	3:E:181:GLN:HA	2.14	0.47
4:F:167:LYS:HB2	4:F:209:ILE:HD12	1.96	0.47
1:A:118:TYR:HB2	1:A:123:LEU:HD21	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:151:LEU:N	4:H:151:LEU:CD2	2.78	0.47
1:A:36:PHE:HD1	1:A:43:PRO:HA	1.78	0.47
1:A:199:VAL:CG1	1:A:200:THR:N	2.77	0.47
2:B:40:LEU:CA	2:B:44:GLU:O	2.56	0.47
2:D:37:VAL:HB	2:D:66:TYR:CE2	2.49	0.47
3:E:133:ASN:O	3:E:136:ASN:N	2.46	0.47
3:E:147:LYS:HD2	3:E:174:TYR:CE2	2.49	0.47
4:F:115:LEU:O	4:F:115:LEU:HG	2.15	0.47
1:A:126:LEU:N	3:E:92:THR:HG21	2.30	0.47
1:A:217:TRP:HE1	1:A:246:ALA:HA	1.79	0.47
1:A:255:GLN:C	1:A:257:TYR:H	2.18	0.47
1:A:274:TRP:CG	1:A:275:GLY:N	2.83	0.47
2:B:31:HIS:HB3	2:B:32:PRO:CD	2.39	0.47
1:C:9:TYR:OH	1:C:74:SER:CB	2.58	0.47
2:D:47:GLU:O	2:D:48:LYS:HG2	2.15	0.47
3:E:92:THR:CG2	3:E:93:TRP:N	2.78	0.47
3:E:148:GLU:N	3:E:148:GLU:OE1	2.44	0.47
4:F:21:ILE:CD1	4:F:94:TYR:HB2	2.45	0.47
4:F:49:LEU:HD13	4:F:69:GLU:CD	2.35	0.47
4:F:55:THR:CB	4:F:56:PRO:CD	2.92	0.47
4:H:164:VAL:HG12	4:H:165:TYR:N	2.29	0.47
1:A:209:TYR:CB	1:A:210:PRO:HD3	2.42	0.47
1:A:234:ARG:NH1	2:B:10:TYR:CD1	2.82	0.47
1:C:129:ASN:HB3	1:C:130:PRO:HD2	1.87	0.47
1:C:205:ALA:O	1:C:206:LEU:HD23	2.14	0.47
3:E:6:GLN:NE2	3:E:86:TYR:O	2.48	0.47
3:E:127:SER:OG	3:E:142:LYS:HB3	2.15	0.47
4:F:21:ILE:HG22	4:F:22:SER:N	2.30	0.47
4:F:72:LYS:O	4:F:79:SER:HA	2.13	0.47
1:A:79:MET:C	1:A:81:LEU:H	2.19	0.47
1:A:153:VAL:HG12	1:A:154:PRO:HD3	1.97	0.47
1:C:126:LEU:HD21	3:G:105:LYS:CE	2.44	0.47
2:D:39:LEU:HD12	2:D:49:VAL:HG21	1.97	0.47
4:F:141:GLU:O	4:F:142:THR:C	2.53	0.47
3:G:47:PHE:CZ	3:G:60:LYS:HA	2.50	0.47
3:G:152:SER:N	3:G:191:SER:O	2.48	0.47
1:A:97:TRP:CG	1:A:116:LEU:HG	2.50	0.47
2:B:24:ASN:ND2	2:B:67:TYR:CB	2.78	0.47
2:B:84:HIS:N	2:B:87:LEU:HD21	2.23	0.47
1:C:28:VAL:O	1:C:29:ASP:C	2.53	0.47
1:C:196:GLU:OE2	1:C:196:GLU:N	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:24:ASN:ND2	2:D:67:TYR:HB2	2.30	0.47
4:H:69:GLU:HA	4:H:82:THR:O	2.15	0.47
1:C:25:VAL:HG21	2:D:54:LEU:O	2.14	0.46
1:C:45:MET:SD	1:C:54:GLN:NE2	2.86	0.46
1:C:129:ASN:O	1:C:131:SER:N	2.49	0.46
4:F:49:LEU:HD13	4:F:69:GLU:OE2	2.15	0.46
4:F:72:LYS:O	4:F:79:SER:HB2	2.15	0.46
3:G:6:GLN:O	3:G:7:SER:O	2.32	0.46
1:A:169:GLN:O	1:A:170:LYS:C	2.52	0.46
1:C:3:HIS:ND1	1:C:3:HIS:N	2.63	0.46
4:F:198:PRO:O	4:F:202:MET:HG3	2.14	0.46
3:G:126:PRO:HG3	3:G:144:PHE:HB2	1.96	0.46
2:B:17:ASN:ND2	2:B:74:GLU:HB2	2.30	0.46
2:D:94:LYS:H	2:D:94:LYS:HG3	1.41	0.46
3:E:32:VAL:CG2	3:E:90:ALA:HB2	2.45	0.46
4:H:16:ASP:N	4:H:86:LEU:O	2.45	0.46
3:E:24:ASN:ND2	6:J:1:NAG:HN2	2.02	0.46
1:A:165:SER:OG	1:A:166:ASP:N	2.47	0.46
1:A:181:ARG:HG2	1:A:182:SER:N	2.30	0.46
1:C:51:TRP:HZ3	1:C:179:LEU:HG	1.81	0.46
3:E:145:TYR:CD2	3:E:146:PRO:CD	2.99	0.46
2:B:39:LEU:O	2:B:45:ARG:HA	2.15	0.46
2:B:42:ASN:ND2	2:B:76:ASP:OD1	2.49	0.46
2:B:69:GLU:N	2:B:69:GLU:OE1	2.47	0.46
2:D:31:HIS:HD1	2:D:32:PRO:N	2.13	0.46
2:D:67:TYR:N	2:D:67:TYR:HD1	2.13	0.46
3:E:139:CYS:HB2	3:E:153:LEU:HD21	1.97	0.46
3:E:200:HIS:O	3:E:201:SER:C	2.54	0.46
4:F:48:PHE:O	4:F:49:LEU:HD23	2.15	0.46
2:B:33:SER:O	2:B:35:ILE:HG22	2.15	0.46
2:B:67:TYR:CD1	2:B:67:TYR:N	2.84	0.46
1:C:219:LEU:O	1:C:220:ASN:HB3	2.15	0.46
2:D:41:LYS:HE2	2:D:42:ASN:ND2	2.30	0.46
3:E:7:SER:CB	3:E:22:ARG:HB2	2.44	0.46
4:F:185:THR:O	4:F:187:ASP:N	2.49	0.46
4:F:212:HIS:ND1	4:F:212:HIS:C	2.69	0.46
3:G:13:LEU:O	3:G:117:GLU:N	2.47	0.46
3:G:47:PHE:HZ	3:G:59:LEU:O	1.98	0.46
3:G:53:THR:CG2	3:G:54:LYS:N	2.79	0.46
1:C:176:LYS:HD3	1:C:180:LEU:HD11	1.97	0.46
3:E:21:LEU:HD22	3:E:112:THR:HG21	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:266:LEU:HD22	1:A:270:LEU:CD1	2.34	0.46
1:C:181:ARG:HG2	1:C:182:SER:H	1.81	0.46
1:C:218:GLN:HG2	1:C:223:GLU:HA	1.97	0.46
3:E:132:LYS:CE	3:E:132:LYS:N	2.74	0.46
4:F:75:SER:C	4:F:77:SER:H	2.19	0.46
4:H:92:ALA:O	4:H:94:TYR:CD1	2.69	0.46
4:H:189:TYR:N	4:H:189:TYR:CD1	2.83	0.46
1:A:155:HIS:NE2	1:A:157:SER:CA	2.65	0.46
1:A:175:GLY:O	1:A:176:LYS:C	2.54	0.46
1:C:4:SER:O	1:C:28:VAL:HA	2.15	0.46
1:C:97:TRP:CG	1:C:116:LEU:HG	2.51	0.46
2:D:13:HIS:HB3	2:D:14:PRO:CD	2.46	0.46
4:F:151:LEU:HD12	4:F:151:LEU:HA	1.79	0.46
3:G:103:THR:HG23	3:G:103:THR:O	2.16	0.46
1:C:25:VAL:HG13	2:D:53:ASP:HB3	1.98	0.45
3:E:43:LEU:HD11	4:F:46:LEU:HD21	1.97	0.45
4:H:9:ILE:O	4:H:113:THR:HG23	2.16	0.45
4:H:133:THR:C	5:L:1:NAG:H62	2.36	0.45
1:A:84:PHE:HE1	3:E:30:ARG:HH21	1.65	0.45
1:A:180:LEU:HD23	1:A:180:LEU:HA	1.62	0.45
2:D:37:VAL:HG13	2:D:82:VAL:HG22	1.97	0.45
4:F:60:PHE:HB3	4:F:70:ALA:HB2	1.98	0.45
1:A:191:ARG:N	1:A:274:TRP:CZ3	2.84	0.45
1:A:196:GLU:H	1:A:196:GLU:HG3	1.53	0.45
2:B:59:ASP:O	2:B:61:SER:N	2.49	0.45
2:B:80:CYS:O	2:B:92:ILE:HA	2.17	0.45
1:C:55:GLU:HA	1:C:55:GLU:OE1	2.16	0.45
3:E:132:LYS:N	3:E:132:LYS:CD	2.79	0.45
3:E:185:SER:HA	3:E:188:VAL:HG23	1.98	0.45
1:A:73:LEU:HD23	1:A:73:LEU:N	2.31	0.45
1:A:103:VAL:HG23	1:A:168:LEU:HD22	1.97	0.45
1:C:97:TRP:CE2	1:C:116:LEU:HD11	2.52	0.45
1:C:234:ARG:HA	1:C:235:PRO:HD3	1.70	0.45
3:E:30:ARG:HG2	3:E:30:ARG:NH1	2.30	0.45
3:E:153:LEU:CD2	3:E:190:CYS:SG	3.05	0.45
3:G:147:LYS:HG3	3:G:174:TYR:CE2	2.44	0.45
1:C:9:TYR:CE2	1:C:11:ALA:HB2	2.52	0.45
1:C:194:ARG:HB2	1:C:198:ASP:C	2.29	0.45
4:F:134:ILE:HG22	4:F:135:PHE:N	2.32	0.45
4:F:215:ASN:OD1	4:F:215:ASN:O	2.34	0.45
3:G:67:GLU:OE1	3:G:69:ARG:CD	2.65	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:5:GLU:HG3	4:H:7:PRO:HD3	1.98	0.45
4:H:51:TYR:H	4:H:51:TYR:HD2	1.64	0.45
4:H:72:LYS:O	4:H:79:SER:HA	2.16	0.45
1:A:6:ARG:HG3	1:A:98:LEU:HD11	1.98	0.45
1:A:97:TRP:CZ3	1:A:116:LEU:HD21	2.52	0.45
2:B:23:LEU:HB3	2:B:68:THR:HG22	1.99	0.45
2:D:5:PRO:HB3	2:D:30:PHE:CB	2.43	0.45
4:F:146:LYS:HG3	4:F:199:GLU:CG	2.46	0.45
1:A:202:ARG:CD	1:A:204:TRP:CZ2	2.97	0.45
1:C:25:VAL:HG12	1:C:27:TYR:CE1	2.52	0.45
1:C:55:GLU:O	1:C:57:ALA:N	2.48	0.45
3:G:26:THR:O	3:G:26:THR:HG22	2.16	0.45
3:G:27:THR:O	3:G:29:MET:SD	2.75	0.45
4:H:6:GLN:HG2	4:H:23:CYS:HB3	1.98	0.45
1:A:79:MET:C	1:A:81:LEU:N	2.70	0.45
1:A:187:ALA:HB3	1:A:270:LEU:CD2	2.47	0.45
2:D:37:VAL:HG22	2:D:82:VAL:HG13	1.99	0.45
1:A:60:TRP:O	1:A:63:GLN:N	2.46	0.45
1:C:95:LEU:HD12	1:C:96:GLN:N	2.32	0.45
3:E:40:ARG:HB3	4:F:163:ARG:NH2	2.32	0.45
3:E:96:SER:OG	3:E:100:GLU:HB2	2.17	0.45
3:G:113:GLN:HG3	3:G:113:GLN:O	2.17	0.45
1:A:64:THR:HG1	1:A:65:ARG:H	1.64	0.44
1:C:235:PRO:HG2	2:D:26:TYR:CE1	2.52	0.44
3:E:35:PHE:CE1	3:E:108:PHE:HE2	2.34	0.44
4:H:21:ILE:HD12	4:H:81:LEU:HD23	1.99	0.44
4:H:33:VAL:HG13	4:H:34:THR:H	1.81	0.44
1:C:126:LEU:CA	3:G:92:THR:HG21	2.47	0.44
3:E:4:VAL:HG13	3:E:25:PHE:CD2	2.52	0.44
3:E:30:ARG:HH22	3:E:103:THR:CG2	2.30	0.44
1:A:103:VAL:CG1	1:A:104:GLU:N	2.80	0.44
1:A:268:GLU:O	1:A:269:PRO:C	2.55	0.44
1:C:117:ALA:HB1	1:C:121:GLU:H	1.83	0.44
1:C:164:CYS:C	1:C:166:ASP:N	2.70	0.44
1:C:232:GLU:HB3	2:D:8:GLN:NE2	2.32	0.44
2:D:13:HIS:HB3	2:D:14:PRO:HD2	1.99	0.44
4:F:7:PRO:HG2	4:F:22:SER:OG	2.17	0.44
4:F:23:CYS:SG	4:F:96:CYS:HB3	2.58	0.44
1:A:73:LEU:CB	1:A:77:ASN:ND2	2.81	0.44
1:C:230:LEU:CD2	1:C:245:ALA:HB2	2.47	0.44
2:D:39:LEU:O	2:D:40:LEU:HD23	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:84:HIS:CE1	2:D:85:VAL:O	2.71	0.44
4:F:63:LYS:O	4:F:63:LYS:HG3	2.18	0.44
4:H:93:ILE:HG22	4:H:95:TYR:CE1	2.53	0.44
1:A:39:LYS:O	1:A:40:GLU:CG	2.64	0.44
1:A:191:ARG:HB3	1:A:274:TRP:CH2	2.53	0.44
1:A:199:VAL:N	1:A:249:VAL:O	2.51	0.44
2:B:31:HIS:O	2:B:32:PRO:C	2.55	0.44
2:B:49:VAL:HG22	2:B:68:THR:HB	2.00	0.44
1:C:191:ARG:CB	1:C:274:TRP:HZ3	2.28	0.44
3:E:89:ALA:HB1	3:E:107:VAL:O	2.17	0.44
3:E:165:ALA:O	3:E:176:ALA:HA	2.17	0.44
4:F:150:TYR:CD2	4:F:225:PHE:HD2	2.35	0.44
4:H:131:LYS:N	4:H:155:GLU:O	2.51	0.44
1:A:16:GLY:C	1:A:18:GLY:N	2.71	0.44
1:A:22:PHE:CZ	1:A:71:GLY:HA3	2.52	0.44
2:B:56:PHE:HB2	2:B:61:SER:O	2.18	0.44
1:C:188:HIS:CE1	1:C:204:TRP:HB2	2.52	0.44
3:E:184:ASP:O	3:E:185:SER:C	2.56	0.44
4:F:159:PRO:O	4:F:160:ASP:CB	2.66	0.44
3:G:89:ALA:HB1	3:G:106:LEU:HG	1.99	0.44
3:G:198:THR:CG2	3:G:199:VAL:N	2.81	0.44
4:H:198:PRO:O	4:H:200:ARG:N	2.51	0.44
1:A:4:SER:HB2	1:A:102:ASP:OD1	2.17	0.44
1:A:76:ARG:O	1:A:79:MET:N	2.48	0.44
1:A:84:PHE:CE1	3:E:30:ARG:NE	2.77	0.44
1:A:234:ARG:HD2	1:A:242:GLN:O	2.17	0.44
2:B:84:HIS:O	2:B:87:LEU:CD2	2.66	0.44
1:C:87:LYS:HD3	1:C:93:HIS:CE1	2.52	0.44
3:E:145:TYR:CD2	3:E:146:PRO:HG3	2.53	0.44
4:F:124:LEU:O	4:F:124:LEU:HG	2.17	0.44
4:F:132:PRO:CG	4:F:221:GLN:HE22	2.30	0.44
4:F:136:LEU:HB3	4:F:137:PRO:CD	2.48	0.44
4:H:193:SER:O	4:H:194:TRP:HB3	2.17	0.44
3:E:131:MET:HB2	3:E:138:ALA:HB3	2.00	0.44
3:E:179:LEU:HD11	4:F:153:LEU:HD22	1.99	0.44
4:F:139:VAL:O	4:F:140:ALA:C	2.55	0.44
4:H:94:TYR:O	4:H:112:GLY:HA2	2.17	0.44
1:A:12:VAL:CG1	1:A:13:SER:N	2.81	0.44
1:A:81:LEU:HD13	1:A:118:TYR:HD1	1.82	0.44
1:A:209:TYR:CB	1:A:210:PRO:CD	2.96	0.44
1:C:35:ARG:HG2	1:C:36:PHE:N	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:81:LEU:HG	1:C:118:TYR:CD1	2.53	0.44
1:C:208:PHE:CZ	1:C:241:PHE:O	2.70	0.44
2:D:29:GLY:HA2	2:D:61:SER:OG	2.18	0.44
3:E:35:PHE:CE1	3:E:108:PHE:CE2	3.06	0.44
3:G:24:ASN:N	3:G:24:ASN:OD1	2.50	0.44
3:G:146:PRO:C	3:G:148:GLU:N	2.71	0.44
4:H:60:PHE:HD2	4:H:60:PHE:H	1.55	0.44
1:C:97:TRP:HD1	1:C:98:LEU:H	1.61	0.43
1:C:254:GLU:C	1:C:256:SER:N	2.71	0.43
2:D:56:PHE:HB2	2:D:61:SER:O	2.18	0.43
4:H:105:PHE:C	4:H:107:LYS:N	2.64	0.43
1:A:10:THR:HG21	2:B:62:PHE:HE2	1.82	0.43
1:A:208:PHE:CD2	1:A:213:ILE:HD12	2.54	0.43
2:B:13:HIS:O	2:B:15:ALA:N	2.51	0.43
4:F:20:GLN:HA	4:F:81:LEU:O	2.19	0.43
4:H:148:GLY:O	4:H:197:VAL:HG23	2.18	0.43
7:M:2:NAG:H82	7:M:2:NAG:C3	2.47	0.43
1:A:231:VAL:CG2	1:A:244:TRP:O	2.67	0.43
2:B:37:VAL:HA	2:B:81:ARG:O	2.18	0.43
1:C:87:LYS:HB3	1:C:93:HIS:CE1	2.41	0.43
1:C:98:LEU:C	1:C:98:LEU:CD1	2.77	0.43
1:C:166:ASP:O	1:C:170:LYS:HG2	2.18	0.43
3:E:6:GLN:OE1	3:E:88:CYS:SG	2.77	0.43
3:G:8:PRO:O	3:G:112:THR:HG23	2.18	0.43
4:H:25:VAL:HG12	4:H:26:PHE:N	2.33	0.43
4:H:157:PHE:CG	4:H:159:PRO:HD2	2.54	0.43
1:A:28:VAL:O	1:A:29:ASP:HB2	2.17	0.43
1:A:38:SER:O	1:A:39:LYS:HB3	2.18	0.43
1:A:238:ASP:OD1	1:A:238:ASP:C	2.57	0.43
1:C:34:LEU:CD2	1:C:35:ARG:N	2.80	0.43
3:E:10:ALA:HB3	3:G:12:SER:HB3	2.00	0.43
4:F:55:THR:HB	4:F:56:PRO:CD	2.48	0.43
1:A:97:TRP:CE2	1:A:116:LEU:HD11	2.54	0.43
2:B:7:ILE:CD1	2:B:82:VAL:HG21	2.49	0.43
1:C:76:ARG:C	1:C:79:MET:HB2	2.38	0.43
2:D:23:LEU:CD2	2:D:39:LEU:HD22	2.48	0.43
3:E:37:GLN:HG2	3:E:87:PHE:HE1	1.84	0.43
4:F:82:THR:HG22	4:F:83:ILE:N	2.33	0.43
4:F:105:PHE:HD2	4:F:107:LYS:HG2	1.82	0.43
4:H:75:SER:C	4:H:77:SER:N	2.72	0.43
1:A:152:THR:HG22	1:A:153:VAL:N	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:54:LEU:HD11	2:B:62:PHE:HD2	1.84	0.43
1:C:231:VAL:HG11	1:C:244:TRP:CZ2	2.54	0.43
1:C:234:ARG:HB2	2:D:10:TYR:OH	2.19	0.43
2:D:98:ASP:C	2:D:99:MET:SD	2.97	0.43
3:E:141:VAL:HG21	3:E:151:ILE:HD11	1.99	0.43
4:F:190:MET:CG	4:F:191:LYS:N	2.82	0.43
3:G:7:SER:CB	3:G:22:ARG:H	2.31	0.43
3:G:143:ASP:CB	3:G:173:LYS:HD2	2.47	0.43
1:A:43:PRO:HG2	1:A:64:THR:HA	2.01	0.43
1:A:69:ILE:O	1:A:70:GLN:C	2.55	0.43
2:B:42:ASN:ND2	2:B:76:ASP:HA	2.29	0.43
1:C:5:LEU:HD12	1:C:27:TYR:O	2.19	0.43
1:C:23:ILE:O	1:C:24:ILE:HG12	2.19	0.43
2:D:56:PHE:CB	2:D:61:SER:O	2.66	0.43
3:E:123:PRO:HA	3:E:146:PRO:HD3	1.99	0.43
4:H:3:LYS:HE3	4:H:27:ILE:HD11	2.01	0.43
4:H:90:ASP:O	4:H:94:TYR:OH	2.37	0.43
4:H:105:PHE:C	4:H:107:LYS:H	2.13	0.43
4:H:147:THR:HG22	4:H:148:GLY:N	2.33	0.43
1:A:8:PHE:HB2	1:A:25:VAL:HG23	2.01	0.43
2:B:54:LEU:HA	2:B:64:LEU:CD2	2.49	0.43
1:C:97:TRP:CD2	1:C:116:LEU:HG	2.53	0.43
1:C:202:ARG:HA	1:C:246:ALA:HB2	2.01	0.43
3:E:31:SER:HA	3:E:50:ALA:HA	2.01	0.43
3:E:46:LEU:O	3:E:47:PHE:CD2	2.71	0.43
3:E:164:PRO:HG3	3:E:178:LYS:CE	2.49	0.43
4:F:75:SER:O	4:F:77:SER:N	2.46	0.43
3:G:125:LYS:HA	3:G:126:PRO:HD3	1.53	0.43
4:H:51:TYR:O	4:H:51:TYR:HD2	2.02	0.43
1:C:8:PHE:CD2	2:D:56:PHE:CE1	3.07	0.43
2:D:41:LYS:HE2	2:D:42:ASN:HD21	1.83	0.43
3:E:4:VAL:HG13	3:E:25:PHE:HD2	1.84	0.43
3:E:122:PRO:O	3:E:123:PRO:O	2.36	0.43
4:F:228:ILE:CG2	4:F:229:LYS:H	2.29	0.43
1:A:185:PRO:CB	1:A:208:PHE:HB3	2.49	0.43
1:C:219:LEU:HB2	1:C:224:LEU:HD11	1.99	0.43
4:F:30:PHE:O	4:F:33:VAL:HG23	2.19	0.43
4:F:132:PRO:HG3	4:F:223:ILE:HD11	2.00	0.43
4:F:212:HIS:O	4:F:213:GLU:C	2.57	0.43
3:G:7:SER:HB3	3:G:22:ARG:H	1.83	0.43
3:G:106:LEU:CB	4:H:38:TYR:OH	2.67	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:108:PHE:N	3:G:108:PHE:CD1	2.85	0.43
3:G:134:GLY:O	3:G:136:ASN:ND2	2.51	0.43
1:A:81:LEU:HD22	1:A:118:TYR:CD1	2.54	0.42
2:B:17:ASN:OD1	2:B:17:ASN:N	2.49	0.42
1:C:262:TYR:N	1:C:262:TYR:CD1	2.87	0.42
2:D:24:ASN:ND2	2:D:67:TYR:HB3	2.33	0.42
4:F:88:GLU:C	4:F:90:ASP:N	2.70	0.42
4:F:90:ASP:O	4:F:115:LEU:HD23	2.19	0.42
4:F:157:PHE:CD1	4:F:157:PHE:C	2.93	0.42
1:A:73:LEU:C	1:A:75:GLU:N	2.72	0.42
1:A:73:LEU:HB2	1:A:77:ASN:ND2	2.34	0.42
1:C:14:ARG:O	1:C:16:GLY:N	2.52	0.42
1:C:51:TRP:CZ3	1:C:179:LEU:HG	2.54	0.42
2:D:95:TRP:CD1	2:D:96:ASP:N	2.87	0.42
3:E:14:HIS:C	3:E:15:GLU:O	2.57	0.42
4:F:63:LYS:O	4:F:64:GLU:HB2	2.18	0.42
3:G:148:GLU:O	3:G:149:VAL:CG2	2.61	0.42
2:B:59:ASP:C	2:B:61:SER:H	2.23	0.42
2:B:73:THR:O	2:B:74:GLU:C	2.58	0.42
1:C:73:LEU:CD1	3:G:99:TYR:HB2	2.46	0.42
1:C:102:ASP:O	1:C:103:VAL:HG23	2.19	0.42
4:F:28:GLU:O	4:F:30:PHE:N	2.52	0.42
4:F:160:ASP:HB2	4:F:189:TYR:CD2	2.54	0.42
4:F:169:LYS:HB2	4:F:207:ARG:HG3	2.00	0.42
3:G:18:ASP:HA	3:G:75:ILE:O	2.19	0.42
3:G:26:THR:O	3:G:26:THR:CG2	2.67	0.42
3:G:46:LEU:HA	3:G:46:LEU:HD23	1.80	0.42
3:G:47:PHE:CZ	3:G:59:LEU:O	2.72	0.42
2:B:87:LEU:HD23	2:B:87:LEU:O	2.20	0.42
2:D:23:LEU:C	2:D:24:ASN:HD22	2.23	0.42
2:D:80:CYS:O	2:D:93:VAL:N	2.49	0.42
3:E:24:ASN:OD1	3:E:24:ASN:C	2.48	0.42
3:E:80:LEU:CD2	3:E:116:VAL:O	2.66	0.42
4:F:144:LEU:HA	4:F:144:LEU:HD22	1.64	0.42
3:G:166:ILE:CG2	3:G:175:SER:O	2.56	0.42
3:G:181:GLN:H	3:G:181:GLN:HG3	1.66	0.42
1:A:83:HIS:O	1:A:85:TYR:N	2.53	0.42
1:A:97:TRP:CD1	1:A:98:LEU:N	2.88	0.42
1:A:190:THR:OG1	1:A:202:ARG:HB3	2.20	0.42
1:A:204:TRP:CH2	1:A:244:TRP:CD1	3.08	0.42
1:C:236:ALA:CB	1:C:240:THR:O	2.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:12:SER:HA	3:E:115:THR:O	2.20	0.42
3:E:135:THR:O	3:E:135:THR:HG22	2.19	0.42
3:E:145:TYR:CG	3:E:146:PRO:N	2.86	0.42
1:A:61:GLU:O	1:A:65:ARG:N	2.38	0.42
2:B:5:PRO:CB	2:B:30:PHE:HB3	2.49	0.42
1:C:22:PHE:CE2	1:C:38:SER:HB3	2.54	0.42
1:C:191:ARG:HB3	1:C:274:TRP:CZ3	2.49	0.42
3:E:6:GLN:O	3:E:7:SER:O	2.37	0.42
3:E:61:SER:CA	3:E:72:THR:O	2.68	0.42
4:F:19:ALA:O	4:F:83:ILE:N	2.53	0.42
3:G:99:TYR:CD1	3:G:99:TYR:N	2.88	0.42
4:H:221:GLN:NE2	4:H:223:ILE:HD11	2.35	0.42
1:A:153:VAL:CG1	1:A:154:PRO:HD3	2.49	0.42
2:B:49:VAL:HG13	2:B:67:TYR:O	2.19	0.42
2:B:75:LYS:HA	2:B:75:LYS:HD3	1.61	0.42
3:E:117:GLU:OE1	3:E:117:GLU:HA	2.20	0.42
4:H:31:ARG:C	4:H:33:VAL:H	2.22	0.42
1:A:103:VAL:O	1:A:104:GLU:HB2	2.18	0.42
1:C:77:ASN:O	1:C:78:LEU:C	2.58	0.42
1:C:219:LEU:HB3	1:C:224:LEU:HD21	2.02	0.42
1:C:234:ARG:H	1:C:234:ARG:HG3	1.40	0.42
1:C:249:VAL:HG21	1:C:257:TYR:CD2	2.55	0.42
3:E:7:SER:HB3	3:E:22:ARG:CB	2.46	0.42
3:G:114:VAL:HG12	3:G:115:THR:N	2.35	0.42
3:G:128:VAL:HG11	3:G:201:SER:HB3	2.01	0.42
1:A:55:GLU:O	1:A:57:ALA:N	2.53	0.42
1:A:83:HIS:C	1:A:86:ASN:H	2.23	0.42
1:A:84:PHE:CD2	1:A:84:PHE:O	2.73	0.42
3:E:90:ALA:O	3:E:107:VAL:HG22	2.20	0.42
3:E:169:SER:HB3	3:E:170:PRO:HD2	2.01	0.42
4:F:39:ARG:HG3	4:F:94:TYR:CE2	2.55	0.42
3:G:59:LEU:C	3:G:60:LYS:HG2	2.40	0.42
1:A:65:ARG:NH1	1:A:158:GLN:CG	2.83	0.42
1:A:185:PRO:HD2	1:A:266:LEU:HD23	2.00	0.42
1:C:233:THR:H	1:C:233:THR:HG22	1.49	0.42
3:E:40:ARG:HA	3:E:40:ARG:HD3	1.67	0.42
3:E:55:GLU:CB	3:E:60:LYS:HG2	2.49	0.42
3:G:26:THR:CG2	3:G:69:ARG:HH11	2.33	0.42
1:A:193:PRO:HG3	1:A:199:VAL:HG22	2.01	0.41
1:C:129:ASN:O	1:C:130:PRO:C	2.58	0.41
1:C:151:SER:O	1:C:153:VAL:HG23	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:210:PRO:O	1:C:211:ALA:C	2.59	0.41
1:C:233:THR:CB	1:C:243:LYS:HZ2	2.33	0.41
2:D:65:LEU:HD12	2:D:66:TYR:H	1.84	0.41
4:F:20:GLN:HA	4:F:82:THR:HA	2.02	0.41
4:F:186:ASN:HD21	6:K:1:NAG:C5	2.31	0.41
1:A:263:HIS:CG	1:A:264:GLU:H	2.37	0.41
2:B:23:LEU:HD23	2:B:39:LEU:CD1	2.43	0.41
1:C:10:THR:HG21	2:D:62:PHE:CE2	2.55	0.41
1:C:234:ARG:HD3	2:D:10:TYR:CZ	2.55	0.41
2:D:79:ALA:CB	2:D:94:LYS:HA	2.49	0.41
3:G:190:CYS:H	3:G:201:SER:HG	1.67	0.41
1:A:8:PHE:CD1	1:A:8:PHE:N	2.88	0.41
1:C:39:LYS:O	1:C:39:LYS:HG2	2.20	0.41
1:C:249:VAL:CG2	1:C:257:TYR:CE2	3.02	0.41
3:E:92:THR:HG22	3:E:93:TRP:O	2.20	0.41
3:E:139:CYS:O	3:E:177:VAL:HA	2.21	0.41
3:G:25:PHE:CD1	3:G:25:PHE:N	2.87	0.41
3:G:101:LEU:HD23	3:G:101:LEU:HA	1.79	0.41
1:A:73:LEU:HD11	3:E:98:GLY:O	2.21	0.41
1:C:23:ILE:CG2	1:C:24:ILE:N	2.70	0.41
1:C:77:ASN:C	1:C:79:MET:N	2.73	0.41
1:C:204:TRP:HE3	1:C:206:LEU:HD21	1.83	0.41
2:D:41:LYS:O	2:D:43:GLY:N	2.53	0.41
3:G:20:ALA:CB	3:G:74:HIS:HA	2.50	0.41
2:B:23:LEU:HG	2:B:24:ASN:N	2.36	0.41
1:C:126:LEU:N	3:G:92:THR:HG21	2.35	0.41
1:C:184:PRO:CG	1:C:265:GLY:O	2.64	0.41
2:D:33:SER:O	2:D:34:ASP:C	2.58	0.41
2:D:40:LEU:HA	2:D:44:GLU:O	2.19	0.41
3:E:35:PHE:N	3:E:87:PHE:O	2.47	0.41
3:E:64:ASP:HB3	3:E:67:GLU:OE1	2.20	0.41
4:F:6:GLN:HA	4:F:7:PRO:HD3	1.84	0.41
4:F:86:LEU:HD23	4:F:86:LEU:HA	1.73	0.41
4:F:137:PRO:HD3	4:F:150:TYR:CD2	2.56	0.41
2:D:19:LYS:HD3	2:D:19:LYS:HA	1.84	0.41
3:E:13:LEU:HB3	3:E:17:THR:CG2	2.49	0.41
4:F:73:ASN:N	4:F:74:PRO:HD3	2.34	0.41
4:F:136:LEU:HB3	4:F:137:PRO:HD2	2.02	0.41
3:G:5:GLU:HA	3:G:5:GLU:OE1	2.20	0.41
3:G:112:THR:O	3:G:112:THR:HG22	2.20	0.41
3:G:163:ASP:HA	3:G:164:PRO:HD3	1.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:3:LYS:HE3	4:H:27:ILE:CD1	2.50	0.41
4:H:91:GLU:HG3	4:H:115:LEU:O	2.20	0.41
2:B:31:HIS:O	2:B:33:SER:N	2.54	0.41
1:C:219:LEU:O	1:C:220:ASN:CB	2.69	0.41
3:E:62:ALA:O	3:E:71:SER:HA	2.21	0.41
3:E:99:TYR:N	3:E:99:TYR:CD1	2.88	0.41
4:F:51:TYR:CD2	4:F:59:ILE:HD13	2.55	0.41
2:B:42:ASN:HD21	2:B:76:ASP:CA	2.30	0.41
2:D:31:HIS:CB	2:D:32:PRO:CD	2.99	0.41
2:D:75:LYS:HD3	2:D:75:LYS:HA	1.93	0.41
2:D:99:MET:SD	2:D:99:MET:N	2.94	0.41
4:F:69:GLU:CB	4:F:82:THR:O	2.68	0.41
4:F:118:ILE:HD11	4:F:124:LEU:HD13	2.02	0.41
4:F:162:ILE:C	4:F:163:ARG:HD3	2.40	0.41
4:H:6:GLN:HG2	4:H:23:CYS:HB2	2.03	0.41
4:H:49:LEU:O	4:H:50:LEU:HG	2.21	0.41
2:B:23:LEU:HD21	2:B:39:LEU:HD22	2.03	0.41
2:B:26:TYR:CD1	2:B:65:LEU:HB2	2.53	0.41
1:C:6:ARG:CD	1:C:100:GLY:HA3	2.50	0.41
1:C:42:THR:HA	1:C:43:PRO:HD3	1.85	0.41
1:C:51:TRP:CH2	1:C:179:LEU:HD21	2.55	0.41
1:C:62:GLN:O	1:C:66:ILE:HG13	2.21	0.41
1:C:84:PHE:HD1	4:H:103:SER:O	2.03	0.41
1:C:202:ARG:HD3	2:D:98:ASP:O	2.21	0.41
2:D:59:ASP:OD1	2:D:59:ASP:O	2.39	0.41
3:E:61:SER:HA	3:E:72:THR:O	2.21	0.41
3:G:15:GLU:N	3:G:117:GLU:O	2.54	0.41
4:H:99:GLY:HA3	4:H:105:PHE:CE2	2.55	0.41
1:A:9:TYR:CD2	1:A:9:TYR:C	2.94	0.41
1:A:17:LEU:HD23	1:A:17:LEU:HA	1.79	0.41
1:A:61:GLU:C	1:A:64:THR:HG1	2.18	0.41
1:A:207:GLY:HA2	1:A:240:THR:CB	2.51	0.41
1:C:10:THR:HG21	2:D:62:PHE:HE2	1.86	0.41
1:C:205:ALA:C	1:C:206:LEU:HD23	2.42	0.41
2:D:83:ASN:HB2	2:D:90:PRO:HB3	2.03	0.41
3:E:17:THR:CG2	3:E:18:ASP:N	2.83	0.41
4:F:145:HIS:O	4:F:146:LYS:CB	2.66	0.41
4:H:13:ARG:HA	4:H:14:PRO:HD3	1.92	0.41
4:H:53:LEU:O	4:H:53:LEU:CG	2.69	0.41
4:H:60:PHE:CD1	4:H:62:ASP:OD1	2.74	0.41
4:H:157:PHE:CE1	4:H:189:TYR:HB2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:14:ARG:CB	1:A:15:PRO:HD3	2.50	0.40
1:A:78:LEU:HD13	1:A:95:LEU:HB3	2.03	0.40
1:A:219:LEU:CD2	1:A:256:SER:O	2.69	0.40
2:B:55:SER:HB3	2:B:63:TYR:OH	2.21	0.40
1:C:121:GLU:O	1:C:122:ASP:C	2.60	0.40
1:C:156:ILE:O	1:C:156:ILE:HG22	2.21	0.40
1:C:164:CYS:O	1:C:166:ASP:N	2.54	0.40
4:F:128:ILE:CG2	4:F:158:PHE:CB	2.93	0.40
3:G:3:GLN:NE2	3:G:26:THR:N	2.52	0.40
3:G:55:GLU:HB2	3:G:60:LYS:HE2	2.03	0.40
1:C:184:PRO:HA	1:C:185:PRO:HD3	1.81	0.40
3:E:145:TYR:CB	3:E:146:PRO:CD	2.99	0.40
4:F:14:PRO:HB2	4:F:17:GLU:CG	2.51	0.40
4:F:91:GLU:OE2	4:F:116:ILE:HA	2.21	0.40
1:A:64:THR:O	1:A:68:THR:OG1	2.38	0.40
1:A:73:LEU:HD12	3:E:99:TYR:O	2.22	0.40
1:A:261:VAL:HB	1:A:270:LEU:HB3	2.03	0.40
1:A:266:LEU:HA	1:A:267:PRO:HD3	1.95	0.40
1:C:155:HIS:CD2	1:C:157:SER:OG	2.74	0.40
1:C:215:LEU:HD12	1:C:245:ALA:CB	2.52	0.40
4:F:54:ALA:C	4:F:55:THR:OG1	2.60	0.40
4:F:156:ALA:C	4:F:188:THR:HG21	2.41	0.40
3:G:11:LEU:HD23	3:G:11:LEU:O	2.21	0.40
4:H:81:LEU:HA	4:H:81:LEU:HD12	1.90	0.40
4:H:96:CYS:O	4:H:96:CYS:SG	2.79	0.40
1:A:36:PHE:HA	1:A:40:GLU:OE1	2.21	0.40
1:C:14:ARG:HA	1:C:15:PRO:HD3	1.93	0.40
1:C:164:CYS:O	1:C:165:SER:C	2.60	0.40
4:F:52:VAL:CG2	4:F:71:SER:HB2	2.47	0.40
4:F:200:ARG:HD3	4:F:200:ARG:HA	1.57	0.40
4:F:202:MET:O	4:F:227:SER:HB2	2.22	0.40
3:G:81:GLU:H	3:G:81:GLU:HG2	1.70	0.40
1:A:76:ARG:O	1:A:77:ASN:C	2.60	0.40
1:C:28:VAL:HG11	1:C:172:LEU:HD21	2.04	0.40
2:D:41:LYS:C	2:D:43:GLY:N	2.73	0.40
4:F:199:GLU:C	4:F:201:ALA:H	2.25	0.40
3:G:58:ARG:CB	3:G:76:ARG:O	2.67	0.40

All (5) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:255:GLN:NE2	4:F:66:LYS:CE[1_545]	1.35	0.85
1:A:53:GLU:OE2	3:E:157:LYS:NZ[1_455]	1.36	0.84
1:C:255:GLN:CD	4:F:66:LYS:NZ[1_545]	1.96	0.24
1:C:255:GLN:CD	4:F:66:LYS:CE[1_545]	2.13	0.07
1:C:255:GLN:NE2	4:F:66:LYS:NZ[1_545]	2.17	0.03

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	258/260 (99%)	181 (70%)	55 (21%)	22 (8%)	0	4
1	C	258/260 (99%)	192 (74%)	45 (17%)	21 (8%)	1	4
2	B	100/102 (98%)	86 (86%)	9 (9%)	5 (5%)	1	11
2	D	100/102 (98%)	79 (79%)	12 (12%)	9 (9%)	0	4
3	E	205/207 (99%)	157 (77%)	30 (15%)	18 (9%)	0	4
3	G	205/207 (99%)	158 (77%)	29 (14%)	18 (9%)	0	4
4	F	228/230 (99%)	167 (73%)	37 (16%)	24 (10%)	0	3
4	H	228/230 (99%)	172 (75%)	34 (15%)	22 (10%)	0	3
All	All	1582/1598 (99%)	1192 (75%)	251 (16%)	139 (9%)	0	4

All (139) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	14	ARG
1	A	15	PRO
1	A	51	TRP
1	A	56	GLU
1	A	129	ASN
1	A	197	GLY
1	A	209	TYR
1	A	220	ASN

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Mol	Chain	Res	Type
1	A	254	GLU
2	B	47	GLU
2	B	60	TRP
2	B	74	GLU
1	C	15	PRO
1	C	56	GLU
1	C	106	ASP
1	C	129	ASN
1	C	150	ASN
1	C	158	GLN
1	C	255	GLN
2	D	31	HIS
2	D	33	SER
2	D	85	VAL
3	E	7	SER
3	E	39	SER
3	E	185	SER
4	F	7	PRO
4	F	56	PRO
4	F	107	LYS
4	F	119	PRO
4	F	122	LYS
4	F	133	THR
4	F	186	ASN
4	F	213	GLU
4	F	214	ASN
4	F	216	LYS
3	G	7	SER
3	G	122	PRO
3	G	188	VAL
4	H	56	PRO
4	H	64	GLU
4	H	121	ASP
4	H	133	THR
4	H	172	ASN
4	H	199	GLU
4	H	209	ILE
1	A	120	SER
1	A	176	LYS
1	A	221	GLY
1	C	212	ASP
1	C	233	THR

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Mol	Chain	Res	Type
1	C	263	HIS
3	E	65	SER
3	E	78	ALA
3	E	97	GLU
3	E	105	LYS
3	E	123	PRO
3	E	134	GLY
3	E	188	VAL
3	E	203	ASP
4	F	4	LEU
4	F	30	PHE
4	F	76	ALA
4	F	89	GLU
4	F	100	GLU
4	F	199	GLU
3	G	28	THR
3	G	52	GLY
3	G	67	GLU
3	G	133	ASN
3	G	145	TYR
3	G	165	ALA
3	G	185	SER
3	G	187	SER
4	H	45	GLY
4	H	85	SER
4	H	107	LYS
4	H	168	GLU
1	A	89	MET
1	A	118	TYR
1	A	158	GLN
1	A	193	PRO
1	A	275	GLY
1	C	24	ILE
1	C	124	PRO
1	C	130	PRO
1	C	133	CYS
1	C	207	GLY
1	C	267	PRO
2	D	1	ILE
2	D	17	ASN
2	D	32	PRO
2	D	90	PRO

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Mol	Chain	Res	Type
3	E	103	THR
4	F	42	PRO
4	F	55	THR
4	F	132	PRO
4	F	159	PRO
4	F	200	ARG
3	G	80	LEU
3	G	96	SER
3	G	123	PRO
3	G	164	PRO
4	H	128	ILE
4	H	226	PRO
1	A	153	VAL
1	C	44	ARG
1	C	210	PRO
1	C	254	GLU
2	D	54	LEU
3	E	51	SER
3	E	145	TYR
4	H	74	PRO
4	H	198	PRO
4	H	216	LYS
4	H	218	GLY
1	A	50	PRO
2	D	88	SER
3	E	16	GLY
3	E	80	LEU
4	F	14	PRO
4	F	158	PHE
3	G	169	SER
4	H	14	PRO
4	H	42	PRO
4	H	158	PHE
1	A	237	GLY
3	E	159	ILE
1	A	104	GLU
2	B	31	HIS
1	C	20	PRO
1	C	104	GLU
4	F	226	PRO
1	A	267	PRO
3	E	57	GLY

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Mol	Chain	Res	Type
3	G	167	VAL
2	B	14	PRO
3	G	170	PRO
4	H	41	LYS
4	H	119	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	233/233 (100%)	207 (89%)	26 (11%)	5	18
1	C	233/233 (100%)	210 (90%)	23 (10%)	6	23
2	B	96/96 (100%)	86 (90%)	10 (10%)	5	21
2	D	96/96 (100%)	86 (90%)	10 (10%)	5	21
3	E	180/180 (100%)	167 (93%)	13 (7%)	12	37
3	G	177/180 (98%)	155 (88%)	22 (12%)	4	14
4	F	206/206 (100%)	177 (86%)	29 (14%)	3	11
4	H	204/206 (99%)	176 (86%)	28 (14%)	3	11
All	All	1425/1430 (100%)	1264 (89%)	161 (11%)	4	18

All (161) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	PHE
1	A	35	ARG
1	A	38	SER
1	A	68	THR
1	A	94	THR
1	A	99	GLN
1	A	102	ASP
1	A	108	HIS
1	A	133	CYS
1	A	151	SER

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Mol	Chain	Res	Type
1	A	152	THR
1	A	181	ARG
1	A	196	GLU
1	A	198	ASP
1	A	213	ILE
1	A	214	THR
1	A	216	THR
1	A	227	ASP
1	A	231	VAL
1	A	233	THR
1	A	234	ARG
1	A	235	PRO
1	A	242	GLN
1	A	247	VAL
1	A	251	LEU
1	A	270	LEU
2	B	4	THR
2	B	12	ARG
2	B	55	SER
2	B	65	LEU
2	B	70	PHE
2	B	73	THR
2	B	87	LEU
2	B	94	LYS
2	B	98	ASP
2	B	99	MET
1	C	7	TYR
1	C	8	PHE
1	C	9	TYR
1	C	37	SER
1	C	53	GLU
1	C	54	GLN
1	C	58	ASP
1	C	78	LEU
1	C	83	HIS
1	C	91	ASP
1	C	94	THR
1	C	98	LEU
1	C	101	CYS
1	C	112	TRP
1	C	125	THR
1	C	127	ASN

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Mol	Chain	Res	Type
1	C	128	GLU
1	C	129	ASN
1	C	214	THR
1	C	215	LEU
1	C	220	ASN
1	C	233	THR
1	C	234	ARG
2	D	4	THR
2	D	7	ILE
2	D	17	ASN
2	D	51	HIS
2	D	56	PHE
2	D	67	TYR
2	D	70	PHE
2	D	84	HIS
2	D	94	LYS
2	D	99	MET
3	E	2	ASP
3	E	6	GLN
3	E	13	LEU
3	E	25	PHE
3	E	30	ARG
3	E	32	VAL
3	E	46	LEU
3	E	72	THR
3	E	132	LYS
3	E	133	ASN
3	E	148	GLU
3	E	150	THR
3	E	152	SER
4	F	18	THR
4	F	23	CYS
4	F	34	THR
4	F	42	PRO
4	F	51	TYR
4	F	53	LEU
4	F	55	THR
4	F	79	SER
4	F	84	TYR
4	F	85	SER
4	F	100	GLU
4	F	106	HIS

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Mol	Chain	Res	Type
4	F	118	ILE
4	F	121	ASP
4	F	133	THR
4	F	135	PHE
4	F	143	ASN
4	F	144	LEU
4	F	155	GLU
4	F	160	ASP
4	F	177	SER
4	F	183	LEU
4	F	185	THR
4	F	192	PHE
4	F	212	HIS
4	F	215	ASN
4	F	221	GLN
4	F	223	ILE
4	F	224	PHE
3	G	11	LEU
3	G	12	SER
3	G	13	LEU
3	G	17	THR
3	G	23	CYS
3	G	25	PHE
3	G	28	THR
3	G	45	SER
3	G	64	ASP
3	G	92	THR
3	G	101	LEU
3	G	104	ASP
3	G	108	PHE
3	G	115	THR
3	G	120	SER
3	G	122	PRO
3	G	133	ASN
3	G	135	THR
3	G	140	LEU
3	G	143	ASP
3	G	181	GLN
3	G	191	SER
4	H	21	ILE
4	H	34	THR
4	H	42	PRO

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Mol	Chain	Res	Type
4	H	51	TYR
4	H	56	PRO
4	H	60	PHE
4	H	62	ASP
4	H	64	GLU
4	H	96	CYS
4	H	105	PHE
4	H	118	ILE
4	H	133	THR
4	H	143	ASN
4	H	144	LEU
4	H	151	LEU
4	H	161	VAL
4	H	163	ARG
4	H	165	TYR
4	H	183	LEU
4	H	184	LYS
4	H	186	ASN
4	H	187	ASP
4	H	189	TYR
4	H	190	MET
4	H	208	CYS
4	H	215	ASN
4	H	228	ILE
4	H	229	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	63	GLN
1	A	70	GLN
1	A	96	GLN
1	A	99	GLN
1	A	127	ASN
2	B	24	ASN
2	B	42	ASN
1	C	32	GLN
1	C	54	GLN
1	C	86	ASN
1	C	96	GLN
1	C	99	GLN
1	C	108	HIS

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Mol	Chain	Res	Type
1	C	155	HIS
1	C	218	GLN
1	C	220	ASN
2	D	24	ASN
2	D	42	ASN
3	E	6	GLN
3	E	33	GLN
3	E	74	HIS
3	E	121	GLN
3	E	133	ASN
4	F	6	GLN
4	F	36	HIS
4	F	178	GLN
4	F	186	ASN
4	F	214	ASN
4	F	215	ASN
3	G	3	GLN
3	G	6	GLN
3	G	24	ASN
3	G	33	GLN
3	G	38	ASN
3	G	136	ASN
4	H	73	ASN
4	H	106	HIS
4	H	206	HIS
4	H	221	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 ⓘ

13 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	$\# Z > 2$
5	NAG	I	1	5,3	15,15,15	0.56	0	21,21,21	0.77	0
5	NAG	I	2	5	15,15,15	0.47	0	21,21,21	0.70	0
5	MAN	I	3	5	12,12,12	0.44	0	17,17,17	0.45	0
6	NAG	J	1	6,3	15,15,15	0.56	0	21,21,21	0.79	0
6	NAG	J	2	6	15,15,15	0.48	0	21,21,21	0.70	0
6	NAG	K	1	6,4	15,15,15	0.56	0	21,21,21	1.13	2 (9%)
6	NAG	K	2	6	15,15,15	0.48	0	21,21,21	0.70	0
5	NAG	L	1	5,3	15,15,15	0.57	0	21,21,21	0.97	1 (4%)
5	NAG	L	2	5	15,15,15	0.48	0	21,21,21	0.70	0
5	MAN	L	3	5	12,12,12	0.44	0	17,17,17	0.45	0
7	NAG	M	1	7,3	15,15,15	1.20	1 (6%)	21,21,21	1.79	5 (23%)
7	NAG	M	2	7	14,14,15	0.78	0	17,19,21	0.84	0
7	FUC	M	3	7	10,10,11	0.97	1 (10%)	14,14,16	2.01	2 (14%)

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
5	NAG	I	1	5,3	1/1/6/7	0/6/26/26	0/1/1/1
5	NAG	I	2	5	-	4/6/26/26	0/1/1/1
5	MAN	I	3	5	-	2/2/22/22	0/1/1/1
6	NAG	J	1	6,3	1/1/6/7	0/6/26/26	0/1/1/1
6	NAG	J	2	6	-	4/6/26/26	0/1/1/1
6	NAG	K	1	6,4	-	0/6/26/26	0/1/1/1
6	NAG	K	2	6	-	4/6/26/26	0/1/1/1
5	NAG	L	1	5,3	1/1/6/7	0/6/26/26	0/1/1/1
5	NAG	L	2	5	-	4/6/26/26	0/1/1/1
5	MAN	L	3	5	-	2/2/22/22	0/1/1/1
7	NAG	M	1	7,3	1/1/6/7	5/6/26/26	0/1/1/1
7	NAG	M	2	7	-	5/6/23/26	0/1/1/1
7	FUC	M	3	7	-	-	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	M	1	NAG	C1-C2	-3.52	1.48	1.52
7	M	3	FUC	C1-C2	2.20	1.57	1.52

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	M	3	FUC	C1-C2-C3	6.49	119.10	109.64
7	M	1	NAG	C3-C4-C5	4.12	117.70	110.23
7	M	1	NAG	C1-C2-C3	-3.60	105.63	110.54
6	K	1	NAG	O1-C1-C2	-3.27	102.42	109.22
7	M	1	NAG	C4-C3-C2	2.54	114.09	110.40
5	L	1	NAG	O1-C1-C2	-2.40	104.23	109.22
7	M	1	NAG	O4-C4-C3	-2.38	104.75	110.38
7	M	1	NAG	O5-C1-C2	-2.30	107.20	109.52
7	M	3	FUC	C2-C3-C4	2.06	114.49	110.86
6	K	1	NAG	O1-C1-O5	-2.02	104.42	110.41

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	I	1	NAG	C1
5	L	1	NAG	C1
6	J	1	NAG	C1
7	M	1	NAG	C1

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	I	2	NAG	C8-C7-N2-C2
5	I	2	NAG	O7-C7-N2-C2
5	L	2	NAG	C8-C7-N2-C2
5	L	2	NAG	O7-C7-N2-C2
6	J	2	NAG	C8-C7-N2-C2
6	J	2	NAG	O7-C7-N2-C2
6	K	2	NAG	C8-C7-N2-C2
6	K	2	NAG	O7-C7-N2-C2
7	M	1	NAG	C3-C2-N2-C7
7	M	1	NAG	C8-C7-N2-C2
7	M	1	NAG	O7-C7-N2-C2
7	M	2	NAG	C8-C7-N2-C2
7	M	2	NAG	O7-C7-N2-C2

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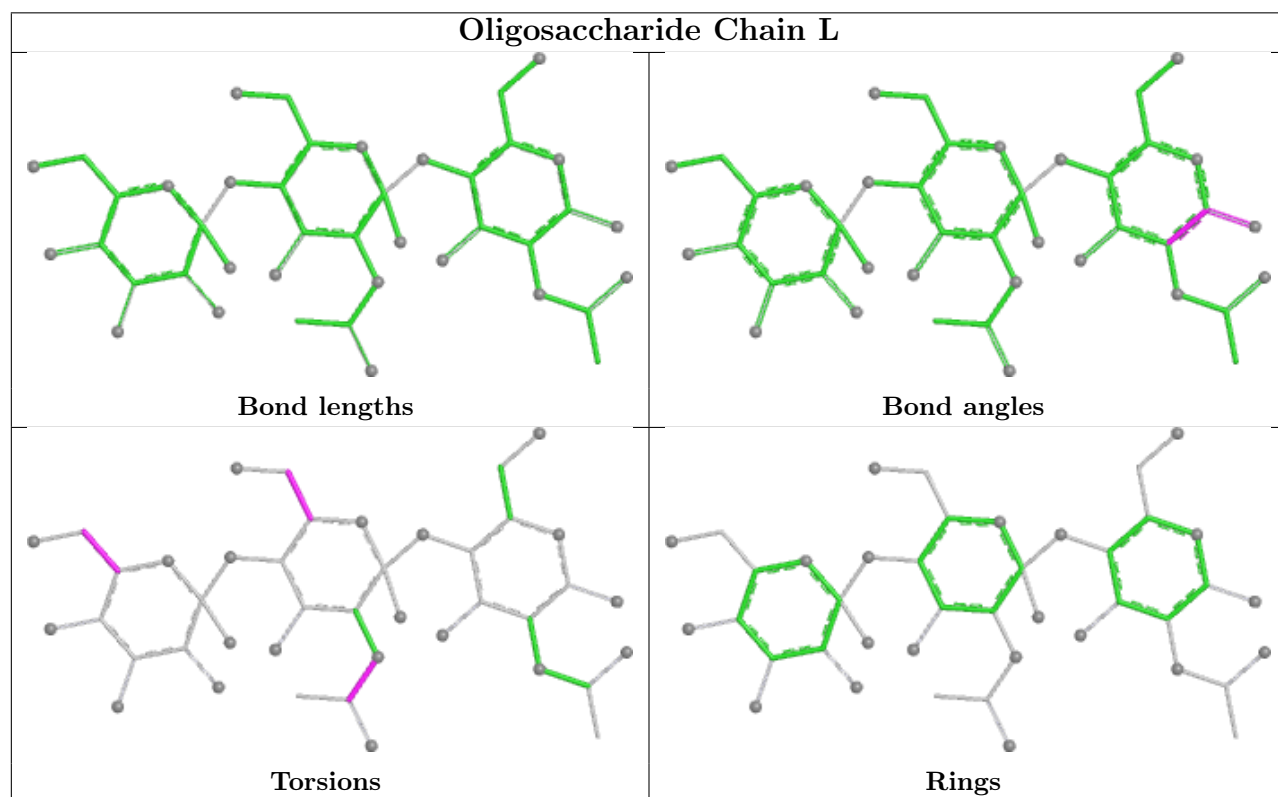
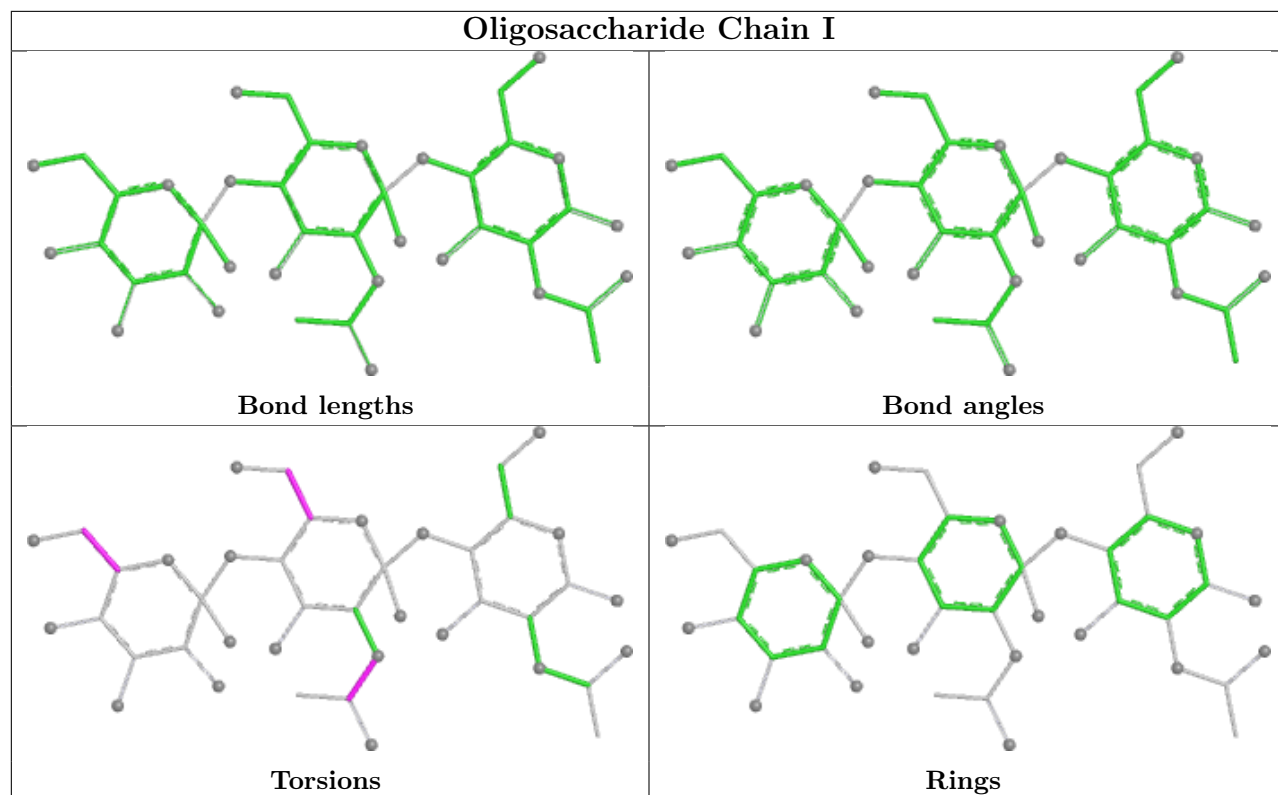
Mol	Chain	Res	Type	Atoms
7	M	1	NAG	C4-C5-C6-O6
7	M	1	NAG	O5-C5-C6-O6
5	I	3	MAN	C4-C5-C6-O6
5	L	3	MAN	C4-C5-C6-O6
5	I	2	NAG	C4-C5-C6-O6
5	L	2	NAG	C4-C5-C6-O6
6	J	2	NAG	C4-C5-C6-O6
6	K	2	NAG	C4-C5-C6-O6
5	I	2	NAG	O5-C5-C6-O6
5	L	2	NAG	O5-C5-C6-O6
6	J	2	NAG	O5-C5-C6-O6
6	K	2	NAG	O5-C5-C6-O6
7	M	2	NAG	O5-C5-C6-O6
7	M	2	NAG	C3-C2-N2-C7
5	L	3	MAN	O5-C5-C6-O6
5	I	3	MAN	O5-C5-C6-O6
7	M	2	NAG	C1-C2-N2-C7

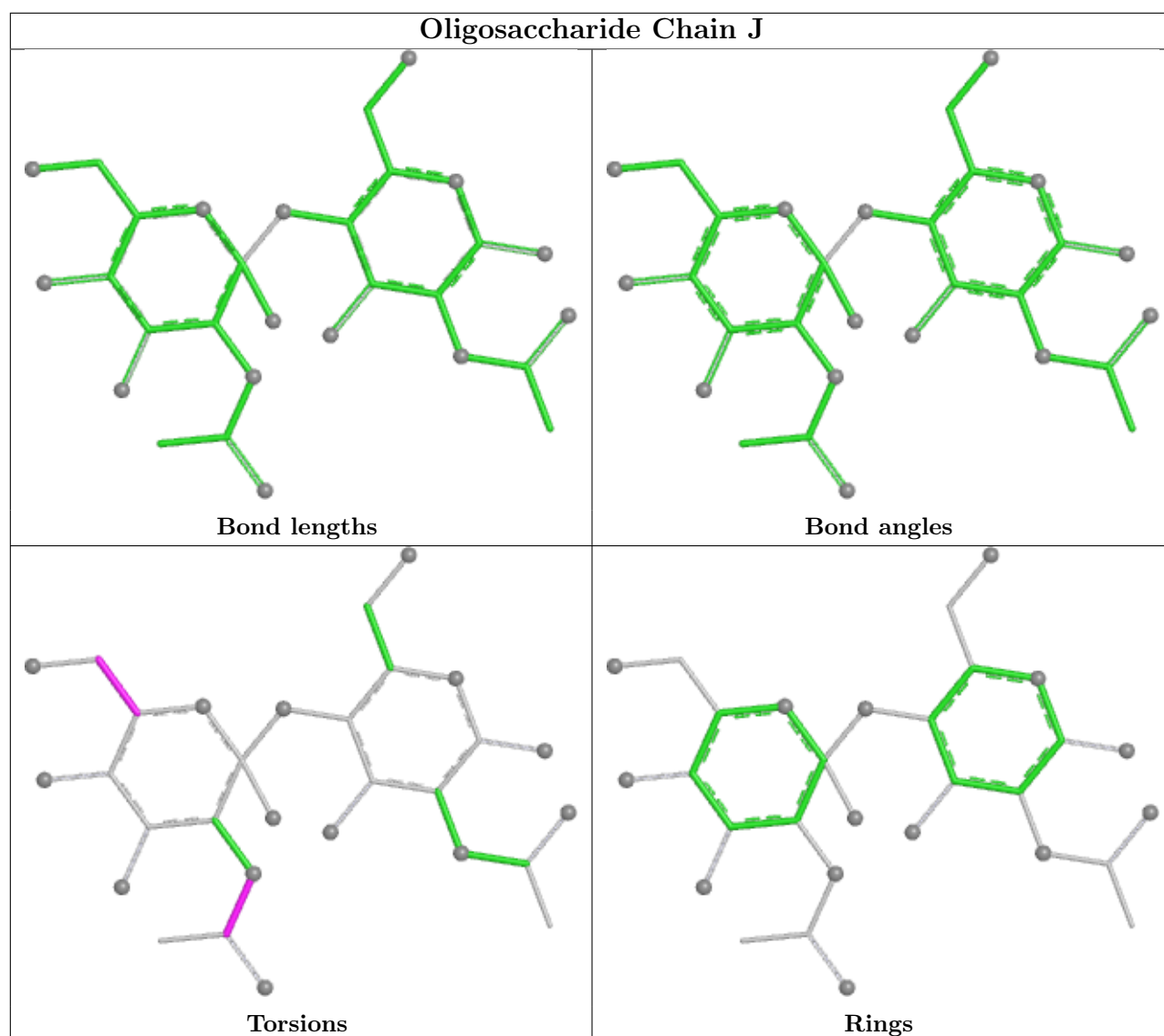
There are no ring outliers.

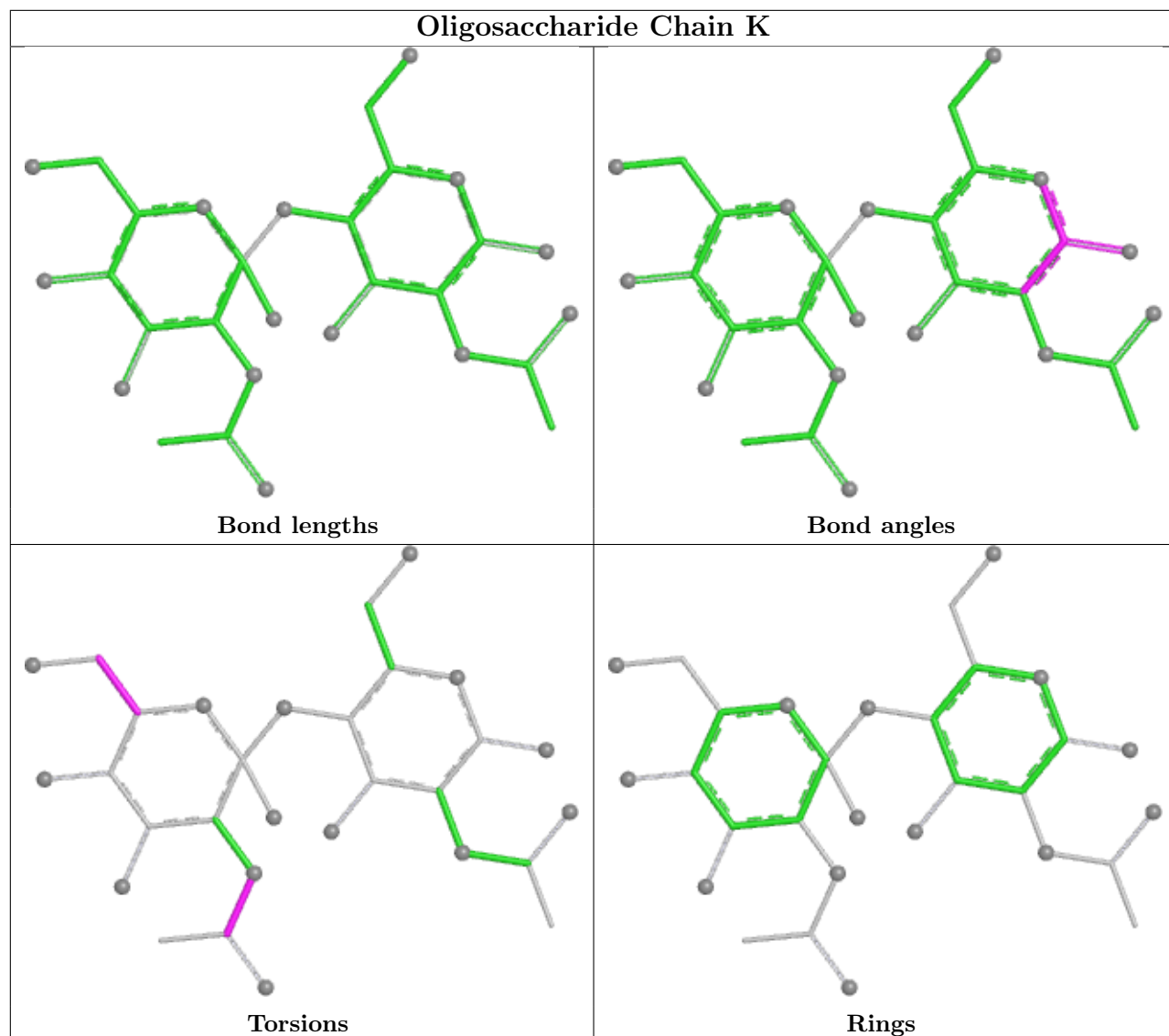
8 monomers are involved in 59 short contacts:

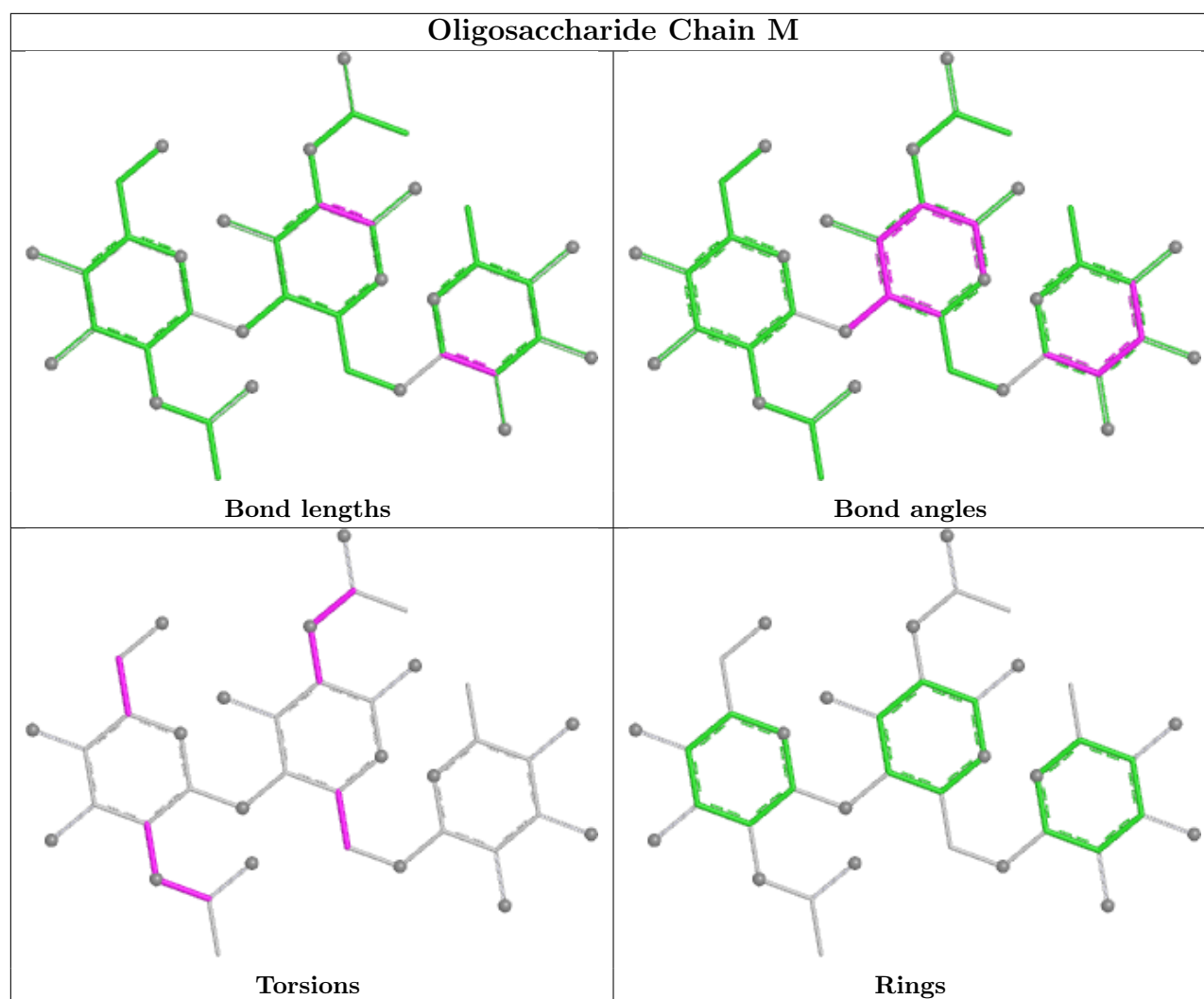
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	J	1	NAG	8	0
6	K	1	NAG	22	0
7	M	1	NAG	10	0
5	L	1	NAG	7	0
6	J	2	NAG	1	0
5	I	1	NAG	6	0
5	I	3	MAN	3	0
7	M	2	NAG	2	0

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.