



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 02:48 AM UTC

PDB ID : 7C2L / pdb_00007c2l
EMDB ID : EMD-30276
Title : S protein of SARS-CoV-2 in complex bound with 4A8
Authors : Yan, R.H.; Zhang, Y.Y.; Guo, Y.Y.; Li, Y.N.; Xia, L.; Zhou, Q.
Deposited on : 2020-05-08
Resolution : 3.10 Å(reported)

This is a Full wwPDB EM 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/EMValidationReportHelp>

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:

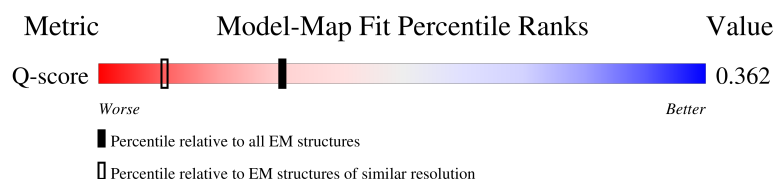
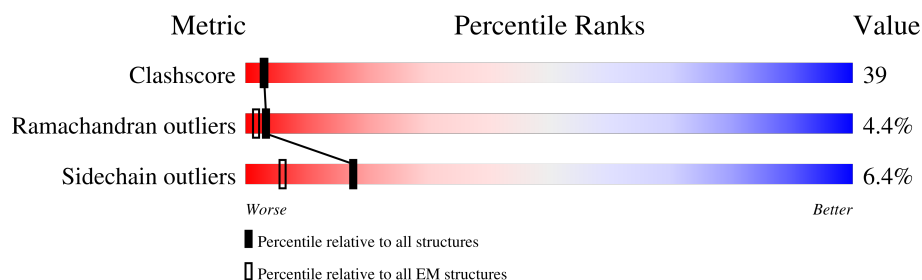
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
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:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.10 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)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14724 (2.60 - 3.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1283	
1	B	1283	
1	C	1283	
2	H	458	

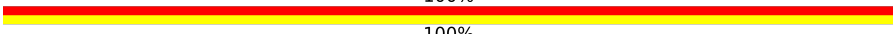
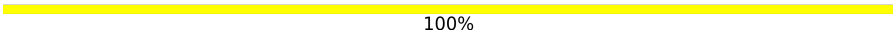
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Mol	Chain	Length	Quality of chain
2	I	458	
2	J	458	
3	L	219	
3	M	219	
3	N	219	
4	D	3	
4	E	3	
4	S	3	
4	T	3	
4	c	3	
4	d	3	
5	F	2	
5	G	2	
5	K	2	
5	O	2	
5	P	2	
5	Q	2	
5	R	2	
5	U	2	
5	V	2	
5	W	2	
5	X	2	
5	Y	2	
5	Z	2	
5	a	2	

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Mol	Chain	Length	Quality of chain
5	b	2	 50% 50%
5	e	2	 100%
5	f	2	 50% 50%
5	g	2	 50% 100%
5	h	2	 100%
5	i	2	 50% 50%
5	j	2	 50% 50%
5	k	2	 100%
5	l	2	 50% 100%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 35988 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1031	Total	C	N	O	S	0	0
			8064	5146	1346	1536	36		
1	B	1055	Total	C	N	O	S	0	0
			8269	5278	1380	1574	37		
1	C	1049	Total	C	N	O	S	0	0
			8227	5254	1374	1562	37		

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	986	PRO	LYS	engineered mutation	UNP P0DTC2
A	987	PRO	VAL	engineered mutation	UNP P0DTC2
A	1274	LEU	-	expression tag	UNP P0DTC2
A	1275	GLU	-	expression tag	UNP P0DTC2
A	1276	ASP	-	expression tag	UNP P0DTC2
A	1277	TYR	-	expression tag	UNP P0DTC2
A	1278	LYS	-	expression tag	UNP P0DTC2
A	1279	ASP	-	expression tag	UNP P0DTC2
A	1280	ASP	-	expression tag	UNP P0DTC2
A	1281	ASP	-	expression tag	UNP P0DTC2
A	1282	ASP	-	expression tag	UNP P0DTC2
A	1283	LYS	-	expression tag	UNP P0DTC2
B	986	PRO	LYS	engineered mutation	UNP P0DTC2
B	987	PRO	VAL	engineered mutation	UNP P0DTC2
B	1274	LEU	-	expression tag	UNP P0DTC2
B	1275	GLU	-	expression tag	UNP P0DTC2
B	1276	ASP	-	expression tag	UNP P0DTC2
B	1277	TYR	-	expression tag	UNP P0DTC2
B	1278	LYS	-	expression tag	UNP P0DTC2
B	1279	ASP	-	expression tag	UNP P0DTC2
B	1280	ASP	-	expression tag	UNP P0DTC2
B	1281	ASP	-	expression tag	UNP P0DTC2
B	1282	ASP	-	expression tag	UNP P0DTC2
B	1283	LYS	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	986	PRO	LYS	engineered mutation	UNP P0DTC2
C	987	PRO	VAL	engineered mutation	UNP P0DTC2
C	1274	LEU	-	expression tag	UNP P0DTC2
C	1275	GLU	-	expression tag	UNP P0DTC2
C	1276	ASP	-	expression tag	UNP P0DTC2
C	1277	TYR	-	expression tag	UNP P0DTC2
C	1278	LYS	-	expression tag	UNP P0DTC2
C	1279	ASP	-	expression tag	UNP P0DTC2
C	1280	ASP	-	expression tag	UNP P0DTC2
C	1281	ASP	-	expression tag	UNP P0DTC2
C	1282	ASP	-	expression tag	UNP P0DTC2
C	1283	LYS	-	expression tag	UNP P0DTC2

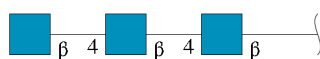
- Molecule 2 is a protein called heavy chain of 4A8.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	229	Total	C	N	O	S	0	0
			1706	1073	273	350	10		
2	I	229	Total	C	N	O	S	0	0
			1706	1073	273	350	10		
2	J	229	Total	C	N	O	S	0	0
			1706	1073	273	350	10		

- Molecule 3 is a protein called light chain of 4A8.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	L	219	Total	C	N	O	S	0	0
			1688	1056	288	338	6		
3	M	219	Total	C	N	O	S	0	0
			1688	1056	288	338	6		
3	N	219	Total	C	N	O	S	0	0
			1688	1056	288	338	6		

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



Mol	Chain	Residues	Atoms				AltConf	Trace
4	D	3	Total	C	N	O	0	0
			42	24	3	15		
4	E	3	Total	C	N	O	0	0
			42	24	3	15		
4	S	3	Total	C	N	O	0	0
			42	24	3	15		
4	T	3	Total	C	N	O	0	0
			42	24	3	15		
4	c	3	Total	C	N	O	0	0
			42	24	3	15		
4	d	3	Total	C	N	O	0	0
			42	24	3	15		

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



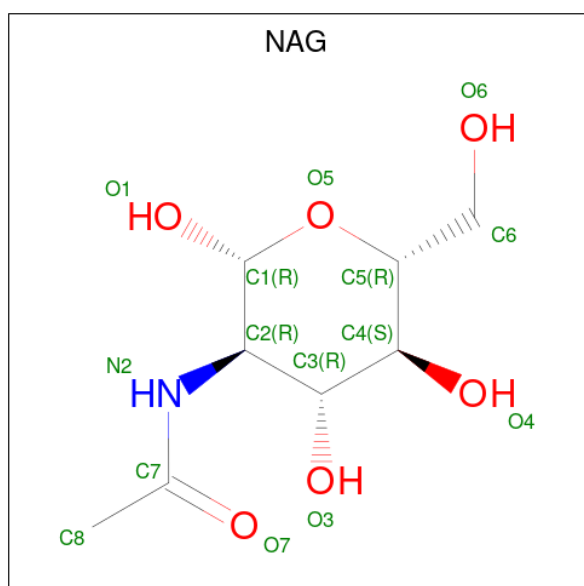
Mol	Chain	Residues	Atoms				AltConf	Trace
5	F	2	Total	C	N	O	0	0
			28	16	2	10		
5	G	2	Total	C	N	O	0	0
			28	16	2	10		
5	K	2	Total	C	N	O	0	0
			28	16	2	10		
5	O	2	Total	C	N	O	0	0
			28	16	2	10		
5	P	2	Total	C	N	O	0	0
			28	16	2	10		
5	Q	2	Total	C	N	O	0	0
			28	16	2	10		
5	R	2	Total	C	N	O	0	0
			28	16	2	10		
5	U	2	Total	C	N	O	0	0
			28	16	2	10		
5	V	2	Total	C	N	O	0	0
			28	16	2	10		
5	W	2	Total	C	N	O	0	0
			28	16	2	10		
5	X	2	Total	C	N	O	0	0
			28	16	2	10		

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Mol	Chain	Residues	Atoms				AltConf	Trace
5	Y	2	Total	C	N	O	0	0
			28	16	2	10		
5	Z	2	Total	C	N	O	0	0
			28	16	2	10		
5	a	2	Total	C	N	O	0	0
			28	16	2	10		
5	b	2	Total	C	N	O	0	0
			28	16	2	10		
5	e	2	Total	C	N	O	0	0
			28	16	2	10		
5	f	2	Total	C	N	O	0	0
			28	16	2	10		
5	g	2	Total	C	N	O	0	0
			28	16	2	10		
5	h	2	Total	C	N	O	0	0
			28	16	2	10		
5	i	2	Total	C	N	O	0	0
			28	16	2	10		
5	j	2	Total	C	N	O	0	0
			28	16	2	10		
5	k	2	Total	C	N	O	0	0
			28	16	2	10		
5	l	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
6	A	1	Total	C	N	O	0
			14	8	1	5	
6	A	1	Total	C	N	O	0
			14	8	1	5	
6	A	1	Total	C	N	O	0
			14	8	1	5	
6	A	1	Total	C	N	O	0
			14	8	1	5	
6	A	1	Total	C	N	O	0
			14	8	1	5	
6	A	1	Total	C	N	O	0
			14	8	1	5	
6	A	1	Total	C	N	O	0
			14	8	1	5	
6	A	1	Total	C	N	O	0
			14	8	1	5	
6	B	1	Total	C	N	O	0
			14	8	1	5	
6	B	1	Total	C	N	O	0
			14	8	1	5	
6	B	1	Total	C	N	O	0
			14	8	1	5	
6	B	1	Total	C	N	O	0
			14	8	1	5	
6	B	1	Total	C	N	O	0
			14	8	1	5	
6	B	1	Total	C	N	O	0
			14	8	1	5	
6	B	1	Total	C	N	O	0
			14	8	1	5	
6	C	1	Total	C	N	O	0
			14	8	1	5	
6	C	1	Total	C	N	O	0
			14	8	1	5	
6	C	1	Total	C	N	O	0
			14	8	1	5	
6	C	1	Total	C	N	O	0
			14	8	1	5	

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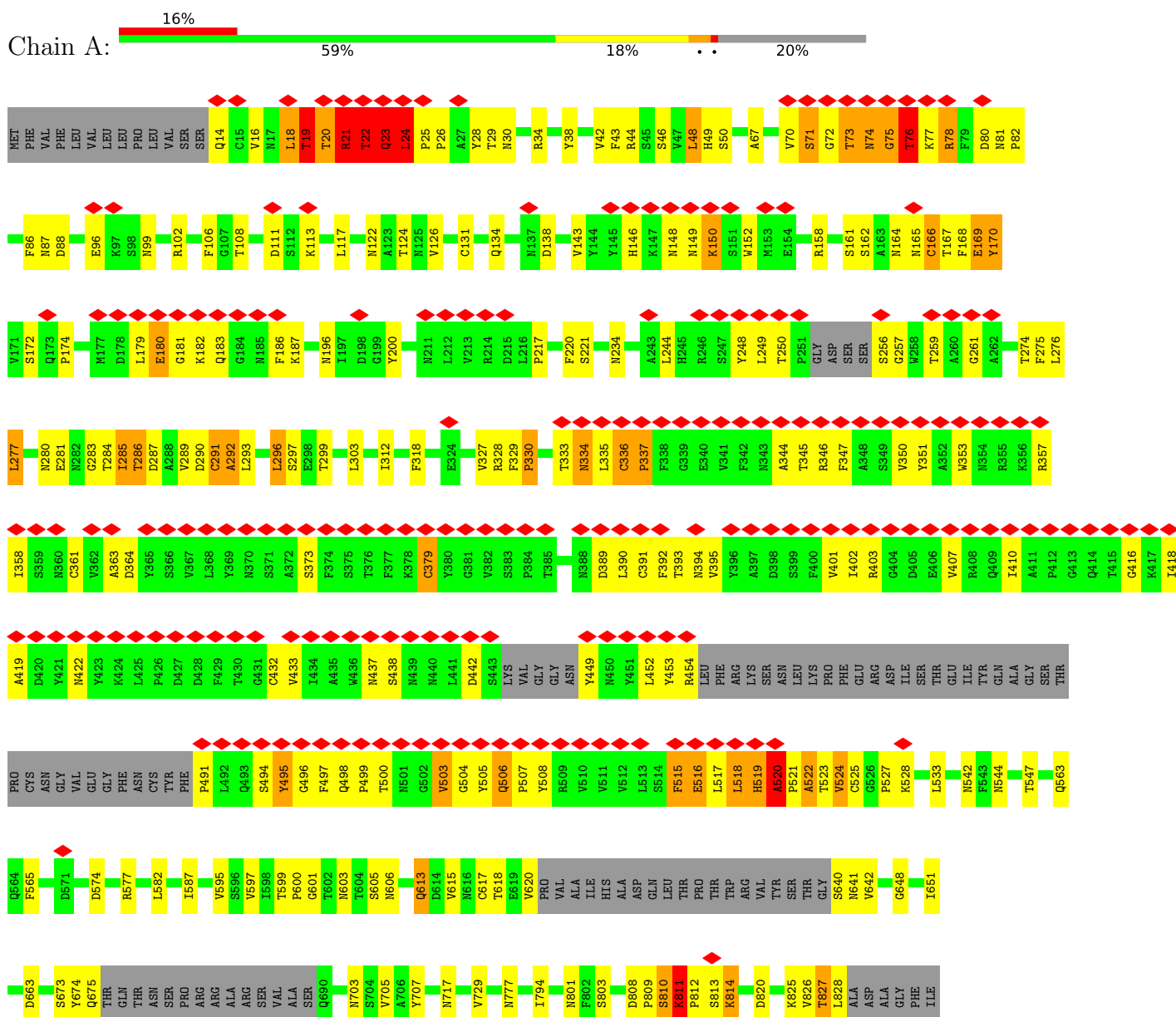
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Mol	Chain	Residues	Atoms				AltConf
6	C	1	Total	C	N	O	0
			14	8	1	5	
6	C	1	Total	C	N	O	0
			14	8	1	5	
6	C	1	Total	C	N	O	0
			14	8	1	5	

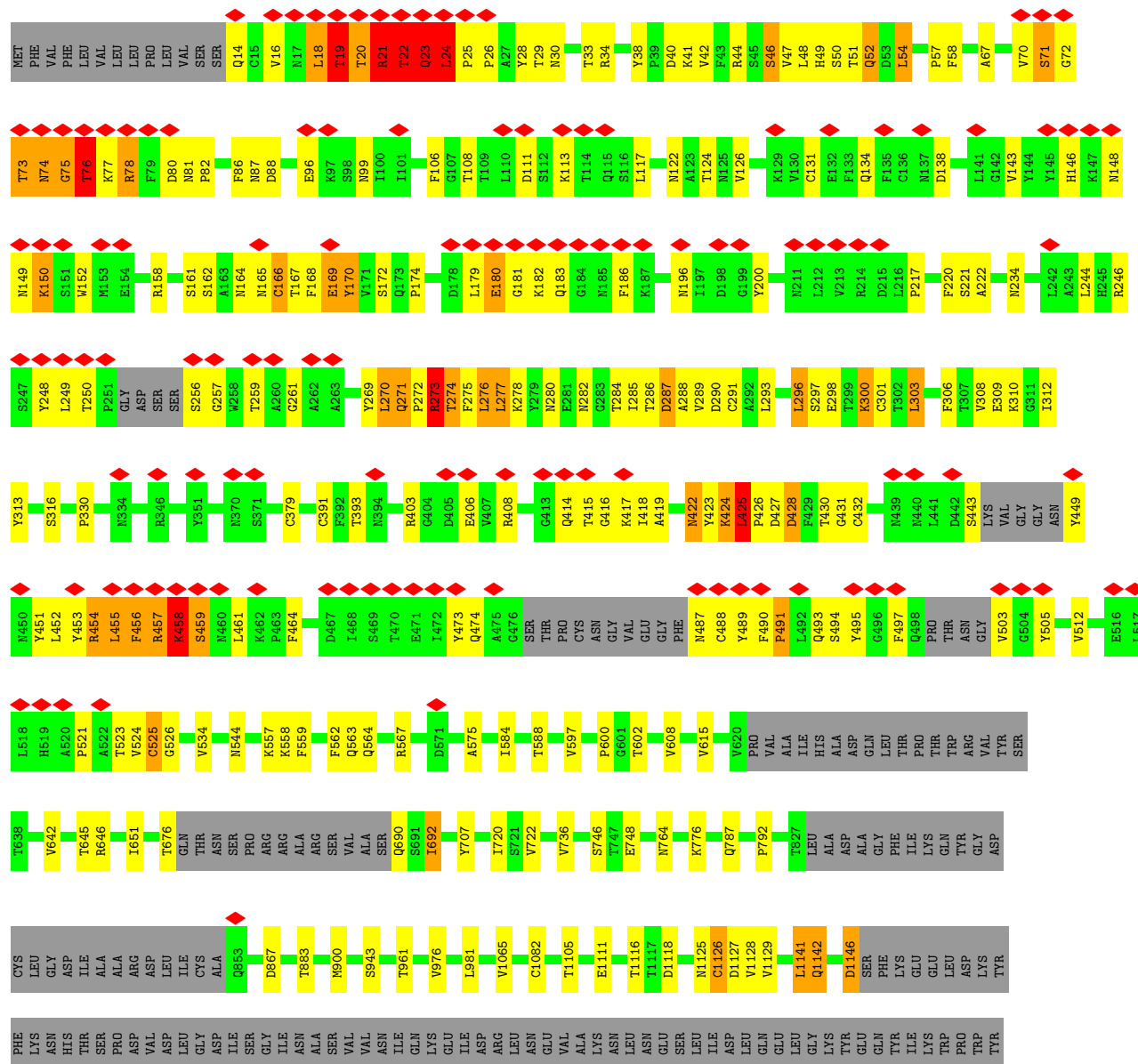
3 Residue-property plots

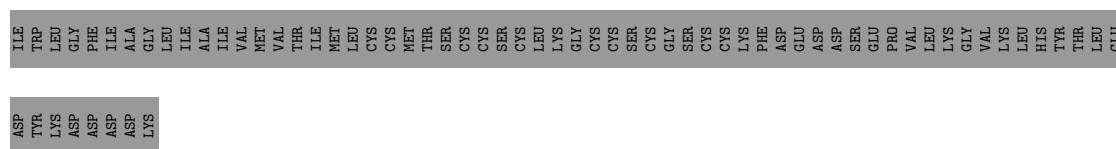
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Spike glycoprotein

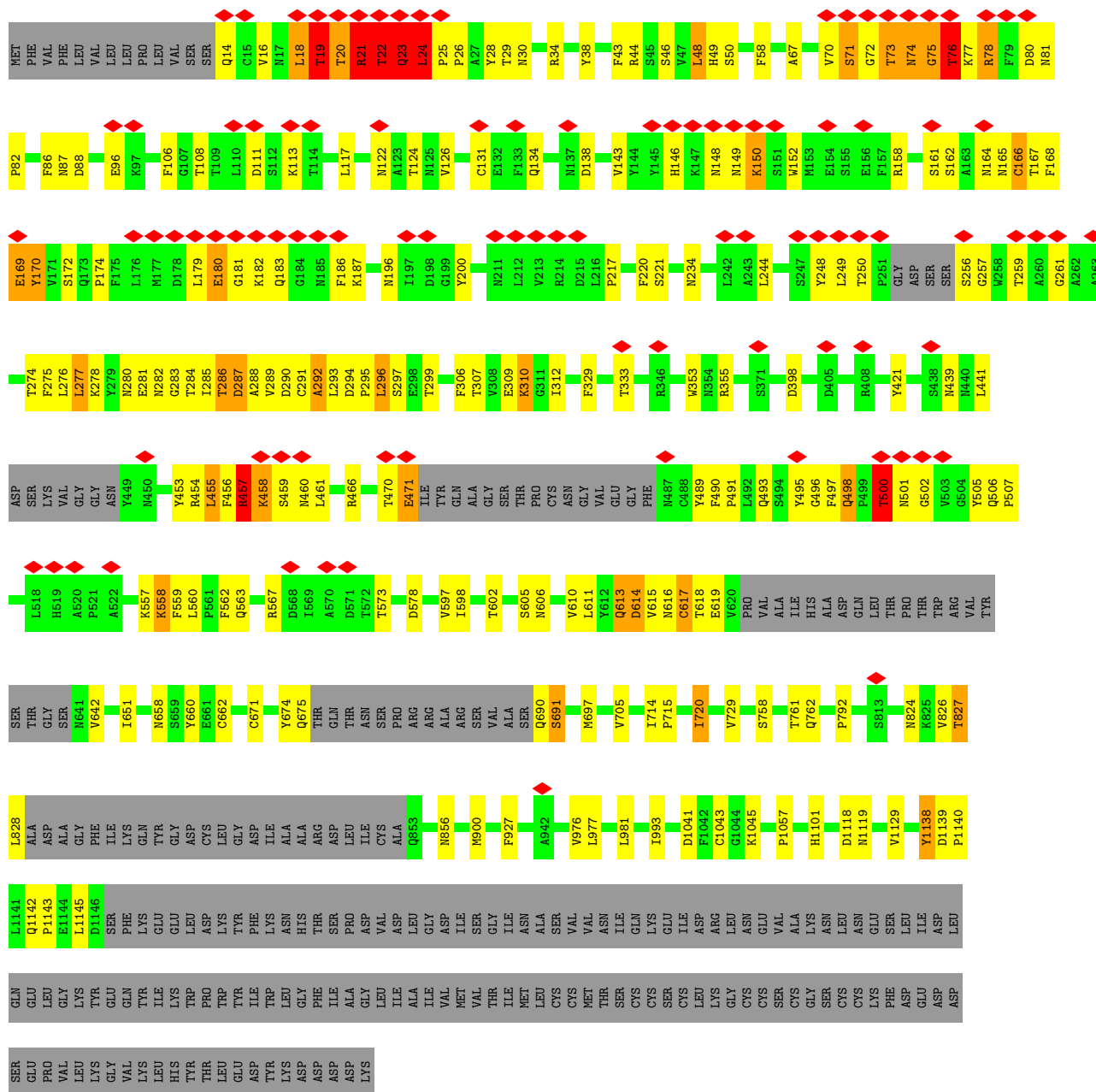


- Molecule 1: Spike glycoprotein

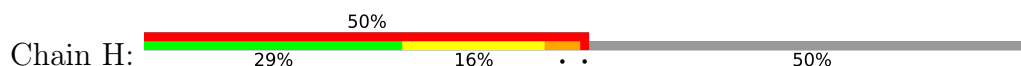




• Molecule 1: Spike glycoprotein

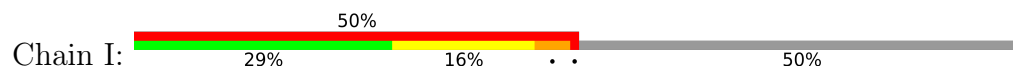


• Molecule 2: heavy chain of 4A8



LEU	THR	VAL	ASP	LYS	SER	ARG	ASP	GLU	THR	GLN	GLY	ASN	ASN	VAL	VAL	PHE	SER	SER	CYS	THR	THR	CYS	VAL	VAL	MET	HIS	THR	GLN	ALA	GLY	PHE	LEU	HIS	ASN	HIS	SER	TYR	THR	GLN	ALA	THR	ASN	GLY	PRO	PRO	GLY	LYS												
THR	LEU	PRO	PRO	SER	ARG	ASP	ASP	GLU	THR	THR	LYS	ASN	ASN	VAL	VAL	VAL	SER	SER	LEU	THR	THR	CYS	VAL	VAL	VAL	THR	THR	THR	GLN	ALA	GLY	PHE	THR	PRO	PRO	SER	ASN	ILE	THR	ILE	ASP	THR	ASN	GLY	GLN	PRO	PRO	GLY	LYS										
LYS	PRO	ARG	GLU	GLN	TYR	ASN	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR											
PRO	ALA	PRO	GLU	LEU	GLY	GLY	PRO	PRO	VAL	PHE	LEU	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO										
F181	P182	A183	V184	L185	Q186	S187	S188	G189	L190	Y191	S192	L193	S194	S195	V196	V197	T198	L199	P200	S201	S202	S203	L204	G205	T206	Q207	T208	Y209	I210	C211	N212	V213	N214	H215	K216	P217	S218	N219	T220	K221	V222	D223	K224	K225	V226	E227	P228	K229	SER	CYS	ASP	LYS	THR	HIS	THR	CYS	PRO	CYS	
G121	T122	T123	V124	T125	V126	S127	S128	A129	S130	T131	K132	G133	P134	S135	V136	F137	P138	L139	A140	P141	S142	S143	K144	S145	T146	S147	G148	G149	T150	A151	A152	L153	G154	C155	L156	V157	K158	D159	Y160	F161	P162	E163	P164	V165	T166	V167	S168	W169	N170	S171	G172	A173	L174	T175	S176	G177	V178	H179	T180
A61	Q62	K63	F64	Q65	G66	R67	V68	T69	W70	T71	E72	D73	T74	S75	T76	D77	T78	A79	Y80	H81	E82	L83	S84	S85	L86	R87	S88	E89	D90	T91	A92	V93	Y94	Y95	C96	A97	T98	S99	T100	A101	P102	A103	G104	T105	P106	D107	L108	F109	D110	Y111	Y112	Y113	G114	M115	D116	V117	W118	G119	Q120
E1	V2	Q3	L4	V5	E6	S7	G8	A9	E10	V11	K12	K13	P14	G15	A16	S17	V18	K19	V20	S21	C22	K23	V24	S25	G26	Y27	T28	L29	T30	E31	L32	S33	M34	H35	W36	V37	R38	Q39	A40	P41	G42	K43	G44	L45	E46	W47	M48	G49	S50	F51	D52	P53	E54	D55	G56	E57	T58	M59	Y60

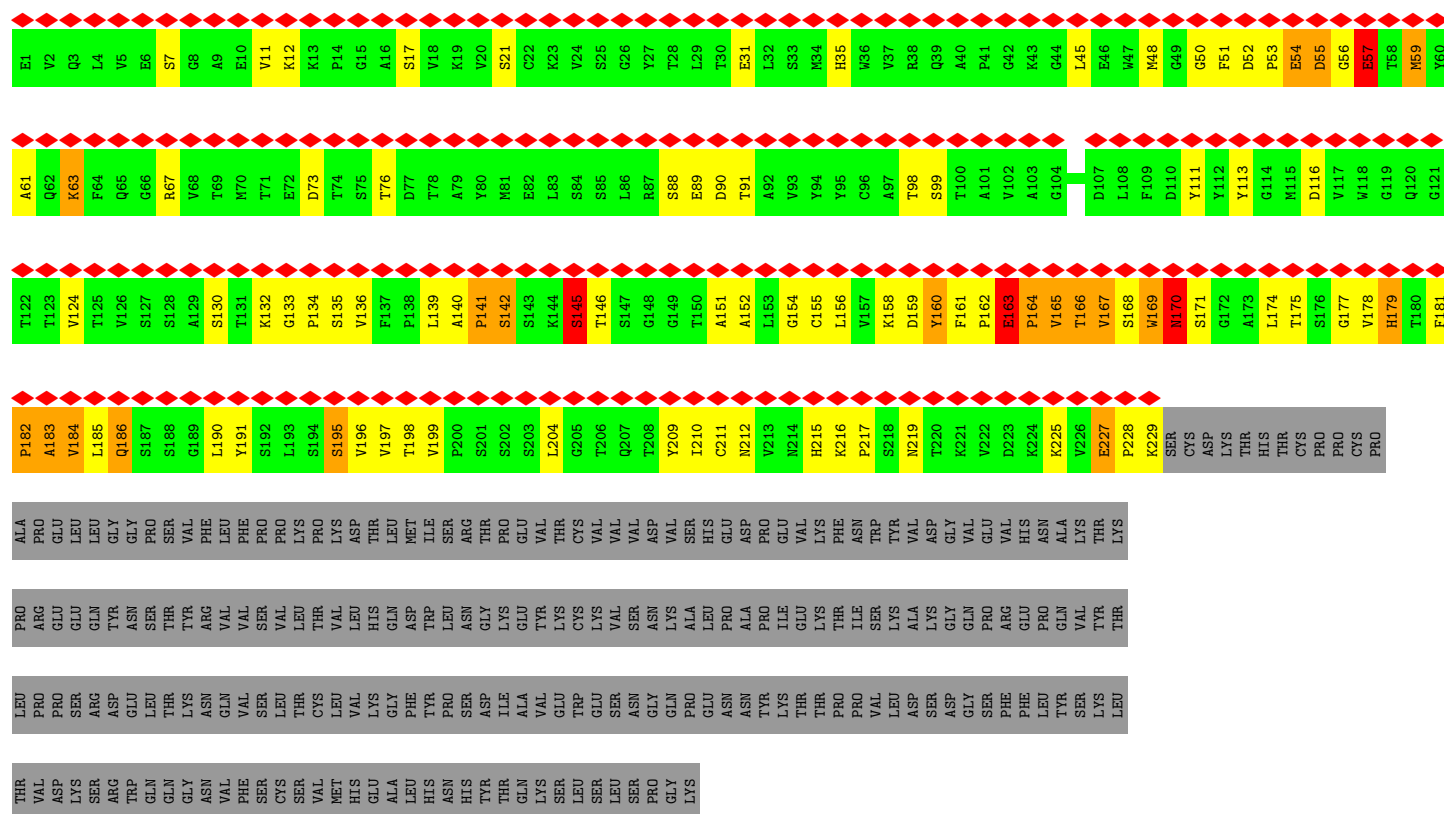
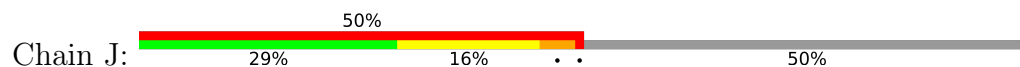
• Molecule 2: heavy chain of 4A8



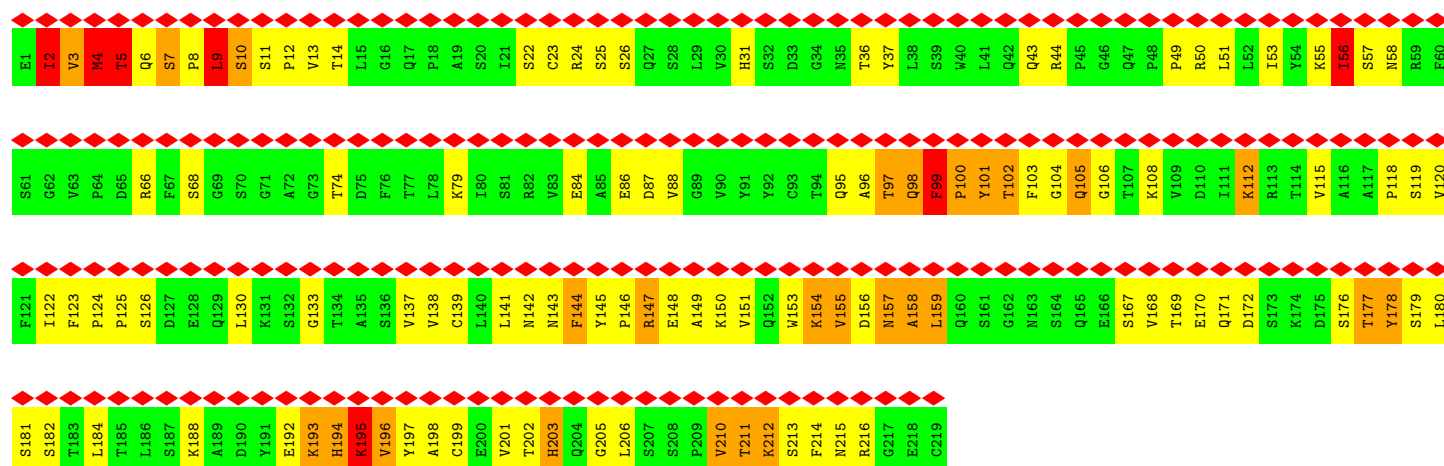
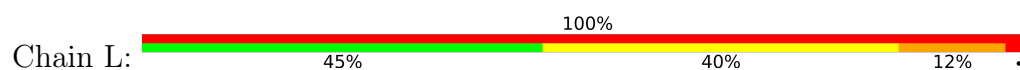
THR	LYS	PRO	ALA	PRO	F181	G121	A61	E1
LEU	PRO	ARG	ALA	PRO	P182	T122	Q62	V2
PRO	ARG	GLU	GLU	GLU	A183	T123	K63	Q3
SER	GLY	LEU	LEU	LEU	V184	V124	F64	L4
ARG	GLN	LEU	LEU	GLY	L185	T125	Q65	V5
ASP	TYR	GLY	GLY	GLY	Q186	V126	G66	E6
GLU	ASN	GLY	GLY	GLY	S187	S127	R67	S7
LEU	SER	PRO	PRO	SER	S188	S128	V68	G8
THR	THR	SER	VAL	THR	G189	A129	T69	A9
ASN	VAL	ARG	PHE	LEU	L190	S130	M70	E10
GLN	VAL	PHE	PHE	LEU	Y191	T131	T71	V11
VAL	VAL	PRO	PRO	PRO	S192	K132	E72	K12
VAL	VAL	PRO	PRO	LYS	L193	G133	D73	K13
THR	LYS	LYS	LYS	PRO	S194	P134	T74	P14
CYS	THR	PRO	PRO	LYS	S195	S135	S75	G15
LEU	VAL	ASP	VAL	ASP	V196	V136	T76	A16
VAL	LEU	THR	THR	THR	V197	F137	D77	S17
GLY	HIS	GLN	LEU	LEU	T198	P138	T78	V18
PHE	ASP	ASP	MET	ILE	V199	L139	A79	K19
TYR	TRP	THR	ILE	SER	P200	A140	Y80	V20
PRO	LEU	SER	SER	ARG	ASN	A140	M81	S21
SER	ASN	ASP	THR	THR	S201	P141	E82	C22
ASP	GLY	THR	PRO	PRO	S202	S142	E82	K23
ILE	LYS	GLU	GLU	GLU	S203	S143	L83	V24
ALA	GLY	VAL	VAL	VAL	L204	K144	S84	G26
VAL	VAL	THR	THR	THR			S85	T28
GLY	LYS	THR	THR	THR			S25	Y27
TRP	CYS	CYS	CYS	CYS	G205	S145	S88	T28
GLY	LYS	VAL	VAL	VAL	T206	T146	E89	L29
GLU	LYS	VAL	VAL	VAL	Q207	S147	D90	T30
SER	ASN	VAL	VAL	VAL	T208	G148	T91	E31
GLY	ASN	ASP	ASP	ASP		G149	A92	L32
GLN	LYS	VAL	VAL	VAL	Y209		V93	S33
PRO	ALA	SER	HIS	LEU	T210	T150	Y94	M34
GLU	LEU	GLU	GLU	PRO	C211	A151	Y95	H35
ASN	ASN	ALA	ASP	ALA	N212	A152	C96	W36
LYS	PRO	ILE	PRO	ILE	V213	L153	A97	V37
THR	GLY	GLY	VAL	VAL	N214	G154	T98	R38
THR	GLY	GLY	VAL	VAL	H215	C155	S99	Q39
THR	LYS	THR	THR	THR	K216	L156	T100	A40
PRO	THR	PRO	PHE	PHE	P217	V157	A101	P41
PRO	ILE	ASN	ASN	ASN	S218	V158	V102	G42
VAL	SER	SER	TRP	TRP	S219	K158	A103	K43
LEU	LYS	LYS	TYR	TYR	N219	D159	G104	G44
ASP	ALA	ALA	VAL	VAL	T220	Y160	T105	L45
SER	LYS	LYS	ASP	ASP	K221	F161	P106	E46
GLY	GLY	GLY	GLY	GLY	T221	A160	D107	W47
GLY	GLN	GLN	VAL	VAL	V222	P162	L108	M48
SER	PRO	PRO	GLU	GLU	V223	E163	F109	G49
PHE	ARG	ARG	VAL	VAL	D223	P164	D110	G50
PHE	PHE	PHE	HIS	HIS	K224	T165	Y111	F51
LEU	PRO	PRO	ASN	THR	K225	T166	Y112	D52
TYR	GLN	GLN	ALA	THR	V226	T166	Y113	P53
SER	VAL	VAL	LYS	THR	E227	V167	G114	E54
LYS	TYR	LYS	THR	CYS	P228	S168	M115	D55
				PRO	K229	W169	D116	G56
				PRO		S170	V117	E57
				CYS		S171	W118	T58
				ASP		G172	G119	M59
				LYS		A173		
				THR		L174		
				HIS		T175		
				THR		S176		
				CYS		G177		
				PRO		V178		
				PRO		H179		
				CYS		T180		
							Q120	Y60

LEU THR VAL ASP LYS SER ARG TRP GLN GLN GLY VAL PHE SER CYS SER VAL MET HIS GLU LEU HIS ASN HIS THR THR GLN LYS SER LEU SER LEU SER PRO GLY LYS

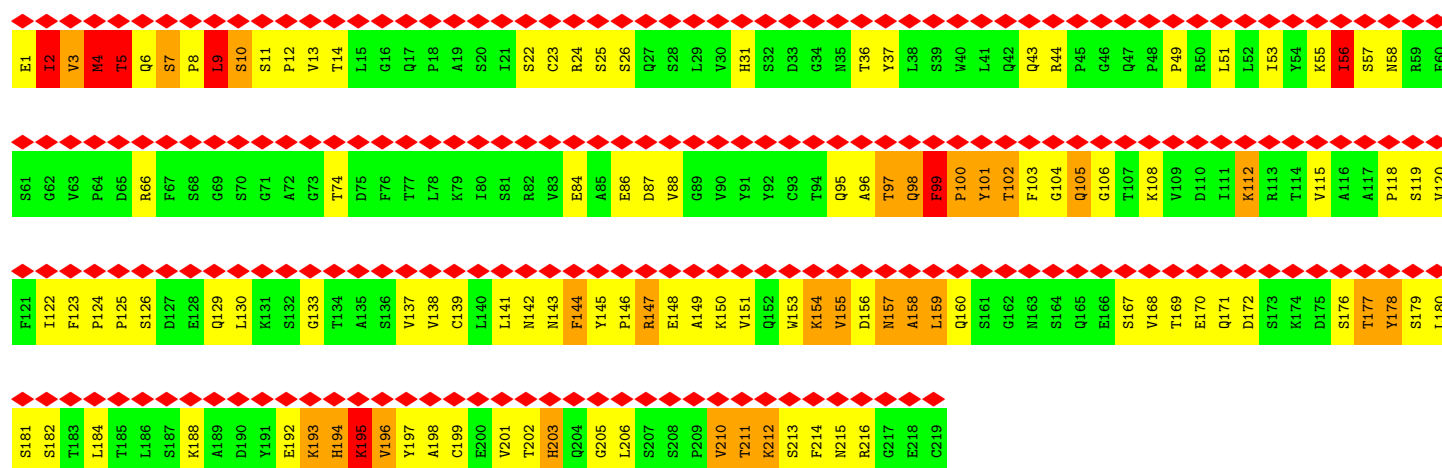
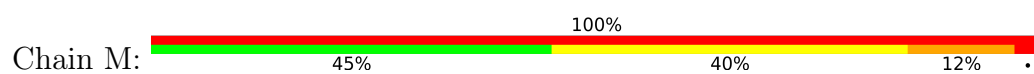
• Molecule 2: heavy chain of 4A8



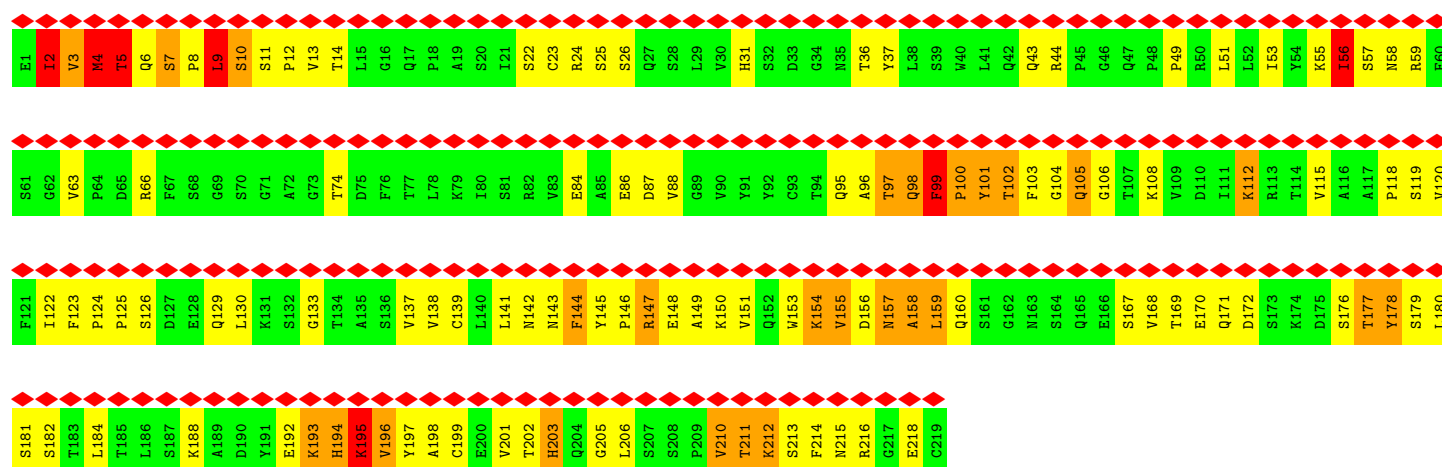
• Molecule 3: light chain of 4A8



• Molecule 3: light chain of 4A8



• Molecule 3: light chain of 4A8



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



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





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



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



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



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



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



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



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



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



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



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



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



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





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



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



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



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



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



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



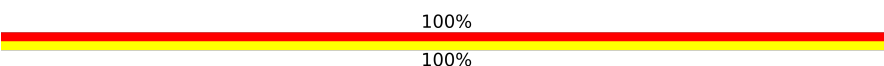


- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain b:  50% 50%

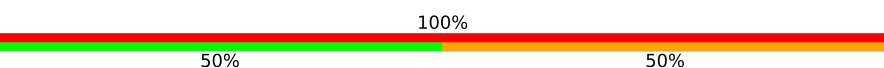


- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain e:  100% 100%



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

Chain f:  100% 50% 50%

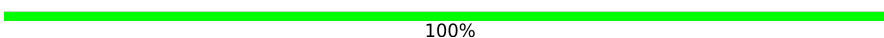


- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain g:  50% 100%



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

Chain h:  100%



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

Chain i:  50% 50% 50%



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



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



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



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	171673	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.144	Depositor
Minimum map value	-0.076	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	313.056, 313.056, 313.056	wwPDB
Map dimensions	288, 288, 288	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.087, 1.087, 1.087	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.52	0/8249	0.74	13/11228 (0.1%)
1	B	0.51	0/8458	0.73	5/11507 (0.0%)
1	C	0.52	0/8417	0.69	4/11454 (0.0%)
2	H	0.53	0/1746	0.78	3/2380 (0.1%)
2	I	0.53	0/1746	0.78	3/2380 (0.1%)
2	J	0.54	0/1746	0.78	3/2380 (0.1%)
3	L	0.47	0/1725	0.73	0/2343
3	M	0.47	0/1725	0.73	0/2343
3	N	0.47	0/1725	0.73	0/2343
All	All	0.51	0/35537	0.73	31/48358 (0.1%)

There are no bond length outliers.

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	145	SER	N-CA-C	-7.80	102.86	111.36
2	H	145	SER	N-CA-C	-7.78	102.88	111.36
2	I	145	SER	N-CA-C	-7.78	102.88	111.36
1	B	274	THR	N-CA-C	-6.54	97.60	108.32
1	B	96	GLU	N-CA-C	6.16	118.72	111.02
1	C	96	GLU	N-CA-C	6.16	118.72	111.02
1	A	96	GLU	N-CA-C	6.14	118.70	111.02
1	B	425	LEU	CA-C-N	-6.06	114.03	120.03
1	B	425	LEU	C-N-CA	-6.06	114.03	120.03
1	A	373	SER	N-CA-C	-6.05	107.13	114.75
1	A	603	ASN	N-CA-C	-6.04	103.64	113.19
1	A	1070	ALA	CA-C-N	5.90	130.10	121.31
1	A	1070	ALA	C-N-CA	5.90	130.10	121.31
1	C	498	GLN	CA-C-N	-5.70	114.08	119.90
1	C	498	GLN	C-N-CA	-5.70	114.08	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	227	GLU	CA-C-N	-5.70	114.08	119.90
2	I	227	GLU	C-N-CA	-5.70	114.08	119.90
2	H	227	GLU	CA-C-N	-5.69	114.10	119.90
2	H	227	GLU	C-N-CA	-5.69	114.10	119.90
2	J	227	GLU	CA-C-N	-5.66	114.13	119.90
2	J	227	GLU	C-N-CA	-5.66	114.13	119.90
1	A	291	CYS	N-CA-C	-5.46	99.62	108.41
1	A	613	GLN	CA-C-N	5.37	131.79	121.54
1	A	613	GLN	C-N-CA	5.37	131.79	121.54
1	A	520	ALA	CA-C-N	-5.35	114.05	119.83
1	A	520	ALA	C-N-CA	-5.35	114.05	119.83
1	A	648	GLY	CA-C-O	-5.22	118.63	122.23
1	A	1142	GLN	O-C-N	5.16	123.83	120.27
1	B	261	GLY	N-CA-C	5.04	120.29	111.78
1	A	261	GLY	N-CA-C	5.04	120.29	111.78
1	C	261	GLY	N-CA-C	5.04	120.29	111.78

There are no chirality outliers.

There are no planarity outliers.

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	8064	0	7849	386	0
1	B	8269	0	8050	342	0
1	C	8227	0	8016	315	0
2	H	1706	0	1654	243	0
2	I	1706	0	1654	248	0
2	J	1706	0	1654	245	0
3	L	1688	0	1647	381	0
3	M	1688	0	1647	381	0
3	N	1688	0	1647	388	0
4	D	42	0	37	0	0
4	E	42	0	37	5	0
4	S	42	0	37	0	0
4	T	42	0	37	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	c	42	0	37	0	0
4	d	42	0	37	5	0
5	F	28	0	25	0	0
5	G	28	0	25	2	0
5	K	28	0	25	0	0
5	O	28	0	25	2	0
5	P	28	0	25	0	0
5	Q	28	0	25	0	0
5	R	28	0	25	0	0
5	U	28	0	25	0	0
5	V	28	0	25	2	0
5	W	28	0	25	0	0
5	X	28	0	25	0	0
5	Y	28	0	25	0	0
5	Z	28	0	25	0	0
5	a	28	0	25	0	0
5	b	28	0	25	0	0
5	e	28	0	25	0	0
5	f	28	0	25	2	0
5	g	28	0	25	0	0
5	h	28	0	25	0	0
5	i	28	0	25	0	0
5	j	28	0	25	0	0
5	k	28	0	25	2	0
5	l	28	0	25	0	0
6	A	126	0	117	1	0
6	B	112	0	104	0	0
6	C	112	0	104	0	0
All	All	35988	0	34940	2731	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 39.

All (2731) 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)
2:H:142:SER:HB3	3:L:214:PHE:CD2	1.35	1.59
2:J:59:MET:HG2	3:N:99:PHE:CD2	1.34	1.59
2:J:142:SER:HB3	3:N:214:PHE:CD2	1.35	1.58
2:H:59:MET:HG2	3:L:99:PHE:CD2	1.34	1.57
2:I:142:SER:HB3	3:M:214:PHE:CD2	1.35	1.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:151:VAL:HG21	3:M:180:LEU:CD2	1.36	1.56
2:I:59:MET:HG2	3:M:99:PHE:CD2	1.34	1.55
3:N:151:VAL:HG21	3:N:180:LEU:CD2	1.36	1.54
2:H:178:VAL:HG12	2:H:197:VAL:CG1	1.38	1.53
3:L:151:VAL:HG21	3:L:180:LEU:CD2	1.36	1.52
3:N:169:THR:CG2	3:N:179:SER:HB2	1.37	1.52
1:C:282:ASN:ND2	5:f:1:NAG:C1	1.71	1.50
2:J:178:VAL:HG12	2:J:197:VAL:CG1	1.38	1.50
3:M:169:THR:CG2	3:M:179:SER:HB2	1.38	1.50
3:L:169:THR:CG2	3:L:179:SER:HB2	1.38	1.49
1:B:282:ASN:ND2	5:V:1:NAG:C1	1.71	1.49
2:I:178:VAL:HG12	2:I:197:VAL:CG1	1.38	1.48
1:C:454:ARG:NH1	1:C:458:LYS:HE3	1.31	1.46
1:C:458:LYS:HG2	1:C:461:LEU:CD1	1.45	1.46
2:H:52:ASP:HB2	3:L:99:PHE:CZ	1.52	1.44
2:J:52:ASP:HB2	3:N:99:PHE:CZ	1.52	1.44
1:A:393:THR:CG2	1:A:518:LEU:HA	1.48	1.42
2:I:52:ASP:HB2	3:M:99:PHE:CZ	1.52	1.42
1:B:452:LEU:CD2	1:B:494:SER:HA	1.51	1.39
1:B:276:LEU:CG	1:B:289:VAL:HB	1.51	1.39
1:A:276:LEU:HB3	1:A:289:VAL:CG1	1.55	1.37
1:A:393:THR:HG23	1:A:518:LEU:CA	1.56	1.35
1:A:22:THR:HG21	1:A:78:ARG:CG	1.60	1.31
1:B:22:THR:HG21	1:B:78:ARG:CG	1.61	1.31
3:M:144:PHE:CZ	3:M:203:HIS:HB2	1.65	1.31
3:N:144:PHE:CZ	3:N:203:HIS:HB2	1.65	1.31
1:C:22:THR:HG21	1:C:78:ARG:CG	1.61	1.30
3:L:144:PHE:CZ	3:L:203:HIS:HB2	1.65	1.30
3:M:153:TRP:CZ2	3:M:182:SER:HB2	1.65	1.30
3:M:118:PRO:HD2	3:M:206:LEU:CG	1.60	1.30
3:L:118:PRO:HD2	3:L:206:LEU:CG	1.60	1.30
3:L:153:TRP:CZ2	3:L:182:SER:HB2	1.65	1.29
3:N:153:TRP:CZ2	3:N:182:SER:HB2	1.65	1.29
3:N:118:PRO:HD2	3:N:206:LEU:CG	1.60	1.28
3:M:7:SER:OG	3:M:8:PRO:HD3	1.11	1.27
2:J:141:PRO:CG	2:J:228:PRO:HA	1.65	1.27
2:I:142:SER:CB	3:M:214:PHE:HD2	1.47	1.27
2:I:141:PRO:CG	2:I:228:PRO:HA	1.65	1.26
2:H:142:SER:CB	3:L:214:PHE:HD2	1.47	1.25
3:M:197:TYR:O	3:M:213:SER:HB2	1.36	1.25
2:J:178:VAL:CG1	2:J:197:VAL:HG13	1.68	1.24

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:142:SER:CB	3:N:214:PHE:HD2	1.47	1.24
1:B:276:LEU:HD11	1:B:289:VAL:CG2	1.67	1.24
2:H:141:PRO:CG	2:H:228:PRO:HA	1.65	1.24
1:C:458:LYS:CG	1:C:461:LEU:HD11	1.67	1.24
3:L:197:TYR:O	3:L:213:SER:HB2	1.36	1.24
2:H:178:VAL:CG1	2:H:197:VAL:HG13	1.67	1.23
3:N:141:LEU:CD2	3:N:201:VAL:HG11	1.69	1.23
3:L:122:ILE:CG2	3:L:213:SER:HA	1.69	1.23
3:N:7:SER:OG	3:N:8:PRO:HD3	1.11	1.23
3:L:141:LEU:CD2	3:L:201:VAL:HG11	1.69	1.22
1:A:392:PHE:CD1	1:A:518:LEU:HD22	1.74	1.22
2:I:169:TRP:CZ3	2:I:211:CYS:HB2	1.74	1.22
2:I:178:VAL:CG1	2:I:197:VAL:HG13	1.68	1.22
3:N:197:TYR:O	3:N:213:SER:HB2	1.36	1.22
1:C:48:LEU:CD2	1:C:276:LEU:HD11	1.70	1.21
3:M:122:ILE:CG2	3:M:213:SER:HA	1.69	1.21
2:J:169:TRP:CZ3	2:J:211:CYS:HB2	1.74	1.21
3:N:122:ILE:CG2	3:N:213:SER:HA	1.69	1.21
3:L:7:SER:OG	3:L:8:PRO:HD3	1.11	1.21
2:J:181:PHE:CZ	3:N:181:SER:HB3	1.76	1.21
2:H:169:TRP:CZ3	2:H:211:CYS:HB2	1.74	1.20
3:M:141:LEU:CD2	3:M:201:VAL:HG11	1.69	1.20
2:H:181:PHE:CZ	3:L:181:SER:HB3	1.76	1.20
2:I:181:PHE:CZ	3:M:181:SER:HB3	1.76	1.19
1:A:48:LEU:CD2	1:A:276:LEU:HD11	1.70	1.19
2:I:142:SER:CB	3:M:214:PHE:CD2	2.24	1.19
3:M:122:ILE:HG21	3:M:213:SER:CA	1.74	1.18
2:H:59:MET:HG2	3:L:99:PHE:CE2	1.79	1.18
2:I:178:VAL:CG1	2:I:197:VAL:CG1	2.22	1.18
3:M:118:PRO:CG	3:M:144:PHE:CE2	2.26	1.18
3:N:118:PRO:CG	3:N:144:PHE:CE2	2.26	1.18
1:B:48:LEU:CD2	1:B:306:PHE:HE1	1.56	1.18
2:H:141:PRO:CD	2:H:228:PRO:HA	1.74	1.17
3:L:118:PRO:CG	3:L:144:PHE:CE2	2.26	1.17
3:L:122:ILE:HG21	3:L:213:SER:CA	1.73	1.17
3:L:144:PHE:CZ	3:L:203:HIS:CB	2.27	1.17
3:N:144:PHE:CZ	3:N:203:HIS:CB	2.27	1.17
3:M:144:PHE:CZ	3:M:203:HIS:CB	2.27	1.17
2:J:59:MET:HG2	3:N:99:PHE:CE2	1.79	1.17
3:N:122:ILE:HG21	3:N:213:SER:CA	1.73	1.17
3:N:153:TRP:CZ2	3:N:182:SER:CB	2.28	1.16

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:141:PRO:CD	2:I:228:PRO:HA	1.74	1.16
1:B:38:TYR:CE1	1:B:222:ALA:HB1	1.79	1.16
2:I:59:MET:HG2	3:M:99:PHE:CE2	1.79	1.16
2:J:59:MET:CG	3:N:99:PHE:CD2	2.29	1.16
1:B:48:LEU:CD2	1:B:306:PHE:CE1	2.29	1.15
3:L:153:TRP:CZ2	3:L:182:SER:CB	2.28	1.15
2:J:141:PRO:CD	2:J:228:PRO:HA	1.74	1.15
2:H:59:MET:CG	3:L:99:PHE:CD2	2.29	1.14
1:B:57:PRO:HB3	1:B:273:ARG:NE	1.61	1.14
3:M:153:TRP:CZ2	3:M:182:SER:CB	2.28	1.14
2:H:178:VAL:CG1	2:H:197:VAL:CG1	2.22	1.14
2:I:59:MET:CG	3:M:99:PHE:CD2	2.29	1.14
2:J:142:SER:CB	3:N:214:PHE:CD2	2.24	1.14
1:C:456:PHE:CD2	1:C:491:PRO:HA	1.83	1.14
2:H:169:TRP:CD1	2:H:197:VAL:CG2	2.30	1.14
3:L:118:PRO:CD	3:L:206:LEU:HG	1.78	1.13
2:J:178:VAL:CG1	2:J:197:VAL:CG1	2.22	1.13
1:B:276:LEU:HD11	1:B:289:VAL:HG21	1.18	1.13
2:J:169:TRP:CD1	2:J:197:VAL:CG2	2.30	1.13
3:M:118:PRO:CD	3:M:206:LEU:HG	1.78	1.13
3:N:7:SER:OG	3:N:8:PRO:CD	1.97	1.12
3:N:169:THR:HG22	3:N:179:SER:CB	1.80	1.12
1:B:276:LEU:HD21	1:B:289:VAL:CG1	1.79	1.12
2:I:169:TRP:CD1	2:I:197:VAL:CG2	2.30	1.12
3:M:118:PRO:HG3	3:M:144:PHE:CZ	1.85	1.12
3:N:118:PRO:CD	3:N:206:LEU:HG	1.78	1.12
1:B:38:TYR:HE1	1:B:222:ALA:HB1	1.04	1.12
3:L:7:SER:OG	3:L:8:PRO:CD	1.97	1.12
3:M:7:SER:OG	3:M:8:PRO:CD	1.97	1.12
3:M:210:VAL:HG12	3:M:211:THR:H	0.97	1.12
3:M:169:THR:HG22	3:M:179:SER:CB	1.80	1.11
3:L:118:PRO:HD2	3:L:206:LEU:CD2	1.80	1.11
3:N:201:VAL:HB	3:N:203:HIS:NE2	1.66	1.11
1:C:48:LEU:HD21	1:C:276:LEU:HD21	1.31	1.11
3:M:151:VAL:HG21	3:M:180:LEU:HD22	1.21	1.11
3:N:118:PRO:HD2	3:N:206:LEU:CD2	1.80	1.11
1:A:825:LYS:NZ	1:A:944:ALA:HB3	1.65	1.11
3:L:118:PRO:HG3	3:L:144:PHE:CZ	1.85	1.11
3:L:169:THR:HG21	3:L:179:SER:HB2	1.19	1.11
3:M:151:VAL:HG21	3:M:180:LEU:HD21	1.13	1.11
3:N:169:THR:HG21	3:N:179:SER:HB2	1.19	1.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:811:LYS:HD3	1:A:820:ASP:OD2	1.51	1.10
3:L:151:VAL:HG21	3:L:180:LEU:HD22	1.21	1.10
3:L:169:THR:HG22	3:L:179:SER:CB	1.80	1.10
1:B:48:LEU:HD21	1:B:306:PHE:CE1	1.87	1.10
3:M:201:VAL:HB	3:M:203:HIS:NE2	1.66	1.10
1:A:22:THR:CG2	1:A:78:ARG:HG3	1.82	1.10
1:B:80:ASP:O	1:B:82:PRO:HD3	1.52	1.10
1:C:22:THR:CG2	1:C:78:ARG:HG3	1.82	1.10
1:B:22:THR:CG2	1:B:78:ARG:HG3	1.82	1.09
3:L:210:VAL:HG12	3:L:211:THR:H	0.97	1.09
3:N:118:PRO:HG3	3:N:144:PHE:CZ	1.85	1.09
1:A:392:PHE:CD1	1:A:518:LEU:CD2	2.35	1.09
1:C:80:ASP:O	1:C:82:PRO:HD3	1.52	1.09
3:M:118:PRO:HD2	3:M:206:LEU:CD2	1.80	1.09
3:N:120:VAL:CG2	3:N:210:VAL:HG11	1.82	1.09
1:A:80:ASP:O	1:A:82:PRO:HD3	1.52	1.09
3:L:201:VAL:HB	3:L:203:HIS:NE2	1.66	1.09
3:M:120:VAL:CG2	3:M:210:VAL:HG11	1.82	1.09
1:B:424:LYS:HB2	1:B:461:LEU:HD23	1.18	1.09
2:H:169:TRP:CZ3	2:H:211:CYS:CB	2.35	1.09
3:L:151:VAL:HG21	3:L:180:LEU:HD21	1.13	1.09
1:A:517:LEU:HD22	1:A:519:HIS:HB2	1.24	1.09
2:J:140:ALA:HB3	2:J:229:LYS:HD3	1.35	1.09
3:L:151:VAL:CG2	3:L:180:LEU:CD2	2.30	1.08
3:L:153:TRP:HE1	3:L:182:SER:HB3	1.18	1.08
3:M:169:THR:HG22	3:M:179:SER:HB2	1.11	1.08
3:N:151:VAL:HG21	3:N:180:LEU:HD22	1.21	1.08
1:A:22:THR:HG21	1:A:78:ARG:CD	1.83	1.08
1:A:48:LEU:HD21	1:A:276:LEU:HD21	1.31	1.08
1:A:392:PHE:O	1:A:522:ALA:HB1	1.51	1.08
3:L:120:VAL:CG2	3:L:210:VAL:HG11	1.82	1.08
3:M:144:PHE:O	3:M:178:TYR:HB2	1.53	1.08
2:J:169:TRP:CZ3	2:J:211:CYS:CB	2.35	1.08
3:N:153:TRP:HE1	3:N:182:SER:HB3	1.18	1.08
1:A:826:VAL:CG1	1:A:1057:PRO:HG2	1.82	1.08
1:C:22:THR:HG21	1:C:78:ARG:CD	1.83	1.08
1:C:457:ARG:H	1:C:457:ARG:HD2	1.12	1.08
2:H:142:SER:CB	3:L:214:PHE:CD2	2.24	1.08
2:H:140:ALA:HB3	2:H:229:LYS:HD3	1.35	1.07
3:L:169:THR:CG2	3:L:179:SER:CB	2.31	1.07
3:M:151:VAL:CG2	3:M:180:LEU:CD2	2.30	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:118:PRO:HG2	3:N:206:LEU:HD11	1.36	1.07
3:N:151:VAL:CG2	3:N:180:LEU:CD2	2.30	1.07
2:I:169:TRP:CZ3	2:I:211:CYS:CB	2.35	1.07
3:N:151:VAL:HG21	3:N:180:LEU:HD21	1.13	1.07
1:B:22:THR:HG21	1:B:78:ARG:CD	1.83	1.07
1:A:392:PHE:HD1	1:A:518:LEU:HD22	0.97	1.07
2:J:178:VAL:HG12	2:J:197:VAL:HG13	1.10	1.07
3:N:144:PHE:O	3:N:178:TYR:HB2	1.53	1.07
3:N:169:THR:CG2	3:N:179:SER:CB	2.31	1.07
3:N:169:THR:HG22	3:N:179:SER:HB2	1.11	1.06
1:C:458:LYS:HG2	1:C:461:LEU:HD12	1.37	1.06
3:M:56:ILE:HG23	3:M:57:SER:H	1.16	1.06
3:N:56:ILE:HG23	3:N:57:SER:H	1.15	1.06
3:N:210:VAL:HG12	3:N:211:THR:H	0.97	1.06
1:A:826:VAL:HG11	1:A:1057:PRO:HG2	1.08	1.06
1:C:454:ARG:HD3	1:C:458:LYS:NZ	1.70	1.06
3:M:169:THR:CG2	3:M:179:SER:CB	2.31	1.06
2:H:178:VAL:HG12	2:H:197:VAL:HG13	1.10	1.06
3:M:169:THR:HG21	3:M:179:SER:HB2	1.19	1.05
3:L:56:ILE:HG23	3:L:57:SER:H	1.15	1.05
2:I:178:VAL:HG12	2:I:197:VAL:HG13	1.10	1.05
1:A:22:THR:CG2	1:A:78:ARG:CG	2.34	1.05
1:B:22:THR:CG2	1:B:78:ARG:CG	2.34	1.05
3:L:153:TRP:NE1	3:L:182:SER:HB3	1.72	1.05
3:M:155:VAL:HG21	3:M:184:LEU:HD21	1.35	1.05
3:N:155:VAL:HG21	3:N:184:LEU:HD21	1.35	1.05
1:C:22:THR:CG2	1:C:78:ARG:CG	2.34	1.05
3:M:153:TRP:HE1	3:M:182:SER:HB3	1.18	1.05
3:M:153:TRP:NE1	3:M:182:SER:HB3	1.72	1.05
1:B:48:LEU:HD21	1:B:306:PHE:CD1	1.92	1.04
2:H:163:GLU:HB3	2:H:164:PRO:HD3	1.39	1.04
3:L:169:THR:HG22	3:L:179:SER:HB2	1.11	1.04
3:L:118:PRO:HG3	3:L:144:PHE:CE2	1.90	1.04
3:L:144:PHE:O	3:L:178:TYR:HB2	1.53	1.04
3:M:153:TRP:HZ2	3:M:182:SER:CB	1.68	1.04
3:N:118:PRO:CG	3:N:144:PHE:CZ	2.41	1.04
3:M:118:PRO:CG	3:M:144:PHE:CZ	2.41	1.04
3:N:2:ILE:O	3:N:3:VAL:HG13	1.58	1.04
3:N:153:TRP:HZ2	3:N:182:SER:CB	1.67	1.04
3:L:155:VAL:HG21	3:L:184:LEU:HD21	1.35	1.04
3:N:153:TRP:NE1	3:N:182:SER:HB3	1.72	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:2:ILE:O	3:L:3:VAL:HG13	1.58	1.03
3:L:118:PRO:CG	3:L:144:PHE:CZ	2.41	1.03
2:I:140:ALA:HB3	2:I:229:LYS:HD3	1.35	1.03
1:B:58:PHE:CE1	1:B:275:PHE:HE2	1.76	1.03
2:H:185:LEU:HD21	2:H:191:TYR:CZ	1.94	1.03
3:M:168:VAL:HG13	3:M:179:SER:O	1.58	1.03
2:J:163:GLU:HB3	2:J:164:PRO:HD3	1.39	1.03
1:B:1082:CYS:SG	1:B:1126:CYS:HB2	1.98	1.03
3:L:144:PHE:CE2	3:L:203:HIS:CG	2.47	1.03
2:J:141:PRO:CG	2:J:228:PRO:CA	2.37	1.03
3:M:2:ILE:O	3:M:3:VAL:HG13	1.58	1.02
3:N:144:PHE:CE2	3:N:203:HIS:CG	2.47	1.02
1:A:48:LEU:HD21	1:A:276:LEU:CD2	1.89	1.02
2:H:52:ASP:HB2	3:L:99:PHE:CE1	1.94	1.02
3:L:118:PRO:CD	3:L:206:LEU:CG	2.36	1.02
3:L:153:TRP:HZ2	3:L:182:SER:CB	1.67	1.02
3:L:210:VAL:HG12	3:L:211:THR:N	1.70	1.02
2:I:52:ASP:HB2	3:M:99:PHE:CE1	1.94	1.02
2:I:178:VAL:HG12	2:I:197:VAL:CB	1.90	1.02
2:I:185:LEU:HD21	2:I:191:TYR:CZ	1.94	1.02
1:A:276:LEU:HB3	1:A:289:VAL:HG13	1.41	1.02
1:A:454:ARG:HD2	1:A:491:PRO:CA	1.90	1.02
1:B:276:LEU:HG	1:B:289:VAL:HB	1.03	1.02
2:I:141:PRO:CG	2:I:228:PRO:CA	2.36	1.02
2:I:163:GLU:HB3	2:I:164:PRO:HD3	1.39	1.02
3:M:118:PRO:HG3	3:M:144:PHE:CE2	1.90	1.02
3:N:151:VAL:CG2	3:N:180:LEU:HD22	1.89	1.02
3:M:118:PRO:HG2	3:M:206:LEU:HD11	1.36	1.02
3:M:144:PHE:CE2	3:M:203:HIS:CG	2.47	1.02
2:J:59:MET:CG	3:N:99:PHE:CE2	2.43	1.02
1:C:48:LEU:HD21	1:C:276:LEU:CD2	1.89	1.02
3:M:210:VAL:HG12	3:M:211:THR:N	1.70	1.02
2:J:52:ASP:HB2	3:N:99:PHE:CE1	1.94	1.02
3:N:168:VAL:HG13	3:N:179:SER:O	1.58	1.02
2:H:178:VAL:HG12	2:H:197:VAL:CB	1.90	1.01
3:M:118:PRO:CD	3:M:206:LEU:CG	2.36	1.01
2:H:141:PRO:CG	2:H:228:PRO:CA	2.36	1.01
3:N:118:PRO:HG3	3:N:144:PHE:CE2	1.90	1.01
3:L:118:PRO:HG2	3:L:144:PHE:CE2	1.93	1.01
2:J:178:VAL:HG12	2:J:197:VAL:CB	1.90	1.01
2:H:140:ALA:CB	2:H:229:LYS:CD	2.39	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:168:VAL:HG13	3:L:179:SER:O	1.58	1.01
2:J:169:TRP:CD1	2:J:197:VAL:HG23	1.96	1.01
1:A:392:PHE:HB3	1:A:518:LEU:HB3	1.43	1.00
1:B:452:LEU:HD22	1:B:494:SER:HA	1.02	1.00
3:L:118:PRO:HG2	3:L:206:LEU:HD11	1.36	1.00
2:J:140:ALA:CB	2:J:229:LYS:CD	2.39	1.00
3:N:118:PRO:HG2	3:N:144:PHE:CE2	1.93	1.00
1:C:454:ARG:HD3	1:C:458:LYS:HZ2	1.17	1.00
2:I:140:ALA:CB	2:I:229:LYS:CD	2.39	1.00
2:I:169:TRP:CD1	2:I:197:VAL:HG23	1.96	1.00
3:M:118:PRO:HG2	3:M:144:PHE:CE2	1.93	1.00
3:N:210:VAL:HG12	3:N:211:THR:N	1.70	1.00
1:A:285:ILE:HG22	1:A:286:THR:H	1.26	1.00
1:C:458:LYS:HG2	1:C:461:LEU:HD11	1.05	1.00
3:L:151:VAL:CG2	3:L:180:LEU:HD22	1.89	1.00
2:I:59:MET:CG	3:M:99:PHE:CE2	2.43	1.00
3:M:118:PRO:HD2	3:M:206:LEU:HG	1.37	1.00
2:J:185:LEU:HD21	2:J:191:TYR:CZ	1.94	1.00
1:B:454:ARG:HG3	1:B:455:LEU:H	1.25	1.00
1:A:276:LEU:HB3	1:A:289:VAL:HG12	1.38	1.00
2:J:142:SER:HA	3:N:214:PHE:HE2	1.26	1.00
3:N:150:LYS:HZ2	3:N:202:THR:HB	1.26	1.00
1:B:220:PHE:CE2	1:B:287:ASP:HA	1.97	0.99
1:B:48:LEU:HD23	1:B:306:PHE:HE1	1.24	0.99
3:L:56:ILE:CG2	3:L:57:SER:H	1.75	0.99
3:M:56:ILE:CG2	3:M:57:SER:H	1.75	0.99
2:H:59:MET:CG	3:L:99:PHE:CE2	2.43	0.99
3:M:210:VAL:CG1	3:M:211:THR:H	1.75	0.99
3:L:210:VAL:CG1	3:L:211:THR:H	1.75	0.99
1:B:1082:CYS:SG	1:B:1126:CYS:CB	2.51	0.99
3:M:2:ILE:HG22	3:M:4:MET:HE2	1.45	0.99
3:M:151:VAL:CG2	3:M:180:LEU:HD22	1.88	0.99
1:C:48:LEU:CD2	1:C:276:LEU:CD1	2.41	0.98
3:L:155:VAL:CG2	3:L:184:LEU:CD2	2.41	0.98
3:N:9:LEU:HD11	3:N:105:GLN:NE2	1.78	0.98
1:B:452:LEU:HD22	1:B:494:SER:CA	1.93	0.98
3:N:210:VAL:CG1	3:N:211:THR:H	1.75	0.98
2:H:169:TRP:CD1	2:H:197:VAL:HG23	1.96	0.98
2:H:178:VAL:HG12	2:H:197:VAL:CG2	1.94	0.98
3:L:2:ILE:CG2	3:L:4:MET:HE2	1.93	0.98
3:L:2:ILE:HG22	3:L:4:MET:HE2	1.45	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:178:VAL:HG12	2:I:197:VAL:CG2	1.94	0.98
1:A:48:LEU:CD2	1:A:276:LEU:CD1	2.41	0.98
3:N:56:ILE:HG23	3:N:57:SER:N	1.75	0.98
3:N:155:VAL:CG2	3:N:184:LEU:CD2	2.41	0.98
2:H:169:TRP:HZ2	2:H:195:SER:O	1.47	0.98
1:B:58:PHE:CE1	1:B:275:PHE:CE2	2.51	0.98
3:M:9:LEU:HD11	3:M:105:GLN:NE2	1.78	0.98
3:N:118:PRO:CD	3:N:206:LEU:CG	2.36	0.98
3:N:141:LEU:HD22	3:N:201:VAL:HG11	1.43	0.98
1:C:454:ARG:NH1	1:C:458:LYS:CE	2.26	0.97
2:J:52:ASP:CB	3:N:99:PHE:CZ	2.47	0.97
2:J:169:TRP:HZ2	2:J:195:SER:O	1.47	0.97
3:N:2:ILE:CG2	3:N:4:MET:HE2	1.93	0.97
2:I:142:SER:HA	3:M:214:PHE:HE2	1.26	0.97
2:I:181:PHE:HB3	3:M:167:SER:HB3	1.46	0.97
1:B:276:LEU:HD21	1:B:289:VAL:HG11	1.43	0.97
2:H:169:TRP:CD1	2:H:197:VAL:HG21	1.99	0.97
3:M:141:LEU:HD22	3:M:201:VAL:HG11	1.43	0.97
1:A:401:VAL:HG13	1:A:508:TYR:O	1.64	0.97
2:H:181:PHE:CZ	3:L:181:SER:CB	2.47	0.97
3:M:2:ILE:CG2	3:M:4:MET:HE2	1.93	0.97
3:M:155:VAL:CG2	3:M:184:LEU:CD2	2.41	0.97
2:H:52:ASP:CB	3:L:99:PHE:CZ	2.47	0.97
2:H:181:PHE:HB3	3:L:167:SER:HB3	1.46	0.97
3:L:9:LEU:HD11	3:L:105:GLN:NE2	1.78	0.97
3:N:2:ILE:CG2	3:N:4:MET:CE	2.43	0.97
3:L:118:PRO:HD2	3:L:206:LEU:HD21	1.47	0.97
2:I:181:PHE:CZ	3:M:181:SER:CB	2.47	0.97
3:M:56:ILE:HG23	3:M:57:SER:N	1.75	0.97
2:J:178:VAL:HG12	2:J:197:VAL:CG2	1.94	0.97
2:J:181:PHE:CZ	3:N:181:SER:CB	2.47	0.97
3:N:56:ILE:CG2	3:N:57:SER:H	1.75	0.97
3:L:141:LEU:HD22	3:L:201:VAL:HG11	1.43	0.96
3:L:154:LYS:CD	3:L:157:ASN:HA	1.96	0.96
3:N:154:LYS:CD	3:N:157:ASN:HA	1.96	0.96
3:N:155:VAL:CG2	3:N:184:LEU:HD21	1.95	0.96
3:L:150:LYS:HZ2	3:L:202:THR:HB	1.29	0.96
3:L:153:TRP:CE2	3:L:182:SER:HB2	2.00	0.96
3:M:153:TRP:CE2	3:M:182:SER:HB2	2.00	0.96
3:M:154:LYS:CD	3:M:157:ASN:HA	1.96	0.96
2:J:181:PHE:HB3	3:N:167:SER:HB3	1.46	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:2:ILE:CG2	3:L:4:MET:CE	2.43	0.96
1:A:449:TYR:CD2	1:A:497:PHE:HD2	1.84	0.96
3:M:2:ILE:CG2	3:M:4:MET:CE	2.43	0.96
2:I:52:ASP:CB	3:M:99:PHE:CZ	2.47	0.96
1:A:391:CYS:HB3	1:A:525:CYS:HA	1.45	0.95
3:L:141:LEU:HD11	3:L:151:VAL:HG13	1.48	0.95
3:N:118:PRO:CG	3:N:206:LEU:HD11	1.96	0.95
1:B:276:LEU:HG	1:B:289:VAL:CB	1.96	0.95
1:B:422:ASN:O	1:B:461:LEU:HD21	1.64	0.95
3:N:118:PRO:HD2	3:N:206:LEU:HG	1.37	0.95
2:H:169:TRP:HZ3	2:H:211:CYS:HB2	1.17	0.95
2:J:169:TRP:CD1	2:J:197:VAL:HG21	1.99	0.95
3:N:118:PRO:HG2	3:N:206:LEU:CD1	1.96	0.95
2:H:184:VAL:O	2:H:191:TYR:CD1	2.20	0.95
1:A:43:PHE:CD2	1:C:559:PHE:CE1	2.54	0.95
2:J:184:VAL:O	2:J:191:TYR:CD1	2.20	0.95
3:L:56:ILE:HG23	3:L:57:SER:N	1.75	0.95
3:L:2:ILE:HD12	3:L:2:ILE:H	1.32	0.95
3:M:118:PRO:CG	3:M:206:LEU:HD11	1.96	0.95
3:M:118:PRO:HG2	3:M:206:LEU:CD1	1.96	0.95
3:L:118:PRO:CG	3:L:206:LEU:HD11	1.96	0.95
3:L:155:VAL:CG2	3:L:184:LEU:HD21	1.96	0.95
2:I:169:TRP:HZ2	2:I:195:SER:O	1.47	0.95
1:C:22:THR:HG21	1:C:78:ARG:NE	1.81	0.95
3:L:118:PRO:HG2	3:L:206:LEU:CD1	1.97	0.94
2:I:169:TRP:CD1	2:I:197:VAL:HG21	1.99	0.94
3:N:153:TRP:CE2	3:N:182:SER:HB2	2.00	0.94
3:N:118:PRO:HD2	3:N:206:LEU:HD21	1.47	0.94
1:A:318:PHE:CE1	1:A:620:VAL:O	2.20	0.94
2:H:142:SER:HA	3:L:214:PHE:HE2	1.26	0.94
3:N:2:ILE:HG22	3:N:4:MET:HE2	1.45	0.94
2:I:184:VAL:O	2:I:191:TYR:CD1	2.20	0.94
3:M:2:ILE:H	3:M:2:ILE:HD12	1.32	0.94
3:M:141:LEU:HD11	3:M:151:VAL:HG13	1.48	0.94
3:N:2:ILE:H	3:N:2:ILE:HD12	1.32	0.94
1:A:403:ARG:O	1:A:407:VAL:HG23	1.67	0.94
1:C:48:LEU:HD21	1:C:276:LEU:CG	1.97	0.94
1:A:454:ARG:CD	1:A:491:PRO:CA	2.45	0.94
1:C:220:PHE:CE2	1:C:287:ASP:HA	2.02	0.94
3:L:120:VAL:HG21	3:L:210:VAL:HB	1.48	0.94
3:M:153:TRP:CE2	3:M:182:SER:CB	2.51	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:126:VAL:HG12	1:B:172:SER:O	1.68	0.94
1:B:22:THR:HG21	1:B:78:ARG:NE	1.81	0.93
1:B:57:PRO:HB3	1:B:273:ARG:CZ	1.98	0.93
3:M:118:PRO:HD2	3:M:206:LEU:HD21	1.47	0.93
1:A:22:THR:HG21	1:A:78:ARG:NE	1.81	0.93
3:L:153:TRP:CE2	3:L:182:SER:CB	2.51	0.93
3:L:153:TRP:HE1	3:L:182:SER:CB	1.81	0.93
1:B:276:LEU:CD1	1:B:289:VAL:HB	1.98	0.93
1:B:452:LEU:CD2	1:B:494:SER:CA	2.45	0.93
3:N:154:LYS:HD3	3:N:157:ASN:HA	1.50	0.93
3:M:153:TRP:NE1	3:M:182:SER:CB	2.32	0.93
3:N:153:TRP:HE1	3:N:182:SER:CB	1.81	0.93
3:N:153:TRP:CE2	3:N:182:SER:CB	2.51	0.93
3:M:144:PHE:HZ	3:M:203:HIS:HB2	1.12	0.93
3:M:155:VAL:CG2	3:M:184:LEU:HD21	1.96	0.93
3:N:141:LEU:HD11	3:N:151:VAL:HG13	1.48	0.93
1:A:126:VAL:HG12	1:A:172:SER:O	1.68	0.93
3:L:7:SER:HG	3:L:8:PRO:HD3	1.26	0.93
1:A:48:LEU:HD21	1:A:276:LEU:CG	1.97	0.92
1:C:22:THR:HG21	1:C:78:ARG:HG3	1.46	0.92
3:M:141:LEU:CD2	3:M:201:VAL:CG1	2.48	0.92
3:M:153:TRP:HE1	3:M:182:SER:CB	1.81	0.92
1:A:826:VAL:HG11	1:A:1057:PRO:CG	1.99	0.92
1:B:418:ILE:HD13	1:B:422:ASN:HD21	1.34	0.92
3:L:154:LYS:HD3	3:L:157:ASN:HA	1.50	0.92
2:I:160:TYR:CD2	2:I:162:PRO:HD2	2.04	0.92
1:B:276:LEU:CG	1:B:289:VAL:CB	2.45	0.92
1:B:276:LEU:CD1	1:B:289:VAL:CG2	2.48	0.92
3:N:120:VAL:HG21	3:N:210:VAL:HB	1.48	0.92
1:A:220:PHE:CG	1:A:286:THR:O	2.22	0.92
2:J:160:TYR:CD2	2:J:162:PRO:HD2	2.04	0.92
2:H:178:VAL:HB	2:H:197:VAL:HG22	1.50	0.92
3:M:150:LYS:HZ2	3:M:202:THR:HB	1.35	0.92
3:N:153:TRP:NE1	3:N:182:SER:CB	2.32	0.92
2:J:141:PRO:HG3	2:J:228:PRO:CB	2.00	0.92
3:M:120:VAL:HG21	3:M:210:VAL:HB	1.48	0.92
2:J:178:VAL:HB	2:J:197:VAL:HG22	1.50	0.92
1:A:517:LEU:CD2	1:A:519:HIS:HB2	1.99	0.92
1:C:454:ARG:HH11	1:C:458:LYS:CE	1.82	0.92
2:I:169:TRP:HZ3	2:I:211:CYS:HB2	1.17	0.92
2:I:141:PRO:HG3	2:I:228:PRO:CB	1.99	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:153:TRP:NE1	3:L:182:SER:CB	2.32	0.91
1:C:126:VAL:HG12	1:C:172:SER:O	1.68	0.91
2:H:163:GLU:HB3	2:H:164:PRO:CD	2.00	0.91
2:J:169:TRP:HD1	2:J:197:VAL:CG2	1.80	0.91
3:N:120:VAL:HG21	3:N:210:VAL:CB	2.00	0.91
2:H:141:PRO:HG3	2:H:228:PRO:CB	1.99	0.91
2:H:160:TYR:CD2	2:H:162:PRO:HD2	2.04	0.91
3:L:2:ILE:HG22	3:L:4:MET:CE	2.00	0.91
3:M:4:MET:HB2	3:M:24:ARG:O	1.70	0.91
3:N:141:LEU:CD2	3:N:201:VAL:CG1	2.48	0.91
2:H:181:PHE:CE2	3:L:181:SER:OG	2.23	0.91
3:L:122:ILE:HD13	3:L:199:CYS:HB2	1.53	0.91
3:M:141:LEU:HD12	3:M:180:LEU:HD22	1.53	0.91
3:L:4:MET:HB2	3:L:24:ARG:O	1.70	0.91
3:L:141:LEU:HD12	3:L:180:LEU:HD22	1.53	0.91
3:N:2:ILE:HG22	3:N:4:MET:CE	2.00	0.91
3:N:4:MET:HB2	3:N:24:ARG:O	1.70	0.91
2:H:169:TRP:HD1	2:H:197:VAL:CG2	1.80	0.91
3:M:122:ILE:HG21	3:M:213:SER:HA	0.91	0.91
3:N:122:ILE:HG21	3:N:213:SER:HA	0.91	0.91
3:N:153:TRP:HZ2	3:N:182:SER:HB2	1.24	0.91
2:J:163:GLU:HB3	2:J:164:PRO:CD	2.00	0.91
1:B:1141:LEU:HD23	1:B:1142:GLN:N	1.86	0.90
3:L:141:LEU:CD2	3:L:201:VAL:CG1	2.48	0.90
2:I:178:VAL:HB	2:I:197:VAL:HG22	1.50	0.90
2:I:181:PHE:CE2	3:M:181:SER:OG	2.23	0.90
2:I:163:GLU:HB3	2:I:164:PRO:CD	2.00	0.90
3:L:139:CYS:N	3:L:153:TRP:CH2	2.40	0.90
3:L:144:PHE:HZ	3:L:203:HIS:HB2	1.12	0.90
2:H:140:ALA:CB	2:H:229:LYS:HD3	2.02	0.90
3:L:120:VAL:HG21	3:L:210:VAL:CG1	2.02	0.90
3:L:120:VAL:HG21	3:L:210:VAL:CB	2.00	0.90
3:M:120:VAL:HG21	3:M:210:VAL:CB	2.00	0.90
1:A:392:PHE:O	1:A:522:ALA:CB	2.20	0.90
2:H:59:MET:CG	3:L:99:PHE:HD2	1.77	0.90
2:I:181:PHE:CB	3:M:167:SER:HB3	2.02	0.90
2:I:169:TRP:HD1	2:I:197:VAL:CG2	1.80	0.90
3:M:120:VAL:HG21	3:M:210:VAL:CG1	2.02	0.90
1:A:220:PHE:CZ	1:A:287:ASP:HA	2.06	0.90
1:C:498:GLN:HG2	1:C:501:ASN:HB2	1.53	0.90
3:M:139:CYS:N	3:M:153:TRP:CH2	2.40	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:141:LEU:HD21	3:L:201:VAL:CG1	2.02	0.90
3:M:141:LEU:HD21	3:M:201:VAL:CG1	2.02	0.90
3:N:139:CYS:N	3:N:153:TRP:CH2	2.40	0.90
3:L:210:VAL:O	3:L:211:THR:OG1	1.91	0.89
2:J:169:TRP:HZ3	2:J:211:CYS:HB2	1.17	0.89
3:N:144:PHE:CZ	3:N:203:HIS:CG	2.61	0.89
3:N:210:VAL:O	3:N:211:THR:OG1	1.91	0.89
2:H:181:PHE:CB	3:L:167:SER:HB3	2.02	0.89
2:J:181:PHE:CE2	3:N:181:SER:OG	2.23	0.89
3:L:122:ILE:HG21	3:L:213:SER:HA	0.91	0.89
2:J:140:ALA:CB	2:J:229:LYS:HD3	2.01	0.89
3:N:120:VAL:HG21	3:N:210:VAL:CG1	2.02	0.89
2:J:169:TRP:NE1	2:J:197:VAL:HG23	1.87	0.89
3:N:141:LEU:HD12	3:N:180:LEU:HD22	1.53	0.89
1:A:393:THR:OG1	1:A:516:GLU:HB3	1.71	0.89
3:M:120:VAL:CG2	3:M:210:VAL:CG1	2.51	0.89
3:M:154:LYS:HD3	3:M:157:ASN:HA	1.50	0.89
2:J:178:VAL:HG12	2:J:197:VAL:HG11	1.53	0.89
1:A:220:PHE:CE2	1:A:287:ASP:HA	2.06	0.89
1:C:454:ARG:HH11	1:C:458:LYS:HE3	1.07	0.89
2:H:178:VAL:HG12	2:H:197:VAL:HG11	1.53	0.89
3:N:122:ILE:HD13	3:N:199:CYS:HB2	1.53	0.89
1:A:454:ARG:CD	1:A:491:PRO:HA	2.03	0.89
1:A:503:VAL:HG12	1:A:504:GLY:H	1.36	0.89
3:M:144:PHE:CZ	3:M:203:HIS:CG	2.61	0.89
2:I:140:ALA:CB	2:I:229:LYS:HD3	2.01	0.89
1:C:558:LYS:HG3	5:G:1:NAG:O7	1.73	0.88
2:H:169:TRP:NE1	2:H:197:VAL:HG23	1.87	0.88
1:C:23:GLN:C	1:C:24:LEU:HD22	1.98	0.88
1:C:501:ASN:O	1:C:505:TYR:HB2	1.72	0.88
3:L:120:VAL:CG2	3:L:210:VAL:CG1	2.51	0.88
2:I:52:ASP:HB2	3:M:99:PHE:HZ	0.95	0.88
3:M:2:ILE:HG22	3:M:4:MET:CE	2.00	0.88
2:J:181:PHE:CB	3:N:167:SER:HB3	2.02	0.88
2:I:169:TRP:NE1	2:I:197:VAL:HG23	1.87	0.88
2:J:59:MET:CG	3:N:99:PHE:HD2	1.77	0.88
1:A:23:GLN:C	1:A:24:LEU:HD22	1.98	0.88
1:B:22:THR:HG23	1:B:78:ARG:HG3	1.55	0.88
2:I:178:VAL:HG12	2:I:197:VAL:HG11	1.53	0.88
3:M:122:ILE:HD13	3:M:199:CYS:HB2	1.53	0.88
1:C:22:THR:HG23	1:C:78:ARG:HG3	1.55	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:52:ASP:CB	3:N:99:PHE:HZ	1.83	0.88
3:N:141:LEU:HD21	3:N:201:VAL:CG1	2.02	0.88
3:N:144:PHE:HZ	3:N:203:HIS:HB2	1.12	0.88
1:A:48:LEU:HD23	1:A:276:LEU:HD11	1.55	0.88
1:B:23:GLN:C	1:B:24:LEU:HD22	1.98	0.88
3:L:144:PHE:CZ	3:L:203:HIS:CG	2.61	0.88
3:N:7:SER:HG	3:N:8:PRO:HD3	1.35	0.87
2:H:181:PHE:CD2	3:L:167:SER:O	2.28	0.87
1:B:57:PRO:HB3	1:B:273:ARG:HE	1.33	0.87
2:H:140:ALA:HB2	2:H:229:LYS:HD2	1.56	0.87
2:I:59:MET:CG	3:M:99:PHE:HD2	1.77	0.87
3:N:120:VAL:CG2	3:N:210:VAL:CG1	2.51	0.87
1:B:220:PHE:CD2	1:B:286:THR:O	2.28	0.87
3:M:210:VAL:O	3:M:211:THR:OG1	1.91	0.87
3:L:98:GLN:OE1	3:L:98:GLN:N	2.08	0.87
2:J:141:PRO:HG3	2:J:228:PRO:HA	1.56	0.87
3:L:141:LEU:HD21	3:L:201:VAL:HG11	1.57	0.87
2:I:141:PRO:HG3	2:I:228:PRO:CA	2.04	0.87
2:I:178:VAL:CB	2:I:197:VAL:HG22	2.05	0.87
3:N:151:VAL:CG2	3:N:180:LEU:HD21	2.01	0.87
2:H:141:PRO:HG3	2:H:228:PRO:CA	2.04	0.87
3:L:10:SER:O	3:L:11:SER:OG	1.93	0.87
3:M:118:PRO:HD2	3:M:206:LEU:CD1	2.05	0.87
2:H:178:VAL:CB	2:H:197:VAL:HG22	2.05	0.86
3:L:120:VAL:CB	3:L:210:VAL:HG11	2.05	0.86
3:M:118:PRO:HD3	3:M:206:LEU:HG	1.55	0.86
2:J:142:SER:HA	3:N:214:PHE:CE2	2.10	0.86
3:N:118:PRO:HD3	3:N:206:LEU:HG	1.55	0.86
2:J:141:PRO:HD2	2:J:228:PRO:HA	1.58	0.86
1:A:392:PHE:HD1	1:A:518:LEU:CD2	1.79	0.86
1:C:456:PHE:HB3	1:C:457:ARG:HH11	1.39	0.86
1:A:454:ARG:HD2	1:A:491:PRO:N	1.90	0.86
3:L:118:PRO:HD3	3:L:206:LEU:HG	1.55	0.86
3:M:10:SER:O	3:M:11:SER:OG	1.93	0.86
2:I:52:ASP:CB	3:M:99:PHE:HZ	1.83	0.86
2:J:181:PHE:CD2	3:N:167:SER:O	2.28	0.86
3:N:150:LYS:O	3:N:203:HIS:CE1	2.28	0.86
1:B:427:ASP:O	1:B:428:ASP:O	1.93	0.86
2:J:178:VAL:CB	2:J:197:VAL:HG22	2.05	0.86
3:N:10:SER:O	3:N:11:SER:OG	1.93	0.86
3:L:150:LYS:O	3:L:203:HIS:CE1	2.28	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:142:SER:HA	3:M:214:PHE:CE2	2.10	0.86
2:I:181:PHE:CD2	3:M:167:SER:O	2.28	0.86
3:M:120:VAL:CB	3:M:210:VAL:HG11	2.05	0.86
2:J:141:PRO:HG3	2:J:228:PRO:CA	2.04	0.86
1:A:22:THR:HG23	1:A:78:ARG:HG3	1.55	0.86
1:C:48:LEU:HD23	1:C:276:LEU:HD11	1.55	0.86
3:M:153:TRP:HZ2	3:M:182:SER:CA	1.88	0.86
1:A:318:PHE:CZ	1:A:620:VAL:O	2.28	0.86
1:C:456:PHE:HD2	1:C:491:PRO:HA	1.38	0.86
2:H:141:PRO:HG3	2:H:228:PRO:HA	1.56	0.85
3:M:98:GLN:OE1	3:M:98:GLN:N	2.08	0.85
2:H:52:ASP:CB	3:L:99:PHE:HZ	1.83	0.85
3:M:141:LEU:HD21	3:M:201:VAL:HG11	1.57	0.85
3:N:98:GLN:N	3:N:98:GLN:OE1	2.08	0.85
1:A:825:LYS:HZ3	1:A:944:ALA:HB3	1.39	0.85
1:B:961:THR:HG21	1:C:762:GLN:HE21	1.41	0.85
1:C:19:THR:O	1:C:20:THR:OG1	1.94	0.85
2:H:142:SER:HB3	3:L:214:PHE:CE2	2.10	0.85
1:A:390:LEU:HG	1:A:391:CYS:H	1.40	0.85
3:L:2:ILE:HG21	3:L:4:MET:CE	2.06	0.85
3:L:118:PRO:HD2	3:L:206:LEU:CD1	2.05	0.85
2:J:140:ALA:HB2	2:J:229:LYS:HD2	1.56	0.85
2:J:142:SER:HB3	3:N:214:PHE:CE2	2.10	0.85
3:N:2:ILE:HG21	3:N:4:MET:CE	2.07	0.85
1:C:454:ARG:CD	1:C:458:LYS:NZ	2.39	0.85
2:H:142:SER:HA	3:L:214:PHE:CE2	2.10	0.85
3:N:120:VAL:CB	3:N:210:VAL:HG11	2.05	0.85
3:N:153:TRP:HZ2	3:N:182:SER:CA	1.89	0.85
2:H:185:LEU:CD2	2:H:191:TYR:CE1	2.59	0.85
3:M:150:LYS:O	3:M:203:HIS:CE1	2.28	0.85
2:H:59:MET:HB2	3:L:99:PHE:CE2	2.11	0.85
2:J:59:MET:HB2	3:N:99:PHE:CE2	2.11	0.85
2:J:185:LEU:CD2	2:J:191:TYR:CE1	2.59	0.85
1:A:19:THR:O	1:A:20:THR:OG1	1.95	0.85
1:A:454:ARG:HD2	1:A:491:PRO:C	2.01	0.85
3:L:153:TRP:HZ2	3:L:182:SER:CA	1.88	0.85
1:C:454:ARG:CZ	1:C:458:LYS:HE3	2.06	0.85
2:I:142:SER:HB3	3:M:214:PHE:CE2	2.10	0.85
2:I:185:LEU:CD2	2:I:191:TYR:CE1	2.59	0.84
1:B:58:PHE:HE1	1:B:275:PHE:HE2	1.24	0.84
1:C:456:PHE:CE2	1:C:491:PRO:HA	2.11	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:140:ALA:HB2	2:I:229:LYS:HD2	1.56	0.84
3:N:118:PRO:HD2	3:N:206:LEU:CD1	2.05	0.84
1:A:276:LEU:CB	1:A:289:VAL:CG1	2.50	0.84
1:B:270:LEU:O	1:B:271:GLN:HB2	1.75	0.84
1:B:276:LEU:HD11	1:B:289:VAL:CB	2.06	0.84
2:H:141:PRO:HD2	2:H:228:PRO:HA	1.58	0.84
2:H:204:LEU:HD11	2:H:228:PRO:HG3	1.59	0.84
3:M:122:ILE:CG2	3:M:213:SER:CA	2.45	0.84
3:L:143:ASN:CG	3:L:177:THR:HG21	2.02	0.84
2:I:140:ALA:HB3	2:I:229:LYS:CD	2.06	0.84
2:I:59:MET:HB2	3:M:99:PHE:CE2	2.11	0.84
3:M:120:VAL:HB	3:M:210:VAL:HG11	1.60	0.84
2:I:204:LEU:HD11	2:I:228:PRO:HG3	1.59	0.84
1:A:48:LEU:HD23	1:A:276:LEU:CD1	2.04	0.84
1:C:827:THR:C	1:C:828:LEU:HD12	2.03	0.84
1:A:276:LEU:CD2	1:A:289:VAL:HG11	2.08	0.84
3:M:171:GLN:HG3	3:M:178:TYR:CZ	2.13	0.84
3:N:120:VAL:HB	3:N:210:VAL:HG11	1.60	0.84
1:B:19:THR:O	1:B:20:THR:OG1	1.95	0.83
3:L:120:VAL:HB	3:L:210:VAL:HG11	1.60	0.83
3:L:144:PHE:O	3:L:178:TYR:CB	2.26	0.83
3:M:141:LEU:CD1	3:M:201:VAL:HG11	2.08	0.83
3:N:143:ASN:CG	3:N:177:THR:HG21	2.02	0.83
3:L:7:SER:HB3	3:L:22:SER:OG	1.79	0.83
1:A:276:LEU:HD23	1:A:289:VAL:HG11	1.61	0.83
1:B:457:ARG:NH2	1:B:491:PRO:HA	1.93	0.83
3:L:171:GLN:HG3	3:L:178:TYR:CZ	2.13	0.83
3:M:139:CYS:HB2	3:M:153:TRP:CZ3	2.13	0.83
3:M:143:ASN:CG	3:M:177:THR:HG21	2.02	0.83
3:M:144:PHE:O	3:M:178:TYR:CB	2.26	0.83
3:L:141:LEU:CD1	3:L:201:VAL:HG11	2.08	0.83
3:L:151:VAL:CG2	3:L:180:LEU:HD21	2.01	0.83
2:I:141:PRO:HD2	2:I:228:PRO:HA	1.57	0.83
3:M:151:VAL:CG2	3:M:180:LEU:HD21	2.01	0.83
3:M:2:ILE:HG21	3:M:4:MET:CE	2.07	0.83
3:N:141:LEU:CD1	3:N:201:VAL:HG11	2.08	0.83
3:N:202:THR:C	3:N:203:HIS:CD2	2.57	0.83
1:B:22:THR:HG21	1:B:78:ARG:HG3	1.46	0.83
3:L:124:PRO:HG3	3:L:214:PHE:CD1	2.13	0.83
3:L:139:CYS:HB2	3:L:153:TRP:CZ3	2.13	0.83
2:I:178:VAL:CG1	2:I:197:VAL:CG2	2.57	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:4:MET:CB	3:N:24:ARG:O	2.26	0.83
3:N:139:CYS:HB2	3:N:153:TRP:CZ3	2.13	0.83
3:M:2:ILE:HG21	3:M:4:MET:HE1	1.61	0.83
3:M:139:CYS:N	3:M:153:TRP:HH2	1.77	0.83
3:N:2:ILE:HG21	3:N:4:MET:HE1	1.61	0.83
3:N:139:CYS:N	3:N:153:TRP:HH2	1.77	0.83
3:L:171:GLN:HA	3:L:177:THR:O	1.79	0.83
3:L:202:THR:C	3:L:203:HIS:CD2	2.57	0.83
3:M:202:THR:C	3:M:203:HIS:CD2	2.57	0.83
2:J:178:VAL:CG1	2:J:197:VAL:CG2	2.57	0.83
3:N:171:GLN:HG3	3:N:178:TYR:CZ	2.13	0.83
3:M:4:MET:CB	3:M:24:ARG:O	2.26	0.82
2:J:204:LEU:HD11	2:J:228:PRO:HG3	1.59	0.82
3:N:171:GLN:HA	3:N:177:THR:O	1.79	0.82
1:C:458:LYS:CG	1:C:461:LEU:CD1	2.35	0.82
2:I:169:TRP:CZ2	2:I:195:SER:O	2.33	0.82
3:M:7:SER:HB3	3:M:22:SER:OG	1.79	0.82
1:A:48:LEU:CD2	1:A:276:LEU:CG	2.57	0.82
1:C:48:LEU:HD23	1:C:276:LEU:CD1	2.04	0.82
2:H:178:VAL:CG1	2:H:197:VAL:CG2	2.57	0.82
3:M:124:PRO:HG3	3:M:214:PHE:CD1	2.13	0.82
3:N:7:SER:HB3	3:N:22:SER:OG	1.79	0.82
1:A:825:LYS:NZ	1:A:944:ALA:CB	2.41	0.82
2:J:181:PHE:CE2	3:N:181:SER:CB	2.62	0.82
1:C:824:ASN:O	1:C:827:THR:HG22	1.80	0.82
2:H:169:TRP:CZ2	2:H:195:SER:O	2.32	0.82
3:L:4:MET:CB	3:L:24:ARG:O	2.26	0.82
1:A:403:ARG:HD3	1:A:505:TYR:HD1	1.45	0.82
3:N:155:VAL:HG22	3:N:184:LEU:CD2	2.09	0.82
1:B:458:LYS:O	1:B:459:SER:HB3	1.78	0.82
1:C:48:LEU:CD2	1:C:276:LEU:CG	2.57	0.82
3:L:139:CYS:N	3:L:153:TRP:HH2	1.77	0.82
3:L:155:VAL:HG22	3:L:184:LEU:CD2	2.09	0.82
3:M:169:THR:HG21	3:M:179:SER:CB	2.05	0.82
3:M:197:TYR:O	3:M:213:SER:CB	2.26	0.82
3:N:124:PRO:HG3	3:N:214:PHE:CD1	2.13	0.82
3:N:144:PHE:O	3:N:178:TYR:CB	2.26	0.81
1:C:421:TYR:O	1:C:458:LYS:HD3	1.79	0.81
2:I:181:PHE:CE2	3:M:181:SER:CB	2.62	0.81
1:B:457:ARG:HH22	1:B:491:PRO:HA	1.43	0.81
1:C:457:ARG:HD2	1:C:457:ARG:N	1.95	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:181:PHE:CE2	3:L:181:SER:CB	2.62	0.81
3:N:197:TYR:O	3:N:213:SER:CB	2.26	0.81
3:L:2:ILE:HG21	3:L:4:MET:HE1	1.61	0.81
3:M:155:VAL:HG22	3:M:184:LEU:CD2	2.09	0.81
2:J:160:TYR:CD2	2:J:162:PRO:CD	2.64	0.81
2:J:169:TRP:CZ3	2:J:211:CYS:HB3	2.16	0.81
2:I:160:TYR:CD2	2:I:162:PRO:CD	2.64	0.81
2:J:169:TRP:CZ2	2:J:195:SER:O	2.32	0.81
3:M:171:GLN:HA	3:M:177:THR:O	1.79	0.81
1:B:276:LEU:CD1	1:B:289:VAL:CB	2.59	0.81
1:B:276:LEU:CD2	1:B:289:VAL:HB	2.10	0.81
3:L:153:TRP:HZ2	3:L:182:SER:HB2	1.24	0.80
1:A:48:LEU:HD22	1:A:276:LEU:HD11	1.64	0.80
2:I:169:TRP:CZ3	2:I:211:CYS:HB3	2.15	0.80
2:J:140:ALA:HB3	2:J:229:LYS:CD	2.06	0.80
2:H:181:PHE:HZ	3:L:181:SER:HB3	1.44	0.80
2:I:181:PHE:HZ	3:M:181:SER:HB3	1.44	0.80
5:O:2:NAG:H3	5:O:2:NAG:H83	1.63	0.80
2:H:160:TYR:CD2	2:H:162:PRO:CD	2.64	0.80
3:N:139:CYS:HB2	3:N:153:TRP:CH2	2.17	0.80
1:A:390:LEU:HG	1:A:391:CYS:N	1.96	0.80
1:A:394:ASN:HB2	1:A:516:GLU:HB2	1.64	0.80
1:B:559:PHE:CE1	1:C:43:PHE:CD2	2.70	0.80
2:I:185:LEU:HD21	2:I:191:TYR:CE1	2.17	0.80
2:J:181:PHE:HZ	3:N:181:SER:HB3	1.44	0.80
1:A:454:ARG:NE	1:A:491:PRO:HA	1.96	0.80
1:C:22:THR:HG21	1:C:78:ARG:HG2	1.64	0.80
3:L:139:CYS:HB2	3:L:153:TRP:CH2	2.17	0.80
1:B:961:THR:CG2	1:C:762:GLN:HE21	1.95	0.80
2:H:185:LEU:HD21	2:H:191:TYR:CE1	2.17	0.80
1:A:78:ARG:HG2	1:A:78:ARG:HH11	1.47	0.80
1:B:473:TYR:O	1:B:489:TYR:CB	2.29	0.79
1:A:38:TYR:HE1	1:A:285:ILE:HG13	1.48	0.79
2:H:160:TYR:HB2	2:H:162:PRO:HD3	1.64	0.79
3:L:139:CYS:CB	3:L:153:TRP:CH2	2.66	0.79
2:I:141:PRO:HG3	2:I:228:PRO:HA	1.56	0.79
3:M:141:LEU:HD12	3:M:151:VAL:HG22	1.64	0.79
3:N:139:CYS:CB	3:N:153:TRP:CH2	2.66	0.79
1:A:391:CYS:HB2	1:A:524:VAL:O	1.81	0.79
1:A:80:ASP:O	1:A:82:PRO:CD	2.30	0.79
2:J:54:GLU:OE1	2:J:111:TYR:HE2	1.66	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:424:LYS:HD3	1:B:425:LEU:N	1.97	0.79
1:C:78:ARG:HG2	1:C:78:ARG:HH11	1.47	0.79
3:L:141:LEU:HD12	3:L:151:VAL:HG22	1.64	0.79
3:L:169:THR:HG21	3:L:179:SER:CB	2.05	0.79
3:M:139:CYS:HB2	3:M:153:TRP:CH2	2.17	0.79
1:A:403:ARG:NH2	1:A:505:TYR:CD1	2.51	0.79
1:A:825:LYS:O	1:A:828:LEU:HD23	1.82	0.79
2:I:54:GLU:OE1	2:I:111:TYR:HE2	1.66	0.79
2:I:160:TYR:HB2	2:I:162:PRO:HD3	1.64	0.79
3:M:145:TYR:CE2	3:M:147:ARG:HB3	2.18	0.79
1:A:22:THR:HG21	1:A:78:ARG:HG2	1.64	0.79
1:A:170:TYR:HE1	1:A:172:SER:HB3	1.48	0.79
1:B:78:ARG:HH11	1:B:78:ARG:HG2	1.47	0.79
3:M:153:TRP:CZ2	3:M:182:SER:O	2.36	0.79
2:J:160:TYR:HB2	2:J:162:PRO:HD3	1.64	0.79
2:H:169:TRP:CZ3	2:H:211:CYS:HB3	2.15	0.78
3:M:141:LEU:CD1	3:M:151:VAL:HG22	2.14	0.78
3:M:153:TRP:CE2	3:M:182:SER:HB3	2.17	0.78
3:N:153:TRP:CZ2	3:N:182:SER:O	2.36	0.78
1:C:48:LEU:HD22	1:C:276:LEU:HD11	1.64	0.78
3:M:139:CYS:CB	3:M:153:TRP:CH2	2.66	0.78
2:J:141:PRO:HG3	2:J:228:PRO:HB3	1.65	0.78
3:N:141:LEU:HD12	3:N:151:VAL:HG22	1.64	0.78
1:B:22:THR:HG21	1:B:78:ARG:HG2	1.64	0.78
2:J:185:LEU:HD21	2:J:191:TYR:CE1	2.17	0.78
3:N:141:LEU:CD1	3:N:151:VAL:HG22	2.14	0.78
1:C:170:TYR:HE1	1:C:172:SER:HB3	1.48	0.78
1:B:276:LEU:C	1:B:277:LEU:HD13	2.09	0.78
3:L:118:PRO:HD2	3:L:206:LEU:HG	1.37	0.78
1:A:422:ASN:HD21	1:A:454:ARG:N	1.81	0.78
3:L:153:TRP:CE2	3:L:182:SER:HB3	2.17	0.78
3:N:150:LYS:NZ	3:N:202:THR:HB	1.99	0.78
3:N:153:TRP:CZ2	3:N:182:SER:C	2.62	0.78
1:A:392:PHE:CD1	1:A:518:LEU:HD23	2.19	0.78
1:C:421:TYR:CE1	1:C:457:ARG:O	2.37	0.78
3:L:141:LEU:CD1	3:L:151:VAL:HG22	2.14	0.78
3:L:153:TRP:CZ2	3:L:182:SER:O	2.36	0.78
3:M:153:TRP:CZ2	3:M:182:SER:C	2.62	0.78
1:B:563:GLN:OE1	1:C:43:PHE:HB2	1.84	0.78
2:I:52:ASP:CB	3:M:99:PHE:CE1	2.67	0.78
1:C:289:VAL:HG23	1:C:306:PHE:CZ	2.17	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:52:ASP:CB	3:L:99:PHE:CE1	2.67	0.77
2:H:54:GLU:OE1	2:H:111:TYR:HE2	1.66	0.77
3:N:9:LEU:O	3:N:10:SER:OG	2.01	0.77
2:H:140:ALA:O	2:H:141:PRO:O	2.02	0.77
3:L:145:TYR:CE2	3:L:147:ARG:HB3	2.18	0.77
2:J:185:LEU:CD2	2:J:191:TYR:CZ	2.67	0.77
3:N:122:ILE:CG2	3:N:213:SER:CA	2.45	0.77
1:C:80:ASP:O	1:C:82:PRO:CD	2.30	0.77
3:L:153:TRP:CZ2	3:L:182:SER:C	2.62	0.77
3:N:216:ARG:HG2	3:N:216:ARG:HH11	1.50	0.77
1:A:220:PHE:CD2	1:A:286:THR:O	2.38	0.77
1:C:299:THR:OG1	1:C:597:VAL:HG21	1.84	0.77
2:H:178:VAL:CG1	2:H:197:VAL:HG22	2.14	0.77
2:I:178:VAL:CG1	2:I:197:VAL:HG22	2.14	0.77
1:C:456:PHE:HB3	1:C:457:ARG:NH1	1.98	0.77
2:J:178:VAL:CG1	2:J:197:VAL:HG22	2.14	0.77
1:B:454:ARG:HG3	1:B:455:LEU:N	2.00	0.77
2:H:185:LEU:CD2	2:H:191:TYR:CZ	2.67	0.77
3:L:122:ILE:CG2	3:L:213:SER:CA	2.45	0.77
1:B:170:TYR:HE1	1:B:172:SER:HB3	1.48	0.77
2:I:155:CYS:HB2	2:I:169:TRP:CH2	2.20	0.77
3:M:150:LYS:NZ	3:M:202:THR:HB	1.99	0.77
2:J:185:LEU:HD23	2:J:191:TYR:CE1	2.19	0.77
3:N:145:TYR:CE2	3:N:147:ARG:HB3	2.18	0.77
2:H:155:CYS:HB2	2:H:169:TRP:CH2	2.20	0.77
2:H:141:PRO:HG3	2:H:228:PRO:HB3	1.65	0.76
3:L:150:LYS:NZ	3:L:202:THR:HB	1.99	0.76
3:L:155:VAL:HG22	3:L:184:LEU:HD22	1.67	0.76
3:M:9:LEU:O	3:M:10:SER:OG	2.01	0.76
3:M:216:ARG:HG2	3:M:216:ARG:HH11	1.50	0.76
3:L:216:ARG:HG2	3:L:216:ARG:HH11	1.50	0.76
2:J:155:CYS:HB2	2:J:169:TRP:CH2	2.20	0.76
1:C:613:GLN:HE21	1:C:613:GLN:HA	1.51	0.76
2:J:59:MET:CB	3:N:99:PHE:CE2	2.68	0.76
3:L:9:LEU:O	3:L:10:SER:OG	2.01	0.76
2:I:185:LEU:HD23	2:I:191:TYR:CE1	2.19	0.76
1:A:299:THR:OG1	1:A:597:VAL:HG21	1.86	0.76
1:B:424:LYS:HD3	1:B:424:LYS:C	2.09	0.76
1:C:291:CYS:O	1:C:292:ALA:CB	2.33	0.76
3:M:2:ILE:HD11	3:M:98:GLN:CG	2.16	0.76
3:L:2:ILE:HD11	3:L:98:GLN:CG	2.16	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:140:ALA:O	2:I:141:PRO:O	2.02	0.76
3:M:122:ILE:CD1	3:M:199:CYS:HB2	2.16	0.76
2:J:140:ALA:O	2:J:141:PRO:O	2.02	0.76
2:I:59:MET:CB	3:M:99:PHE:CE2	2.68	0.76
3:N:122:ILE:CD1	3:N:199:CYS:HB2	2.16	0.76
1:B:424:LYS:HB2	1:B:461:LEU:CD2	2.10	0.76
3:N:118:PRO:CD	3:N:206:LEU:CD1	2.64	0.76
3:N:155:VAL:HG22	3:N:184:LEU:HD22	1.67	0.76
2:H:59:MET:CB	3:L:99:PHE:CE2	2.68	0.76
2:I:141:PRO:HG3	2:I:228:PRO:HB3	1.65	0.76
2:H:166:THR:C	2:H:167:VAL:HG23	2.11	0.75
3:L:122:ILE:CD1	3:L:199:CYS:HB2	2.16	0.75
3:L:197:TYR:O	3:L:213:SER:CB	2.26	0.75
2:I:166:THR:C	2:I:167:VAL:HG23	2.11	0.75
1:C:78:ARG:HG2	1:C:78:ARG:NH1	2.02	0.75
2:J:166:THR:C	2:J:167:VAL:HG23	2.11	0.75
2:I:169:TRP:HD1	2:I:197:VAL:HG21	1.43	0.75
3:N:2:ILE:HD11	3:N:98:GLN:CG	2.16	0.75
3:M:118:PRO:CD	3:M:206:LEU:CD1	2.64	0.75
2:J:52:ASP:HB2	3:N:99:PHE:HZ	0.95	0.75
2:J:169:TRP:HD1	2:J:197:VAL:HG21	1.43	0.75
1:A:393:THR:CG2	1:A:518:LEU:CA	2.35	0.75
1:B:80:ASP:O	1:B:82:PRO:CD	2.30	0.75
2:I:185:LEU:CD2	2:I:191:TYR:CZ	2.67	0.75
3:M:118:PRO:HG2	3:M:144:PHE:CZ	2.16	0.75
2:H:185:LEU:HD23	2:H:191:TYR:CE1	2.19	0.75
3:L:118:PRO:HG2	3:L:144:PHE:CZ	2.16	0.75
3:N:169:THR:HG21	3:N:179:SER:CB	2.04	0.75
1:A:22:THR:HG21	1:A:78:ARG:HG3	1.45	0.75
2:I:141:PRO:CG	2:I:228:PRO:CB	2.64	0.75
2:J:141:PRO:CG	2:J:228:PRO:CB	2.64	0.75
2:H:178:VAL:HG13	2:H:197:VAL:HG13	1.68	0.75
1:B:24:LEU:HD13	1:B:24:LEU:N	2.02	0.74
1:A:220:PHE:CZ	1:A:287:ASP:OD1	2.40	0.74
1:C:456:PHE:HB3	1:C:457:ARG:HD2	1.69	0.74
2:H:169:TRP:CE3	2:H:211:CYS:CB	2.69	0.74
1:A:517:LEU:O	1:A:517:LEU:HD23	1.86	0.74
1:A:517:LEU:O	1:A:518:LEU:HG	1.87	0.74
1:A:811:LYS:CD	1:A:820:ASP:OD2	2.33	0.74
1:C:24:LEU:HD13	1:C:24:LEU:N	2.02	0.74
1:B:220:PHE:HE2	1:B:287:ASP:OD1	1.71	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:289:VAL:HG23	1:C:306:PHE:CE2	2.23	0.74
2:I:169:TRP:CE3	2:I:211:CYS:CB	2.69	0.74
1:A:811:LYS:HG2	1:A:812:PRO:HD3	1.69	0.74
3:M:155:VAL:HG22	3:M:184:LEU:HD22	1.67	0.74
2:J:169:TRP:CE3	2:J:211:CYS:CB	2.69	0.74
1:B:220:PHE:CZ	1:B:288:ALA:N	2.51	0.74
3:L:118:PRO:CD	3:L:206:LEU:CD1	2.64	0.74
2:I:54:GLU:HA	2:I:54:GLU:OE2	1.88	0.74
2:I:165:VAL:HG13	2:I:166:THR:N	2.03	0.74
2:J:54:GLU:OE2	2:J:54:GLU:HA	1.88	0.74
2:J:181:PHE:CE2	3:N:181:SER:HB3	2.21	0.74
1:A:454:ARG:CZ	1:A:491:PRO:HA	2.18	0.74
1:A:503:VAL:HG12	1:A:504:GLY:N	2.02	0.74
2:H:54:GLU:HA	2:H:54:GLU:OE2	1.88	0.74
2:J:52:ASP:CB	3:N:99:PHE:CE1	2.67	0.74
2:I:181:PHE:CE2	3:M:181:SER:HB3	2.21	0.73
1:A:24:LEU:HD13	1:A:24:LEU:N	2.02	0.73
2:H:141:PRO:CG	2:H:228:PRO:HB3	2.18	0.73
3:M:156:ASP:CB	3:M:194:HIS:CE1	2.71	0.73
2:J:174:LEU:HD11	2:J:209:TYR:CD2	2.23	0.73
2:I:174:LEU:HD11	2:I:209:TYR:CD2	2.23	0.73
3:N:141:LEU:HD21	3:N:201:VAL:HG11	1.57	0.73
2:I:204:LEU:HD11	2:I:228:PRO:CG	2.18	0.73
1:B:52:GLN:HG3	1:B:52:GLN:O	1.88	0.73
1:B:277:LEU:HD13	1:B:277:LEU:N	2.02	0.73
1:B:179:LEU:HD23	1:B:179:LEU:C	2.14	0.73
1:C:457:ARG:NH2	1:C:489:TYR:CG	2.56	0.73
3:M:36:THR:CG2	3:M:56:ILE:HD13	2.19	0.73
2:J:141:PRO:CG	2:J:228:PRO:HB3	2.18	0.73
1:A:454:ARG:NE	1:A:491:PRO:CA	2.52	0.73
2:H:52:ASP:HB2	3:L:99:PHE:HZ	0.95	0.73
3:N:2:ILE:HD12	3:N:2:ILE:N	2.03	0.73
1:A:179:LEU:HD23	1:A:179:LEU:C	2.14	0.73
2:I:141:PRO:CG	2:I:228:PRO:HB3	2.18	0.73
3:M:156:ASP:HB2	3:M:194:HIS:CE1	2.24	0.73
2:J:204:LEU:HD11	2:J:228:PRO:CG	2.18	0.73
3:N:36:THR:CG2	3:N:56:ILE:HD13	2.19	0.73
3:N:153:TRP:CE2	3:N:182:SER:HB3	2.17	0.73
1:A:454:ARG:CD	1:A:491:PRO:N	2.52	0.72
2:H:141:PRO:CG	2:H:228:PRO:CB	2.64	0.72
2:H:181:PHE:CE2	3:L:181:SER:HB3	2.21	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:36:THR:CG2	3:L:56:ILE:HD13	2.19	0.72
2:I:184:VAL:HG22	2:I:185:LEU:N	2.03	0.72
1:B:418:ILE:HD13	1:B:422:ASN:ND2	2.02	0.72
1:C:613:GLN:O	1:C:615:VAL:HG23	1.87	0.72
2:H:204:LEU:HD11	2:H:228:PRO:CG	2.18	0.72
3:L:156:ASP:CB	3:L:194:HIS:CE1	2.71	0.72
1:B:48:LEU:CD2	1:B:306:PHE:CD1	2.66	0.72
1:B:276:LEU:CD2	1:B:301:CYS:SG	2.78	0.72
1:B:418:ILE:CD1	1:B:422:ASN:ND2	2.52	0.72
2:J:141:PRO:HG2	2:J:228:PRO:CA	2.20	0.72
2:H:174:LEU:HD11	2:H:209:TYR:CD2	2.23	0.72
3:L:2:ILE:H	3:L:2:ILE:CD1	2.02	0.72
3:N:2:ILE:H	3:N:2:ILE:CD1	2.02	0.72
3:N:122:ILE:HD13	3:N:199:CYS:CB	2.19	0.72
1:C:179:LEU:HD23	1:C:179:LEU:C	2.14	0.72
2:H:184:VAL:HG22	2:H:185:LEU:N	2.03	0.72
3:M:36:THR:HG21	3:M:56:ILE:HD13	1.72	0.72
3:N:55:LYS:O	3:N:56:ILE:HG22	1.90	0.72
3:N:122:ILE:CG2	3:N:213:SER:C	2.63	0.72
1:B:418:ILE:HA	1:B:422:ASN:ND2	2.05	0.72
2:H:48:MET:HA	2:H:61:ALA:HB2	1.71	0.72
2:I:178:VAL:HA	2:I:197:VAL:HA	1.72	0.72
1:A:498:GLN:HB3	1:A:499:PRO:HD2	1.72	0.72
3:M:2:ILE:O	3:M:3:VAL:CG1	2.37	0.72
3:M:155:VAL:HG21	3:M:184:LEU:CD2	2.09	0.72
2:J:184:VAL:HG22	2:J:185:LEU:N	2.03	0.72
3:N:156:ASP:CB	3:N:194:HIS:CE1	2.71	0.72
3:L:36:THR:HG21	3:L:56:ILE:HD13	1.72	0.72
3:L:122:ILE:CG2	3:L:213:SER:C	2.63	0.72
3:L:122:ILE:HD13	3:L:199:CYS:CB	2.19	0.72
1:B:78:ARG:HG2	1:B:78:ARG:NH1	2.02	0.72
2:H:178:VAL:HA	2:H:197:VAL:HA	1.72	0.72
3:M:2:ILE:H	3:M:2:ILE:CD1	2.02	0.72
3:M:2:ILE:HD12	3:M:2:ILE:N	2.03	0.72
2:J:48:MET:HA	2:J:61:ALA:HB2	1.71	0.72
2:H:165:VAL:HG13	2:H:166:THR:N	2.03	0.71
3:L:156:ASP:HB2	3:L:194:HIS:CE1	2.24	0.71
2:I:141:PRO:HG2	2:I:228:PRO:CA	2.20	0.71
3:M:96:ALA:HA	3:M:101:TYR:HD2	1.55	0.71
3:N:144:PHE:CE2	3:N:203:HIS:ND1	2.58	0.71
3:M:122:ILE:HD13	3:M:199:CYS:CB	2.19	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:169:THR:HG22	3:M:179:SER:CA	2.20	0.71
2:J:165:VAL:HG13	2:J:166:THR:N	2.03	0.71
3:M:122:ILE:CG2	3:M:213:SER:C	2.63	0.71
3:N:96:ALA:HA	3:N:101:TYR:HD2	1.55	0.71
3:L:55:LYS:O	3:L:56:ILE:HG22	1.90	0.71
3:L:153:TRP:HZ2	3:L:182:SER:C	1.98	0.71
3:M:118:PRO:CD	3:M:206:LEU:HD11	2.20	0.71
1:A:291:CYS:O	1:A:292:ALA:CB	2.37	0.71
1:A:318:PHE:HE1	1:A:620:VAL:O	1.74	0.71
2:H:181:PHE:CE2	3:L:167:SER:O	2.44	0.71
3:M:153:TRP:HZ2	3:M:182:SER:C	1.98	0.71
2:J:181:PHE:CE2	3:N:167:SER:O	2.44	0.71
3:N:155:VAL:HG21	3:N:184:LEU:CD2	2.09	0.71
1:C:454:ARG:HD3	1:C:458:LYS:CE	2.20	0.71
2:I:48:MET:HA	2:I:61:ALA:HB2	1.71	0.71
3:M:55:LYS:O	3:M:56:ILE:HG22	1.90	0.71
3:M:120:VAL:HG23	3:M:210:VAL:HG11	1.73	0.71
2:H:141:PRO:HG2	2:H:228:PRO:CA	2.20	0.71
3:N:7:SER:CB	3:N:22:SER:OG	2.39	0.71
3:N:118:PRO:HG2	3:N:144:PHE:CZ	2.16	0.71
1:A:291:CYS:O	1:A:292:ALA:HB2	1.89	0.71
2:H:140:ALA:HB3	2:H:229:LYS:CD	2.06	0.71
2:I:181:PHE:CE2	3:M:167:SER:O	2.44	0.71
2:J:204:LEU:HD21	2:J:228:PRO:CG	2.20	0.71
3:N:156:ASP:HB2	3:N:194:HIS:CE1	2.24	0.71
1:A:449:TYR:CD2	1:A:497:PHE:CD2	2.76	0.71
1:B:426:PRO:CD	1:B:464:PHE:CE2	2.74	0.71
3:L:144:PHE:CE2	3:L:203:HIS:ND1	2.58	0.71
2:I:169:TRP:CE3	2:I:169:TRP:HA	2.25	0.71
3:M:155:VAL:CG2	3:M:184:LEU:HD22	2.20	0.71
2:J:178:VAL:HA	2:J:197:VAL:HA	1.72	0.71
1:A:1142:GLN:NE2	1:A:1142:GLN:HA	2.06	0.71
3:L:2:ILE:HD12	3:L:2:ILE:N	2.03	0.71
1:C:291:CYS:O	1:C:292:ALA:HB3	1.91	0.70
2:J:169:TRP:CE3	2:J:169:TRP:HA	2.25	0.70
3:N:36:THR:HG21	3:N:56:ILE:HD13	1.72	0.70
1:B:454:ARG:O	1:B:455:LEU:HB2	1.91	0.70
3:L:118:PRO:CG	3:L:206:LEU:CD1	2.64	0.70
3:N:169:THR:HG22	3:N:179:SER:CA	2.20	0.70
1:A:449:TYR:HB2	1:A:497:PHE:HB2	1.73	0.70
1:A:600:PRO:HB3	1:A:674:TYR:HB2	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:169:TRP:CE3	2:H:169:TRP:HA	2.25	0.70
2:H:204:LEU:HD21	2:H:228:PRO:CG	2.21	0.70
3:L:99:PHE:O	3:L:101:TYR:N	2.25	0.70
2:I:204:LEU:HD21	2:I:228:PRO:CG	2.21	0.70
3:M:144:PHE:CE2	3:M:203:HIS:ND1	2.58	0.70
3:N:2:ILE:O	3:N:3:VAL:CG1	2.37	0.70
3:N:43:GLN:HE21	3:N:49:PRO:HG3	1.57	0.70
3:L:118:PRO:CD	3:L:206:LEU:HD11	2.20	0.70
3:L:169:THR:HG22	3:L:179:SER:CA	2.20	0.70
3:M:115:VAL:HG12	3:M:205:GLY:HA2	1.73	0.70
1:A:78:ARG:HG2	1:A:78:ARG:NH1	2.02	0.70
1:A:277:LEU:HD13	1:A:277:LEU:N	2.07	0.70
1:B:276:LEU:CD2	1:B:289:VAL:CG1	2.66	0.70
3:L:43:GLN:HE21	3:L:49:PRO:HG3	1.57	0.70
3:L:155:VAL:CG2	3:L:184:LEU:HD22	2.20	0.70
3:N:115:VAL:HG12	3:N:205:GLY:HA2	1.73	0.70
1:B:1082:CYS:HG	1:B:1126:CYS:CB	1.98	0.70
3:N:99:PHE:O	3:N:101:TYR:N	2.25	0.70
1:B:38:TYR:HE1	1:B:222:ALA:CB	1.95	0.70
2:I:166:THR:O	2:I:167:VAL:HG23	1.92	0.70
2:J:166:THR:O	2:J:167:VAL:HG23	1.92	0.70
3:N:169:THR:CG2	3:N:179:SER:H	2.04	0.70
3:N:172:ASP:O	3:N:176:SER:HA	1.92	0.70
3:N:195:LYS:HD3	3:N:216:ARG:HB3	1.72	0.70
1:A:46:SER:OG	1:A:281:GLU:N	2.25	0.70
1:C:46:SER:OG	1:C:281:GLU:N	2.25	0.70
3:N:120:VAL:HG23	3:N:210:VAL:HG11	1.73	0.70
1:B:1142:GLN:OE1	1:B:1142:GLN:HA	1.92	0.70
3:L:172:ASP:O	3:L:176:SER:HA	1.92	0.70
3:M:118:PRO:CG	3:M:206:LEU:CD1	2.64	0.70
3:M:169:THR:CG2	3:M:179:SER:H	2.04	0.70
1:A:1116:THR:HA	1:A:1138:TYR:O	1.92	0.70
1:B:961:THR:HG21	1:C:762:GLN:NE2	2.06	0.70
1:C:826:VAL:O	1:C:828:LEU:N	2.25	0.70
3:L:115:VAL:HG12	3:L:205:GLY:HA2	1.73	0.70
3:L:169:THR:CG2	3:L:179:SER:H	2.04	0.70
3:M:105:GLN:HG2	3:M:105:GLN:O	1.92	0.70
3:N:118:PRO:CD	3:N:206:LEU:HD11	2.20	0.70
1:C:286:THR:OG1	1:C:287:ASP:N	2.22	0.69
2:H:166:THR:O	2:H:167:VAL:HG23	1.92	0.69
3:L:7:SER:CB	3:L:22:SER:OG	2.39	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:7:SER:CB	3:M:22:SER:OG	2.39	0.69
2:J:178:VAL:HG13	2:J:197:VAL:HG13	1.68	0.69
3:N:13:VAL:O	3:N:112:LYS:N	2.25	0.69
1:A:285:ILE:HG22	1:A:286:THR:N	2.06	0.69
3:L:105:GLN:O	3:L:105:GLN:HG2	1.92	0.69
3:L:195:LYS:HD3	3:L:216:ARG:HB3	1.72	0.69
3:M:7:SER:HG	3:M:8:PRO:HD3	1.53	0.69
3:M:195:LYS:HD3	3:M:216:ARG:HB3	1.72	0.69
1:A:518:LEU:HD12	1:A:518:LEU:O	1.92	0.69
2:H:165:VAL:HG22	2:H:166:THR:H	1.58	0.69
2:J:181:PHE:HB3	2:J:182:PRO:HD2	1.74	0.69
1:A:454:ARG:NE	1:A:491:PRO:N	2.40	0.69
2:H:169:TRP:HD1	2:H:197:VAL:HG21	1.43	0.69
3:L:13:VAL:O	3:L:112:LYS:N	2.25	0.69
3:M:43:GLN:HE21	3:M:49:PRO:HG3	1.57	0.69
3:M:172:ASP:O	3:M:176:SER:HA	1.92	0.69
1:C:276:LEU:HB3	1:C:289:VAL:HB	1.75	0.69
3:L:141:LEU:CD1	3:L:201:VAL:CG1	2.71	0.69
2:I:181:PHE:HD2	3:M:167:SER:C	2.01	0.69
3:N:118:PRO:CG	3:N:206:LEU:CD1	2.64	0.69
1:B:452:LEU:HD22	1:B:493:GLN:O	1.92	0.69
1:C:49:HIS:O	1:C:277:LEU:N	2.26	0.69
3:L:96:ALA:HA	3:L:101:TYR:HD2	1.55	0.69
2:I:167:VAL:O	2:I:169:TRP:N	2.23	0.69
3:M:99:PHE:O	3:M:101:TYR:N	2.25	0.69
1:B:458:LYS:O	1:B:459:SER:CB	2.39	0.69
1:C:277:LEU:N	1:C:277:LEU:HD13	2.07	0.69
1:C:458:LYS:CD	1:C:461:LEU:HD11	2.23	0.69
2:I:59:MET:CG	3:M:99:PHE:HE2	2.06	0.69
2:I:178:VAL:HG13	2:I:197:VAL:HG13	1.68	0.69
3:M:145:TYR:CD1	3:M:146:PRO:HD2	2.28	0.69
2:J:181:PHE:CD2	3:N:167:SER:C	2.71	0.69
2:J:181:PHE:HD2	3:N:167:SER:C	2.01	0.69
3:N:145:TYR:CD1	3:N:146:PRO:HD2	2.28	0.69
2:H:181:PHE:HD2	3:L:167:SER:C	2.01	0.69
1:A:49:HIS:O	1:A:277:LEU:N	2.26	0.69
2:H:167:VAL:O	2:H:169:TRP:N	2.23	0.69
3:L:2:ILE:O	3:L:3:VAL:CG1	2.37	0.69
3:L:145:TYR:CD1	3:L:146:PRO:HD2	2.28	0.69
2:J:142:SER:CB	3:N:214:PHE:CE2	2.74	0.69
1:B:180:GLU:O	1:B:182:LYS:HG2	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:470:THR:HG22	1:C:471:GLU:N	2.07	0.68
1:C:1118:ASP:OD2	1:C:1140:PRO:HG3	1.93	0.68
2:I:160:TYR:CB	2:I:162:PRO:HD3	2.23	0.68
2:H:160:TYR:CB	2:H:162:PRO:HD3	2.23	0.68
3:N:153:TRP:HZ2	3:N:182:SER:C	1.98	0.68
1:C:289:VAL:CG2	1:C:306:PHE:CE2	2.75	0.68
2:H:181:PHE:CD2	3:L:167:SER:C	2.71	0.68
3:L:96:ALA:HA	3:L:101:TYR:CD2	2.27	0.68
2:J:59:MET:CG	3:N:99:PHE:HE2	2.06	0.68
2:J:165:VAL:HG22	2:J:166:THR:H	1.58	0.68
1:A:42:VAL:C	1:C:563:GLN:HG2	2.18	0.68
1:A:180:GLU:O	1:A:182:LYS:HG2	1.93	0.68
2:I:181:PHE:HB3	2:I:182:PRO:HD2	1.74	0.68
3:M:13:VAL:O	3:M:112:LYS:N	2.25	0.68
3:N:96:ALA:HA	3:N:101:TYR:CD2	2.27	0.68
3:N:105:GLN:O	3:N:105:GLN:HG2	1.92	0.68
3:N:141:LEU:CD1	3:N:201:VAL:CG1	2.71	0.68
3:N:171:GLN:HG3	3:N:178:TYR:CE1	2.28	0.68
3:N:97:THR:HG22	3:N:98:GLN:OE1	1.94	0.68
2:I:181:PHE:CD2	3:M:167:SER:C	2.71	0.68
3:M:97:THR:HG22	3:M:98:GLN:OE1	1.94	0.68
3:M:141:LEU:CD1	3:M:201:VAL:CG1	2.71	0.68
3:M:171:GLN:HG3	3:M:178:TYR:CE1	2.28	0.68
3:N:155:VAL:CG2	3:N:184:LEU:HD22	2.20	0.68
2:J:178:VAL:CG1	2:J:197:VAL:HG11	2.16	0.68
2:H:160:TYR:CG	2:H:162:PRO:HD2	2.28	0.68
3:M:2:ILE:HD11	3:M:98:GLN:HG2	1.75	0.68
2:J:160:TYR:CB	2:J:162:PRO:HD3	2.23	0.68
3:L:171:GLN:HG3	3:L:178:TYR:CE1	2.28	0.68
3:M:96:ALA:HA	3:M:101:TYR:CD2	2.27	0.68
2:H:181:PHE:HB3	2:H:182:PRO:HD2	1.74	0.67
1:A:276:LEU:CB	1:A:289:VAL:HG12	2.20	0.67
1:B:425:LEU:HD13	1:B:430:THR:HG21	1.76	0.67
2:J:59:MET:HG2	3:N:99:PHE:HD2	0.87	0.67
1:C:170:TYR:CE1	1:C:172:SER:HB3	2.29	0.67
2:I:160:TYR:CG	2:I:162:PRO:HD2	2.28	0.67
3:N:2:ILE:HD11	3:N:98:GLN:HG2	1.75	0.67
1:C:180:GLU:O	1:C:182:LYS:HG2	1.93	0.67
1:A:276:LEU:HD23	1:A:289:VAL:CG1	2.23	0.67
3:L:97:THR:HG22	3:L:98:GLN:OE1	1.94	0.67
3:L:120:VAL:CG2	3:L:210:VAL:CB	2.72	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:120:VAL:CG2	3:M:210:VAL:CB	2.72	0.67
3:N:120:VAL:HG12	3:N:212:LYS:HB2	1.77	0.67
1:B:170:TYR:CE1	1:B:172:SER:HB3	2.29	0.67
2:H:177:GLY:O	2:H:198:THR:N	2.28	0.67
3:L:2:ILE:HG22	3:L:3:VAL:N	2.09	0.67
2:I:165:VAL:HG22	2:I:166:THR:H	1.58	0.67
3:N:171:GLN:HG2	3:N:177:THR:O	1.95	0.67
1:B:452:LEU:HD21	1:B:494:SER:HA	1.69	0.67
3:L:2:ILE:HD11	3:L:98:GLN:HG2	1.76	0.67
3:L:171:GLN:HG2	3:L:177:THR:O	1.95	0.67
2:I:177:GLY:O	2:I:198:THR:N	2.28	0.67
2:J:160:TYR:CG	2:J:162:PRO:HD2	2.29	0.67
1:A:170:TYR:CE1	1:A:172:SER:HB3	2.29	0.67
2:I:169:TRP:HA	2:I:169:TRP:HE3	1.60	0.67
3:M:2:ILE:HG22	3:M:3:VAL:N	2.09	0.67
3:M:155:VAL:HG12	3:M:156:ASP:OD2	1.95	0.67
3:M:171:GLN:HG2	3:M:177:THR:O	1.95	0.67
2:H:142:SER:CB	3:L:214:PHE:CE2	2.74	0.66
1:B:18:LEU:O	1:B:19:THR:HG23	1.95	0.66
3:M:13:VAL:O	3:M:112:LYS:CB	2.44	0.66
3:N:155:VAL:HG12	3:N:156:ASP:OD2	1.95	0.66
1:C:18:LEU:O	1:C:19:THR:HG23	1.95	0.66
2:H:141:PRO:HG2	2:H:228:PRO:HA	1.73	0.66
3:L:13:VAL:O	3:L:112:LYS:CB	2.43	0.66
2:J:177:GLY:O	2:J:198:THR:N	2.28	0.66
3:L:120:VAL:HG12	3:L:212:LYS:HB2	1.77	0.66
3:M:120:VAL:HG12	3:M:212:LYS:HB2	1.77	0.66
1:A:24:LEU:CB	1:A:25:PRO:HD2	2.25	0.66
1:A:38:TYR:CE1	1:A:285:ILE:HG13	2.31	0.66
1:A:422:ASN:HD21	1:A:454:ARG:H	1.42	0.66
3:L:118:PRO:HD2	3:L:206:LEU:HD11	1.77	0.66
3:L:141:LEU:CG	3:L:201:VAL:HG11	2.26	0.66
1:A:18:LEU:O	1:A:19:THR:HG23	1.95	0.66
2:H:168:SER:O	2:H:169:TRP:HB2	1.96	0.66
2:J:167:VAL:O	2:J:169:TRP:N	2.23	0.66
3:N:2:ILE:HG22	3:N:3:VAL:N	2.09	0.66
3:N:13:VAL:O	3:N:112:LYS:CB	2.43	0.66
1:A:179:LEU:HD23	1:A:180:GLU:N	2.12	0.65
1:C:18:LEU:O	1:C:18:LEU:HD12	1.96	0.65
2:H:142:SER:CA	3:L:214:PHE:CE2	2.79	0.65
3:L:155:VAL:HG12	3:L:156:ASP:OD2	1.95	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:156:ASP:CG	3:L:194:HIS:CG	2.74	0.65
2:J:169:TRP:HA	2:J:169:TRP:HE3	1.59	0.65
1:B:290:ASP:O	1:B:297:SER:HB3	1.96	0.65
2:H:169:TRP:HA	2:H:169:TRP:HE3	1.59	0.65
3:M:156:ASP:CG	3:M:194:HIS:CG	2.74	0.65
1:A:18:LEU:O	1:A:18:LEU:HD12	1.96	0.65
3:N:141:LEU:CG	3:N:201:VAL:HG11	2.26	0.65
1:C:24:LEU:CB	1:C:25:PRO:HD2	2.26	0.65
1:C:179:LEU:HD23	1:C:180:GLU:N	2.12	0.65
1:A:1144:GLU:OE1	1:A:1144:GLU:HA	1.96	0.65
1:B:179:LEU:HD23	1:B:180:GLU:N	2.12	0.65
3:M:141:LEU:HD21	3:M:201:VAL:HG13	1.78	0.65
2:I:142:SER:CB	3:M:214:PHE:CE2	2.74	0.65
3:M:141:LEU:HD12	3:M:151:VAL:CG2	2.27	0.65
2:J:67:ARG:NH1	2:J:90:ASP:OD2	2.30	0.65
1:A:497:PHE:O	1:A:498:GLN:HG2	1.96	0.65
1:B:24:LEU:CB	1:B:25:PRO:HD2	2.26	0.65
1:C:21:ARG:O	1:C:23:GLN:HG3	1.97	0.65
2:I:142:SER:CA	3:M:214:PHE:CE2	2.79	0.65
3:N:99:PHE:HB3	3:N:100:PRO:CD	2.27	0.65
1:A:21:ARG:O	1:A:23:GLN:HG3	1.97	0.65
1:A:220:PHE:HZ	1:A:287:ASP:OD1	1.79	0.65
1:C:48:LEU:CD2	1:C:276:LEU:HG	2.27	0.65
2:I:168:SER:O	2:I:169:TRP:HB2	1.96	0.65
3:M:4:MET:O	3:M:5:THR:HG22	1.97	0.65
1:A:48:LEU:CD2	1:A:276:LEU:HG	2.27	0.65
1:A:613:GLN:O	1:A:615:VAL:HG13	1.97	0.65
1:B:18:LEU:O	1:B:18:LEU:HD12	1.96	0.65
3:N:4:MET:O	3:N:5:THR:HG22	1.97	0.65
3:N:141:LEU:HD12	3:N:151:VAL:CG2	2.27	0.65
1:C:164:ASN:ND2	4:d:1:NAG:H82	2.12	0.64
3:L:4:MET:O	3:L:5:THR:HG22	1.97	0.64
3:L:141:LEU:HD21	3:L:201:VAL:HG13	1.78	0.64
3:N:156:ASP:CG	3:N:194:HIS:CG	2.74	0.64
1:B:164:ASN:ND2	4:T:1:NAG:H82	2.12	0.64
3:L:155:VAL:HG21	3:L:184:LEU:CD2	2.09	0.64
2:J:142:SER:CA	3:N:214:PHE:CE2	2.79	0.64
2:I:67:ARG:NH1	2:I:90:ASP:OD2	2.30	0.64
2:J:168:SER:O	2:J:169:TRP:HB2	1.96	0.64
3:N:141:LEU:HD21	3:N:201:VAL:HG13	1.78	0.64
1:A:391:CYS:CB	1:A:524:VAL:O	2.44	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:825:LYS:HZ2	1:A:944:ALA:HB3	1.58	0.64
1:B:21:ARG:O	1:B:23:GLN:HG3	1.97	0.64
2:H:54:GLU:OE1	2:H:111:TYR:CE2	2.50	0.64
3:L:120:VAL:HG23	3:L:210:VAL:HG11	1.73	0.64
3:L:141:LEU:HD12	3:L:151:VAL:CG2	2.27	0.64
2:J:54:GLU:OE1	2:J:111:TYR:CE2	2.50	0.64
1:A:164:ASN:ND2	4:E:1:NAG:H82	2.12	0.64
1:A:437:ASN:OD1	1:A:506:GLN:HG3	1.97	0.64
1:B:48:LEU:HD21	1:B:306:PHE:HD1	1.57	0.64
1:B:457:ARG:C	1:B:458:LYS:HG2	2.23	0.64
2:H:165:VAL:HG13	2:H:166:THR:H	1.63	0.64
3:N:120:VAL:CG2	3:N:210:VAL:CB	2.72	0.64
1:A:24:LEU:HB3	1:A:25:PRO:HD2	1.79	0.64
1:A:329:PHE:HB3	1:A:330:PRO:HD2	1.80	0.64
1:A:350:VAL:CG1	1:A:453:TYR:HB2	2.28	0.64
1:B:422:ASN:O	1:B:461:LEU:CD2	2.42	0.64
3:L:99:PHE:HB3	3:L:100:PRO:CD	2.27	0.64
2:J:160:TYR:CG	2:J:162:PRO:CD	2.81	0.64
1:A:391:CYS:CB	1:A:525:CYS:HA	2.25	0.64
1:B:276:LEU:HD21	1:B:289:VAL:CB	2.28	0.64
1:C:278:LYS:HE3	1:C:287:ASP:HB2	1.78	0.64
3:L:122:ILE:HG21	3:L:213:SER:C	2.23	0.64
2:I:165:VAL:HG13	2:I:166:THR:H	1.63	0.64
3:N:146:PRO:O	3:N:147:ARG:HB2	1.97	0.64
1:C:613:GLN:HE21	1:C:613:GLN:CA	2.11	0.64
2:H:67:ARG:NH1	2:H:90:ASP:OD2	2.30	0.64
2:H:178:VAL:CG1	2:H:197:VAL:HG11	2.16	0.64
1:A:393:THR:HG23	1:A:518:LEU:HA	0.71	0.63
1:B:455:LEU:O	1:B:457:ARG:HG2	1.99	0.63
1:C:24:LEU:HB3	1:C:25:PRO:HD2	1.80	0.63
2:H:160:TYR:CG	2:H:162:PRO:CD	2.81	0.63
3:L:158:ALA:O	3:L:159:LEU:O	2.17	0.63
3:L:210:VAL:C	3:L:211:THR:HG1	2.02	0.63
3:M:99:PHE:HB3	3:M:100:PRO:CD	2.27	0.63
3:M:146:PRO:O	3:M:147:ARG:HB2	1.97	0.63
1:A:48:LEU:HD21	1:A:276:LEU:CD1	2.24	0.63
1:C:220:PHE:HE2	1:C:287:ASP:OD1	1.80	0.63
2:I:204:LEU:HD21	2:I:228:PRO:HG3	1.80	0.63
3:M:122:ILE:HG21	3:M:213:SER:C	2.23	0.63
2:I:160:TYR:CG	2:I:162:PRO:CD	2.81	0.63
3:M:158:ALA:O	3:M:159:LEU:O	2.17	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:269:TYR:O	1:B:270:LEU:O	2.17	0.63
1:C:690:GLN:O	1:C:691:SER:HB3	1.98	0.63
1:B:24:LEU:HB3	1:B:25:PRO:HD2	1.79	0.63
1:B:182:LYS:HG3	1:B:186:PHE:CZ	2.33	0.63
1:B:298:GLU:OE2	1:B:316:SER:HB3	1.98	0.63
1:A:38:TYR:CE2	1:C:562:PHE:HZ	2.17	0.63
1:B:426:PRO:CD	1:B:464:PHE:HE2	2.11	0.63
1:C:182:LYS:HG3	1:C:186:PHE:CZ	2.33	0.63
1:C:457:ARG:C	1:C:459:SER:H	2.06	0.63
3:L:2:ILE:CG2	3:L:4:MET:HE1	2.23	0.63
1:B:453:TYR:O	1:B:454:ARG:HB2	1.97	0.63
1:C:307:THR:HA	1:C:602:THR:HG21	1.80	0.63
1:B:473:TYR:O	1:B:489:TYR:HB3	1.99	0.63
2:I:184:VAL:O	2:I:191:TYR:HD1	1.78	0.63
2:J:52:ASP:OD1	2:J:54:GLU:N	2.29	0.63
1:A:392:PHE:CB	1:A:518:LEU:HB3	2.25	0.62
3:L:145:TYR:HE2	3:L:147:ARG:HB3	1.62	0.62
3:N:214:PHE:CE1	3:N:215:ASN:O	2.52	0.62
2:H:52:ASP:OD1	2:H:54:GLU:N	2.29	0.62
2:H:59:MET:HG2	3:L:99:PHE:HD2	0.87	0.62
3:M:25:SER:OG	3:M:26:SER:N	2.30	0.62
1:A:416:GLY:H	1:A:419:ALA:HB3	1.65	0.62
1:B:1125:ASN:O	1:B:1127:ASP:N	2.32	0.62
3:M:141:LEU:CG	3:M:201:VAL:HG11	2.26	0.62
3:N:122:ILE:HG21	3:N:213:SER:C	2.23	0.62
1:B:473:TYR:O	1:B:489:TYR:HB2	1.98	0.62
3:L:4:MET:HE1	3:L:95:GLN:HG2	1.81	0.62
3:L:141:LEU:CD1	3:L:151:VAL:HG13	2.26	0.62
3:L:214:PHE:CE1	3:L:215:ASN:O	2.53	0.62
3:N:25:SER:OG	3:N:26:SER:N	2.30	0.62
3:N:158:ALA:O	3:N:159:LEU:O	2.17	0.62
2:I:54:GLU:CD	2:I:111:TYR:HE2	2.08	0.62
2:J:54:GLU:CD	2:J:111:TYR:HE2	2.08	0.62
1:A:182:LYS:HG3	1:A:186:PHE:CZ	2.33	0.62
3:L:141:LEU:HD22	3:L:201:VAL:CG1	2.25	0.62
3:L:146:PRO:O	3:L:147:ARG:HB2	1.97	0.62
1:C:558:LYS:HA	1:C:558:LYS:HE3	1.81	0.62
3:L:25:SER:OG	3:L:26:SER:N	2.30	0.62
1:A:351:TYR:HB3	1:A:453:TYR:HA	1.81	0.62
2:H:140:ALA:HB2	2:H:229:LYS:CD	2.16	0.62
3:M:141:LEU:CD1	3:M:151:VAL:HG13	2.26	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:204:LEU:HD21	2:J:228:PRO:HG3	1.80	0.62
3:N:198:ALA:HA	3:N:213:SER:HB3	1.82	0.62
2:I:54:GLU:OE1	2:I:111:TYR:CE2	2.50	0.62
2:J:184:VAL:O	2:J:191:TYR:HD1	1.78	0.62
1:A:290:ASP:O	1:A:297:SER:HB3	2.00	0.62
1:A:814:LYS:N	1:A:814:LYS:HZ3	1.97	0.62
1:B:425:LEU:CD1	1:B:430:THR:HG21	2.30	0.62
2:I:169:TRP:CE3	2:I:211:CYS:HB3	2.34	0.62
3:M:214:PHE:CE1	3:M:215:ASN:O	2.53	0.62
2:H:54:GLU:CD	2:H:111:TYR:HE2	2.08	0.61
2:J:165:VAL:HG13	2:J:166:THR:H	1.63	0.61
3:N:118:PRO:HD2	3:N:206:LEU:HD11	1.77	0.61
3:N:145:TYR:HE2	3:N:147:ARG:HB3	1.62	0.61
1:B:276:LEU:CD2	1:B:289:VAL:CB	2.77	0.61
3:L:2:ILE:HD11	3:L:98:GLN:HG3	1.82	0.61
2:I:59:MET:HG2	3:M:99:PHE:HD2	0.87	0.61
3:M:118:PRO:HG3	3:M:144:PHE:CE1	2.34	0.61
1:A:24:LEU:CB	1:A:25:PRO:CD	2.79	0.61
1:A:826:VAL:O	1:A:828:LEU:N	2.30	0.61
3:L:150:LYS:HB3	3:L:202:THR:O	2.00	0.61
2:I:174:LEU:HD11	2:I:209:TYR:CE2	2.35	0.61
3:M:118:PRO:HD2	3:M:206:LEU:HD11	1.77	0.61
3:M:9:LEU:HD11	3:M:105:GLN:HE22	1.62	0.61
1:A:811:LYS:HB3	1:A:812:PRO:CD	2.31	0.61
1:C:421:TYR:CD1	1:C:458:LYS:HB3	2.35	0.61
3:L:158:ALA:O	3:L:159:LEU:C	2.44	0.61
3:M:2:ILE:CG2	3:M:4:MET:HE1	2.23	0.61
3:M:198:ALA:HA	3:M:213:SER:HB3	1.82	0.61
2:J:174:LEU:HD11	2:J:209:TYR:CE2	2.35	0.61
1:A:22:THR:CG2	1:A:78:ARG:NE	2.62	0.61
3:M:145:TYR:HE2	3:M:147:ARG:HB3	1.62	0.61
3:N:150:LYS:HB3	3:N:202:THR:O	2.00	0.61
3:M:2:ILE:HD11	3:M:98:GLN:HG3	1.82	0.61
3:N:4:MET:HE1	3:N:95:GLN:HG2	1.81	0.61
1:B:419:ALA:O	1:B:424:LYS:HG2	2.01	0.61
1:B:423:TYR:HE2	1:B:512:VAL:HG21	1.66	0.61
2:I:52:ASP:OD1	2:I:54:GLU:N	2.29	0.61
2:J:169:TRP:CE3	2:J:211:CYS:HB3	2.34	0.61
3:N:118:PRO:HG3	3:N:144:PHE:CE1	2.34	0.61
1:A:357:ARG:HH12	1:B:167:THR:HA	1.65	0.61
1:B:47:VAL:HG23	1:B:47:VAL:O	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:276:LEU:HD21	1:B:289:VAL:HG12	1.79	0.61
1:B:961:THR:CG2	1:C:762:GLN:NE2	2.62	0.61
3:N:2:ILE:HD11	3:N:98:GLN:HG3	1.82	0.61
3:N:151:VAL:HG21	3:N:180:LEU:CG	2.27	0.61
1:B:24:LEU:CB	1:B:25:PRO:CD	2.79	0.61
1:B:426:PRO:HD3	1:B:464:PHE:CE2	2.34	0.61
1:C:22:THR:CG2	1:C:78:ARG:NE	2.62	0.61
3:L:198:ALA:HA	3:L:213:SER:HB3	1.82	0.61
1:C:674:TYR:HD1	1:C:691:SER:O	1.84	0.60
2:H:174:LEU:HD11	2:H:209:TYR:CE2	2.35	0.60
3:L:141:LEU:HD11	3:L:201:VAL:CG1	2.31	0.60
2:I:55:ASP:C	2:I:57:GLU:H	2.09	0.60
3:N:141:LEU:HD11	3:N:201:VAL:CG1	2.31	0.60
2:H:55:ASP:C	2:H:57:GLU:H	2.09	0.60
3:M:4:MET:HE1	3:M:95:GLN:HG2	1.81	0.60
3:M:150:LYS:HB3	3:M:202:THR:O	2.00	0.60
2:H:184:VAL:O	2:H:191:TYR:HD1	1.78	0.60
2:H:204:LEU:HD21	2:H:228:PRO:HG3	1.80	0.60
3:M:141:LEU:HD11	3:M:201:VAL:CG1	2.31	0.60
3:N:193:LYS:O	3:N:193:LYS:HG3	2.01	0.60
1:A:334:ASN:C	1:A:336:CYS:H	2.10	0.60
1:B:289:VAL:HG23	1:B:306:PHE:CZ	2.36	0.60
1:B:473:TYR:C	1:B:489:TYR:CB	2.74	0.60
1:C:454:ARG:C	1:C:455:LEU:HG	2.26	0.60
3:L:168:VAL:CG1	3:L:179:SER:O	2.44	0.60
3:L:193:LYS:HG3	3:L:193:LYS:O	2.01	0.60
2:I:184:VAL:CG2	2:I:185:LEU:N	2.65	0.60
3:N:141:LEU:HD22	3:N:201:VAL:CG1	2.25	0.60
1:B:23:GLN:OE1	1:B:24:LEU:N	2.34	0.60
1:B:456:PHE:O	1:B:457:ARG:NE	2.35	0.60
2:I:11:VAL:HG11	2:I:161:PHE:HE2	1.67	0.60
1:C:23:GLN:OE1	1:C:24:LEU:N	2.34	0.60
1:B:563:GLN:NE2	1:C:43:PHE:HA	2.17	0.60
1:C:22:THR:HG21	1:C:78:ARG:CZ	2.32	0.60
1:C:24:LEU:CB	1:C:25:PRO:CD	2.79	0.60
1:C:616:ASN:C	1:C:618:THR:H	2.10	0.60
3:L:138:VAL:C	3:L:153:TRP:CH2	2.80	0.60
3:M:193:LYS:HG3	3:M:193:LYS:O	2.01	0.60
1:A:276:LEU:CD2	1:A:289:VAL:CG1	2.79	0.60
3:L:118:PRO:HG3	3:L:144:PHE:CE1	2.34	0.60
3:M:138:VAL:C	3:M:153:TRP:CH2	2.80	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:9:LEU:HD11	3:N:105:GLN:HE22	1.61	0.60
3:N:141:LEU:CD1	3:N:151:VAL:HG13	2.26	0.60
1:A:23:GLN:OE1	1:A:24:LEU:N	2.34	0.60
1:B:170:TYR:CE1	1:B:172:SER:CB	2.85	0.60
1:B:277:LEU:HG	1:B:285:ILE:HD13	1.83	0.60
1:C:457:ARG:NE	1:C:489:TYR:CD2	2.70	0.60
2:H:11:VAL:HG11	2:H:161:PHE:HE2	1.67	0.60
2:H:12:LYS:NZ	2:H:17:SER:O	2.35	0.60
2:J:55:ASP:C	2:J:57:GLU:H	2.09	0.60
3:N:158:ALA:O	3:N:159:LEU:C	2.44	0.60
1:A:170:TYR:CE1	1:A:172:SER:CB	2.85	0.59
1:C:170:TYR:CE1	1:C:172:SER:CB	2.85	0.59
3:L:4:MET:HB3	3:L:24:ARG:O	2.02	0.59
3:L:153:TRP:CH2	3:L:182:SER:O	2.56	0.59
2:J:184:VAL:CG2	2:J:185:LEU:N	2.65	0.59
3:N:138:VAL:C	3:N:153:TRP:CH2	2.80	0.59
2:H:59:MET:CG	3:L:99:PHE:HE2	2.06	0.59
2:I:165:VAL:HG22	2:I:166:THR:N	2.17	0.59
2:I:178:VAL:CG1	2:I:197:VAL:HG11	2.16	0.59
3:M:168:VAL:CG1	3:M:179:SER:O	2.44	0.59
2:J:12:LYS:NZ	2:J:17:SER:O	2.35	0.59
2:H:169:TRP:HE1	2:H:197:VAL:HG23	1.67	0.59
1:C:690:GLN:O	1:C:690:GLN:HG3	2.02	0.59
3:N:153:TRP:CH2	3:N:182:SER:O	2.56	0.59
1:C:290:ASP:O	1:C:297:SER:HB3	2.02	0.59
1:A:393:THR:CG2	1:A:518:LEU:C	2.75	0.59
1:B:22:THR:HG21	1:B:78:ARG:CZ	2.32	0.59
1:B:454:ARG:HD2	1:B:456:PHE:CD1	2.38	0.59
2:J:160:TYR:HD2	2:J:162:PRO:HG2	1.68	0.59
1:A:22:THR:HG21	1:A:78:ARG:CZ	2.32	0.59
1:A:43:PHE:HD2	1:C:559:PHE:CE1	2.17	0.59
1:A:826:VAL:C	1:A:828:LEU:H	2.11	0.59
1:B:131:CYS:HA	1:B:166:CYS:HA	1.85	0.59
1:B:422:ASN:OD1	1:B:422:ASN:N	2.35	0.59
1:B:456:PHE:C	1:B:457:ARG:HG2	2.26	0.59
1:C:454:ARG:CD	1:C:458:LYS:HZ2	2.00	0.59
2:H:184:VAL:CG2	2:H:185:LEU:N	2.65	0.59
3:L:154:LYS:O	3:L:156:ASP:N	2.36	0.59
2:I:45:LEU:HD23	3:M:103:PHE:CE2	2.38	0.59
2:I:161:PHE:N	2:I:162:PRO:HD3	2.18	0.59
3:N:154:LYS:O	3:N:156:ASP:N	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:168:VAL:CG1	3:N:179:SER:O	2.44	0.59
2:H:161:PHE:N	2:H:162:PRO:HD3	2.18	0.59
2:I:52:ASP:OD2	3:M:99:PHE:CE1	2.56	0.59
3:M:158:ALA:O	3:M:159:LEU:C	2.44	0.59
2:J:11:VAL:HG11	2:J:161:PHE:HE2	1.67	0.59
2:J:165:VAL:O	2:J:166:THR:OG1	2.16	0.59
1:B:57:PRO:HB3	1:B:273:ARG:NH2	2.16	0.59
1:B:575:ALA:HB1	1:B:584:ILE:HD11	1.84	0.59
2:I:169:TRP:HE1	2:I:197:VAL:HG23	1.67	0.59
2:I:181:PHE:CZ	3:M:181:SER:OG	2.54	0.59
2:J:45:LEU:HD23	3:N:103:PHE:CE2	2.38	0.59
1:B:473:TYR:C	1:B:489:TYR:HB3	2.27	0.58
1:A:131:CYS:HA	1:A:166:CYS:HA	1.85	0.58
1:A:403:ARG:HG2	1:A:505:TYR:O	2.02	0.58
1:B:563:GLN:CD	1:C:43:PHE:HB2	2.28	0.58
1:B:1146:ASP:OD1	1:B:1146:ASP:N	2.36	0.58
2:I:160:TYR:HD2	2:I:162:PRO:HG2	1.68	0.58
3:M:4:MET:HB3	3:M:25:SER:HA	1.85	0.58
3:M:153:TRP:CH2	3:M:182:SER:O	2.55	0.58
1:C:674:TYR:CE1	1:C:691:SER:N	2.71	0.58
2:H:45:LEU:HD23	3:L:103:PHE:CE2	2.38	0.58
2:H:165:VAL:HG22	2:H:166:THR:N	2.17	0.58
2:H:165:VAL:O	2:H:166:THR:OG1	2.16	0.58
2:H:169:TRP:CE3	2:H:211:CYS:HB3	2.34	0.58
3:L:102:THR:C	3:L:103:PHE:HD1	2.12	0.58
2:I:54:GLU:CD	2:I:111:TYR:CE2	2.82	0.58
2:J:165:VAL:HG22	2:J:166:THR:N	2.17	0.58
1:B:34:ARG:NH1	1:B:221:SER:OG	2.37	0.58
1:B:525:CYS:SG	1:B:526:GLY:N	2.76	0.58
2:H:54:GLU:CD	2:H:111:TYR:CE2	2.82	0.58
3:L:3:VAL:HG23	3:L:3:VAL:O	2.03	0.58
2:I:152:ALA:HA	2:I:198:THR:HA	1.85	0.58
2:J:161:PHE:N	2:J:162:PRO:HD3	2.18	0.58
1:A:640:SER:OG	1:A:641:ASN:N	2.36	0.58
2:H:152:ALA:HA	2:H:198:THR:HA	1.85	0.58
3:L:10:SER:HA	3:L:108:LYS:O	2.04	0.58
1:C:34:ARG:NH1	1:C:221:SER:OG	2.37	0.58
1:C:131:CYS:HA	1:C:166:CYS:HA	1.85	0.58
2:H:184:VAL:O	2:H:191:TYR:HA	2.03	0.58
3:L:9:LEU:HD11	3:L:105:GLN:HE22	1.61	0.58
2:I:184:VAL:O	2:I:191:TYR:HA	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:3:VAL:HG23	3:M:3:VAL:O	2.03	0.58
3:M:154:LYS:O	3:M:156:ASP:N	2.36	0.58
1:B:418:ILE:HG23	1:B:422:ASN:ND2	2.19	0.58
1:B:427:ASP:O	1:B:428:ASP:C	2.47	0.58
1:C:164:ASN:HD22	4:d:1:NAG:H82	1.67	0.58
1:C:497:PHE:O	1:C:498:GLN:HB3	2.04	0.58
2:I:178:VAL:HG12	2:I:197:VAL:HG22	1.77	0.58
2:J:52:ASP:OD2	3:N:99:PHE:CE1	2.56	0.58
1:C:274:THR:C	1:C:275:PHE:HD1	2.12	0.58
2:I:12:LYS:NZ	2:I:17:SER:O	2.35	0.58
3:M:4:MET:HB3	3:M:24:ARG:O	2.02	0.58
2:J:181:PHE:CZ	3:N:181:SER:OG	2.54	0.58
2:H:52:ASP:OD2	3:L:99:PHE:CE1	2.56	0.58
3:N:4:MET:HB3	3:N:25:SER:HA	1.85	0.58
1:C:827:THR:HG23	1:C:827:THR:O	2.02	0.58
2:H:169:TRP:O	2:H:210:ILE:O	2.21	0.58
2:I:166:THR:O	2:I:167:VAL:CB	2.52	0.58
2:J:54:GLU:CD	2:J:111:TYR:CE2	2.82	0.58
2:J:184:VAL:O	2:J:191:TYR:HA	2.04	0.58
3:N:120:VAL:HG23	3:N:210:VAL:HG21	1.86	0.58
1:C:312:ILE:HD12	1:C:598:ILE:HG12	1.84	0.57
2:H:160:TYR:HD2	2:H:162:PRO:HG2	1.68	0.57
3:N:5:THR:OG1	3:N:6:GLN:N	2.37	0.57
1:A:422:ASN:HD21	1:A:454:ARG:CA	2.16	0.57
1:B:78:ARG:CG	1:B:78:ARG:HH11	2.16	0.57
1:C:353:TRP:O	1:C:466:ARG:NH2	2.36	0.57
1:C:457:ARG:NE	1:C:489:TYR:CE2	2.70	0.57
2:J:169:TRP:HE1	2:J:197:VAL:HG23	1.67	0.57
1:A:520:ALA:HB1	1:A:521:PRO:CD	2.34	0.57
1:B:562:PHE:HZ	1:C:38:TYR:CE2	2.22	0.57
3:N:102:THR:C	3:N:103:PHE:HD1	2.12	0.57
1:B:108:THR:OG1	1:B:234:ASN:O	2.22	0.57
2:I:165:VAL:O	2:I:166:THR:OG1	2.16	0.57
2:I:169:TRP:O	2:I:210:ILE:O	2.21	0.57
3:N:3:VAL:HG23	3:N:3:VAL:O	2.03	0.57
3:N:4:MET:C	3:N:5:THR:CG2	2.78	0.57
3:N:171:GLN:CG	3:N:178:TYR:CE1	2.88	0.57
1:A:164:ASN:HD22	4:E:1:NAG:H82	1.67	0.57
1:B:562:PHE:HZ	1:C:38:TYR:CD2	2.23	0.57
1:C:470:THR:HG22	1:C:471:GLU:H	1.68	0.57
3:M:5:THR:OG1	3:M:6:GLN:N	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:55:ASP:O	2:J:57:GLU:N	2.37	0.57
1:A:274:THR:C	1:A:275:PHE:HD1	2.12	0.57
1:B:164:ASN:HD22	4:T:1:NAG:H82	1.67	0.57
2:H:166:THR:O	2:H:167:VAL:CB	2.52	0.57
3:M:120:VAL:HG23	3:M:210:VAL:HG21	1.86	0.57
2:J:162:PRO:O	2:J:164:PRO:HD2	2.04	0.57
3:N:145:TYR:CE2	3:N:147:ARG:CB	2.87	0.57
1:A:334:ASN:ND2	1:A:361:CYS:HA	2.19	0.57
1:C:46:SER:OG	1:C:281:GLU:CA	2.53	0.57
1:C:456:PHE:CD1	1:C:457:ARG:NH1	2.73	0.57
2:H:55:ASP:O	2:H:57:GLU:N	2.37	0.57
3:L:5:THR:OG1	3:L:6:GLN:N	2.37	0.57
3:M:102:THR:C	3:M:103:PHE:HD1	2.12	0.57
2:J:169:TRP:O	2:J:210:ILE:O	2.21	0.57
1:A:46:SER:OG	1:A:281:GLU:CA	2.53	0.57
1:A:599:THR:HG22	1:A:601:GLY:H	1.70	0.57
1:B:276:LEU:HD23	1:B:301:CYS:SG	2.44	0.57
1:C:108:THR:OG1	1:C:234:ASN:O	2.22	0.57
2:J:179:HIS:N	2:J:179:HIS:CD2	2.73	0.57
3:N:10:SER:HA	3:N:108:LYS:O	2.04	0.57
1:B:277:LEU:HG	1:B:285:ILE:CD1	2.35	0.57
1:B:426:PRO:HD2	1:B:464:PHE:CE2	2.40	0.57
2:H:216:LYS:O	2:H:219:ASN:ND2	2.38	0.57
3:L:154:LYS:HD3	3:L:157:ASN:CA	2.31	0.57
3:L:171:GLN:CG	3:L:178:TYR:CE1	2.88	0.57
3:M:4:MET:C	3:M:5:THR:CG2	2.78	0.57
3:M:145:TYR:CE2	3:M:147:ARG:CB	2.87	0.57
1:A:34:ARG:NH1	1:A:221:SER:OG	2.37	0.57
1:A:577:ARG:HD3	1:A:582:LEU:HD13	1.87	0.57
1:B:24:LEU:HD13	1:B:24:LEU:H	1.69	0.57
1:B:424:LYS:HG3	1:B:461:LEU:O	2.05	0.57
1:C:168:PHE:CD1	1:C:169:GLU:N	2.73	0.57
1:C:196:ASN:ND2	1:C:200:TYR:O	2.38	0.57
2:H:181:PHE:CZ	3:L:181:SER:OG	2.54	0.57
2:I:162:PRO:O	2:I:164:PRO:HD2	2.04	0.57
3:M:10:SER:HA	3:M:108:LYS:O	2.04	0.57
1:B:22:THR:CG2	1:B:78:ARG:NE	2.62	0.56
2:H:179:HIS:N	2:H:179:HIS:CD2	2.73	0.56
1:A:422:ASN:ND2	1:A:454:ARG:H	2.02	0.56
2:J:140:ALA:CB	2:J:229:LYS:CG	2.84	0.56
1:A:108:THR:OG1	1:A:234:ASN:O	2.22	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:196:ASN:ND2	1:A:200:TYR:O	2.38	0.56
1:A:334:ASN:HD22	1:A:361:CYS:HA	1.70	0.56
2:H:139:LEU:HD21	2:H:156:LEU:HD12	1.88	0.56
2:H:162:PRO:O	2:H:164:PRO:HD2	2.04	0.56
3:L:120:VAL:HG23	3:L:210:VAL:HG21	1.86	0.56
2:I:139:LEU:HD21	2:I:156:LEU:HD12	1.88	0.56
2:I:140:ALA:CB	2:I:229:LYS:CG	2.84	0.56
3:M:171:GLN:CG	3:M:178:TYR:CE1	2.88	0.56
2:J:152:ALA:HA	2:J:198:THR:HA	1.85	0.56
1:C:439:ASN:ND2	1:C:506:GLN:OE1	2.39	0.56
3:L:169:THR:CG2	3:L:179:SER:N	2.68	0.56
1:A:168:PHE:CD1	1:A:169:GLU:N	2.73	0.56
2:H:170:ASN:HD22	2:H:171:SER:H	1.54	0.56
3:L:4:MET:HB3	3:L:25:SER:HA	1.85	0.56
2:I:216:LYS:O	2:I:219:ASN:ND2	2.38	0.56
2:J:170:ASN:HD22	2:J:171:SER:H	1.54	0.56
3:M:103:PHE:HD1	3:M:103:PHE:N	2.04	0.56
2:J:141:PRO:HG2	2:J:228:PRO:HA	1.73	0.56
1:B:168:PHE:CD1	1:B:169:GLU:N	2.73	0.56
1:B:558:LYS:O	1:C:43:PHE:CE1	2.59	0.56
2:H:181:PHE:CG	3:L:167:SER:HB3	2.41	0.56
3:L:4:MET:C	3:L:5:THR:CG2	2.78	0.56
2:I:55:ASP:O	2:I:57:GLU:N	2.37	0.56
2:J:166:THR:O	2:J:167:VAL:CB	2.52	0.56
1:A:38:TYR:CD2	1:C:562:PHE:HZ	2.24	0.56
3:L:120:VAL:HB	3:L:210:VAL:CG1	2.35	0.56
3:M:193:LYS:O	3:M:194:HIS:CG	2.59	0.56
2:J:216:LYS:O	2:J:219:ASN:ND2	2.38	0.56
1:B:58:PHE:HE1	1:B:275:PHE:CE2	2.09	0.56
1:C:24:LEU:HD13	1:C:24:LEU:H	1.69	0.56
1:C:48:LEU:HD21	1:C:276:LEU:HG	1.85	0.56
3:N:120:VAL:HB	3:N:210:VAL:CG1	2.35	0.56
3:N:169:THR:CG2	3:N:179:SER:N	2.68	0.56
1:A:353:TRP:NE1	1:A:422:ASN:O	2.38	0.56
2:H:52:ASP:CG	3:L:99:PHE:CE1	2.84	0.56
3:M:104:GLY:C	3:M:106:GLY:H	2.13	0.56
3:N:4:MET:HB3	3:N:24:ARG:O	2.02	0.56
1:A:21:ARG:HG2	1:A:22:THR:N	2.21	0.55
1:A:24:LEU:HD13	1:A:24:LEU:H	1.69	0.55
1:B:196:ASN:ND2	1:B:200:TYR:O	2.38	0.55
3:L:103:PHE:HD1	3:L:103:PHE:N	2.04	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:145:TYR:CE2	3:L:147:ARG:CB	2.87	0.55
3:L:193:LYS:O	3:L:194:HIS:CG	2.59	0.55
1:A:827:THR:HG23	1:A:827:THR:O	2.06	0.55
2:J:181:PHE:CG	3:N:167:SER:HB3	2.41	0.55
1:B:521:PRO:HG3	1:B:564:GLN:HE21	1.70	0.55
2:I:160:TYR:CD2	2:I:162:PRO:HG2	2.42	0.55
2:I:170:ASN:HD22	2:I:171:SER:H	1.54	0.55
3:N:103:PHE:HD1	3:N:103:PHE:N	2.04	0.55
1:B:277:LEU:HD22	1:B:277:LEU:H	1.70	0.55
2:H:169:TRP:C	2:H:210:ILE:O	2.49	0.55
3:M:13:VAL:O	3:M:112:LYS:HB2	2.06	0.55
2:J:166:THR:O	2:J:167:VAL:CG2	2.54	0.55
3:N:104:GLY:C	3:N:106:GLY:H	2.13	0.55
1:B:146:HIS:ND1	1:B:148:ASN:O	2.35	0.55
1:B:557:LYS:HD3	1:C:43:PHE:HE2	1.71	0.55
2:H:166:THR:O	2:H:167:VAL:CG2	2.54	0.55
2:I:52:ASP:CG	3:M:99:PHE:CE1	2.84	0.55
2:I:166:THR:O	2:I:167:VAL:CG2	2.54	0.55
2:J:52:ASP:CG	3:N:99:PHE:CE1	2.84	0.55
1:A:454:ARG:CD	1:A:491:PRO:C	2.76	0.55
1:A:812:PRO:O	1:A:813:SER:OG	2.22	0.55
2:I:179:HIS:CD2	2:I:179:HIS:N	2.73	0.55
3:N:13:VAL:O	3:N:112:LYS:HB2	2.06	0.55
3:N:156:ASP:CG	3:N:194:HIS:ND1	2.65	0.55
3:N:198:ALA:CB	3:N:213:SER:HB3	2.37	0.55
1:B:427:ASP:C	1:B:428:ASP:O	2.50	0.55
2:H:51:PHE:CD1	2:H:51:PHE:C	2.85	0.55
3:L:151:VAL:HG21	3:L:180:LEU:CG	2.27	0.55
3:M:103:PHE:N	3:M:103:PHE:CD1	2.75	0.55
2:J:169:TRP:C	2:J:210:ILE:O	2.49	0.55
2:J:215:HIS:O	2:J:219:ASN:N	2.40	0.55
1:A:618:THR:HG21	6:A:1417:NAG:H5	1.89	0.55
1:B:54:LEU:HD23	1:B:54:LEU:N	2.19	0.55
3:L:156:ASP:CG	3:L:194:HIS:ND1	2.65	0.55
2:I:181:PHE:CG	3:M:167:SER:HB3	2.41	0.55
3:N:193:LYS:O	3:N:194:HIS:CG	2.59	0.55
1:A:73:THR:O	1:A:74:ASN:HB2	2.06	0.55
1:B:73:THR:O	1:B:74:ASN:HB2	2.06	0.55
1:B:473:TYR:CB	1:B:489:TYR:HB3	2.37	0.55
1:B:503:VAL:HG22	1:B:505:TYR:H	1.72	0.55
1:C:674:TYR:CD1	1:C:691:SER:O	2.59	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:104:GLY:C	3:L:106:GLY:H	2.13	0.55
3:M:120:VAL:HB	3:M:210:VAL:CG1	2.35	0.55
3:M:156:ASP:CG	3:M:194:HIS:ND1	2.65	0.55
3:M:216:ARG:HG2	3:M:216:ARG:NH1	2.21	0.55
1:A:403:ARG:CZ	1:A:505:TYR:CD1	2.90	0.55
1:A:453:TYR:C	1:A:453:TYR:CD1	2.85	0.55
1:A:453:TYR:HE2	1:A:495:TYR:CZ	2.25	0.55
1:B:220:PHE:CE1	1:B:288:ALA:HB3	2.41	0.55
1:B:418:ILE:HA	1:B:422:ASN:CG	2.31	0.55
1:B:562:PHE:CZ	1:C:38:TYR:HD2	2.25	0.55
3:L:198:ALA:CB	3:L:213:SER:HB3	2.37	0.55
2:I:51:PHE:CD1	2:I:51:PHE:C	2.85	0.55
2:J:139:LEU:HD21	2:J:156:LEU:HD12	1.88	0.55
3:N:141:LEU:HD13	3:N:201:VAL:HG11	1.87	0.55
1:A:170:TYR:CD1	1:A:170:TYR:C	2.85	0.54
1:B:170:TYR:CD1	1:B:170:TYR:C	2.85	0.54
1:B:457:ARG:NH2	1:B:490:PHE:O	2.40	0.54
2:H:179:HIS:HB3	3:L:179:SER:OG	2.07	0.54
3:M:198:ALA:CB	3:M:213:SER:HB3	2.37	0.54
3:N:138:VAL:C	3:N:153:TRP:CZ3	2.85	0.54
1:B:454:ARG:NH1	1:B:456:PHE:CZ	2.75	0.54
1:C:21:ARG:HG2	1:C:22:THR:N	2.21	0.54
1:C:170:TYR:CD1	1:C:170:TYR:C	2.85	0.54
2:H:140:ALA:CB	2:H:229:LYS:CG	2.84	0.54
2:H:160:TYR:CD2	2:H:162:PRO:HG2	2.42	0.54
3:L:151:VAL:CG2	3:L:180:LEU:CD1	2.85	0.54
2:I:169:TRP:C	2:I:210:ILE:O	2.49	0.54
3:M:151:VAL:CG2	3:M:180:LEU:CD1	2.85	0.54
3:M:169:THR:CG2	3:M:179:SER:N	2.68	0.54
3:N:2:ILE:CG2	3:N:4:MET:HE1	2.23	0.54
3:N:103:PHE:N	3:N:103:PHE:CD1	2.75	0.54
3:N:151:VAL:CG2	3:N:180:LEU:CD1	2.85	0.54
1:A:437:ASN:OD1	1:A:506:GLN:CG	2.55	0.54
1:A:663:ASP:HB3	1:A:673:SER:HB3	1.89	0.54
3:L:13:VAL:O	3:L:112:LYS:HB2	2.06	0.54
2:I:215:HIS:O	2:I:219:ASN:N	2.40	0.54
2:J:160:TYR:CD2	2:J:162:PRO:HG2	2.42	0.54
2:J:167:VAL:C	2:J:169:TRP:H	2.15	0.54
1:A:336:CYS:HB2	1:A:363:ALA:HA	1.90	0.54
3:M:141:LEU:HD13	3:M:201:VAL:HG11	1.87	0.54
3:N:7:SER:HB3	3:N:22:SER:HG	1.69	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:125:PRO:HG2	3:M:130:LEU:CD2	2.37	0.54
3:N:125:PRO:HG2	3:N:130:LEU:CD2	2.37	0.54
3:N:193:LYS:O	3:N:194:HIS:CD2	2.61	0.54
1:A:542:ASN:ND2	1:A:547:THR:OG1	2.41	0.54
1:B:562:PHE:CZ	1:C:38:TYR:CD2	2.95	0.54
2:H:215:HIS:O	2:H:219:ASN:N	2.40	0.54
2:J:179:HIS:HB3	3:N:179:SER:OG	2.07	0.54
1:B:57:PRO:CB	1:B:273:ARG:HE	2.15	0.54
1:C:73:THR:O	1:C:74:ASN:HB2	2.06	0.54
3:N:118:PRO:HG3	3:N:144:PHE:CD2	2.42	0.54
1:A:285:ILE:CG2	1:A:286:THR:H	2.06	0.54
1:B:21:ARG:HG2	1:B:22:THR:N	2.21	0.54
1:B:278:LYS:HB2	1:B:306:PHE:CE1	2.43	0.54
2:H:98:THR:OG1	2:H:99:SER:N	2.40	0.54
3:L:138:VAL:C	3:L:153:TRP:CZ3	2.85	0.54
3:L:141:LEU:HD11	3:L:201:VAL:HG12	1.90	0.54
1:C:78:ARG:CG	1:C:78:ARG:HH11	2.16	0.54
3:L:115:VAL:HG12	3:L:205:GLY:CA	2.38	0.54
1:A:244:LEU:HD22	1:A:259:THR:HA	1.90	0.54
1:C:456:PHE:HD1	1:C:457:ARG:HH12	1.55	0.54
2:H:140:ALA:CB	2:H:229:LYS:HD2	2.16	0.54
3:M:138:VAL:C	3:M:153:TRP:CZ3	2.85	0.54
1:B:418:ILE:HG23	1:B:422:ASN:HD22	1.73	0.53
1:C:616:ASN:O	1:C:618:THR:N	2.41	0.53
3:L:193:LYS:O	3:L:194:HIS:CD2	2.61	0.53
1:A:503:VAL:CG1	1:A:504:GLY:H	2.14	0.53
1:C:455:LEU:CD1	1:C:493:GLN:HB2	2.38	0.53
2:I:179:HIS:HB3	3:M:179:SER:OG	2.07	0.53
3:M:141:LEU:HD11	3:M:201:VAL:HG12	1.90	0.53
2:J:51:PHE:C	2:J:51:PHE:CD1	2.85	0.53
3:N:141:LEU:HD11	3:N:201:VAL:HG12	1.90	0.53
1:A:285:ILE:O	1:A:286:THR:OG1	2.22	0.53
1:A:364:ASP:HA	1:A:527:PRO:HD3	1.90	0.53
1:B:473:TYR:O	1:B:489:TYR:CD2	2.62	0.53
1:C:296:LEU:O	1:C:296:LEU:HD22	2.09	0.53
1:A:23:GLN:CD	1:A:24:LEU:H	2.17	0.53
1:A:43:PHE:N	1:C:563:GLN:HG2	2.23	0.53
1:A:256:SER:OG	1:A:257:GLY:N	2.42	0.53
1:A:296:LEU:O	1:A:296:LEU:HD22	2.09	0.53
3:M:139:CYS:H	3:M:153:TRP:HH2	1.56	0.53
1:A:498:GLN:HB3	1:A:499:PRO:CD	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:23:GLN:CD	1:C:24:LEU:H	2.17	0.53
2:H:132:LYS:HG2	2:H:133:GLY:H	1.74	0.53
2:I:98:THR:OG1	2:I:99:SER:N	2.40	0.53
3:M:193:LYS:O	3:M:194:HIS:CD2	2.61	0.53
3:N:139:CYS:H	3:N:153:TRP:HH2	1.56	0.53
1:A:813:SER:C	1:A:814:LYS:HZ3	2.16	0.53
1:B:164:ASN:ND2	4:T:1:NAG:C8	2.72	0.53
3:L:103:PHE:N	3:L:103:PHE:CD1	2.75	0.53
2:I:132:LYS:HG2	2:I:133:GLY:H	1.74	0.53
3:M:115:VAL:HG12	3:M:205:GLY:CA	2.38	0.53
2:J:132:LYS:HG2	2:J:133:GLY:H	1.74	0.53
1:A:811:LYS:NZ	1:A:820:ASP:OD2	2.38	0.53
1:B:244:LEU:HD22	1:B:259:THR:HA	1.90	0.53
1:B:256:SER:OG	1:B:257:GLY:N	2.42	0.53
1:C:48:LEU:HD21	1:C:276:LEU:CD1	2.24	0.53
3:L:125:PRO:HG2	3:L:130:LEU:CD2	2.37	0.53
3:M:143:ASN:OD1	3:M:177:THR:HG21	2.09	0.53
2:J:98:THR:OG1	2:J:99:SER:N	2.40	0.53
1:A:1144:GLU:C	1:A:1146:ASP:H	2.17	0.53
1:B:296:LEU:O	1:B:296:LEU:HD22	2.09	0.53
3:N:216:ARG:HG2	3:N:216:ARG:NH1	2.21	0.53
1:A:146:HIS:ND1	1:A:148:ASN:O	2.35	0.53
1:A:809:PRO:O	1:A:810:SER:HB3	2.09	0.53
1:A:1116:THR:OG1	1:A:1118:ASP:OD1	2.22	0.53
1:B:23:GLN:CD	1:B:24:LEU:H	2.17	0.53
1:C:72:GLY:O	1:C:73:THR:HB	2.09	0.53
3:L:143:ASN:OD1	3:L:177:THR:HG21	2.09	0.53
2:J:184:VAL:CG2	2:J:185:LEU:H	2.22	0.53
1:A:453:TYR:CE2	1:A:495:TYR:OH	2.60	0.52
1:C:146:HIS:ND1	1:C:148:ASN:O	2.35	0.52
1:C:256:SER:OG	1:C:257:GLY:N	2.42	0.52
3:L:141:LEU:HD13	3:L:201:VAL:HG11	1.87	0.52
2:I:170:ASN:HD22	2:I:171:SER:N	2.07	0.52
3:M:7:SER:CB	3:M:8:PRO:CD	2.84	0.52
1:C:498:GLN:CG	1:C:501:ASN:HB2	2.31	0.52
2:I:184:VAL:CG2	2:I:185:LEU:H	2.22	0.52
3:N:151:VAL:HG21	3:N:180:LEU:CD1	2.39	0.52
1:A:801:ASN:OD1	1:A:803:SER:HB3	2.09	0.52
1:B:473:TYR:C	1:B:489:TYR:HB2	2.35	0.52
1:B:559:PHE:CD1	1:C:43:PHE:CD2	2.97	0.52
1:C:244:LEU:HD22	1:C:259:THR:HA	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:135:SER:OG	2:I:158:LYS:O	2.27	0.52
3:N:154:LYS:HD3	3:N:157:ASN:CA	2.31	0.52
1:A:50:SER:HA	1:A:275:PHE:O	2.10	0.52
1:A:454:ARG:HD2	1:A:491:PRO:O	2.08	0.52
1:A:981:LEU:HD21	1:A:993:ILE:HD11	1.91	0.52
1:C:164:ASN:ND2	4:d:1:NAG:C8	2.72	0.52
3:L:139:CYS:H	3:L:153:TRP:HH2	1.56	0.52
3:L:151:VAL:HG21	3:L:180:LEU:CD1	2.39	0.52
1:C:73:THR:HG23	1:C:74:ASN:N	2.25	0.52
2:H:170:ASN:HD22	2:H:171:SER:N	2.07	0.52
2:I:167:VAL:C	2:I:169:TRP:H	2.15	0.52
1:A:452:LEU:HG	1:A:494:SER:HA	1.92	0.52
1:A:1142:GLN:HA	1:A:1142:GLN:HE21	1.72	0.52
1:C:22:THR:O	1:C:23:GLN:HG3	2.10	0.52
1:C:220:PHE:CD2	1:C:287:ASP:HA	2.43	0.52
3:L:2:ILE:HG22	3:L:3:VAL:H	1.74	0.52
3:L:8:PRO:C	3:L:10:SER:N	2.67	0.52
3:M:115:VAL:CG1	3:M:205:GLY:HA2	2.39	0.52
3:M:120:VAL:CG1	3:M:212:LYS:HB2	2.40	0.52
1:A:393:THR:CB	1:A:518:LEU:HA	2.33	0.52
1:B:425:LEU:HD13	1:B:430:THR:CG2	2.40	0.52
1:C:22:THR:CG2	1:C:78:ARG:HG2	2.31	0.52
1:C:453:TYR:CE1	1:C:455:LEU:HD21	2.45	0.52
1:A:164:ASN:ND2	4:E:1:NAG:C8	2.72	0.52
1:B:418:ILE:HD12	1:B:422:ASN:ND2	2.25	0.52
1:C:50:SER:HA	1:C:275:PHE:O	2.10	0.52
1:C:613:GLN:CA	1:C:613:GLN:NE2	2.73	0.52
2:J:170:ASN:HD22	2:J:171:SER:N	2.07	0.52
3:N:2:ILE:HG22	3:N:3:VAL:H	1.74	0.52
3:N:143:ASN:OD1	3:N:177:THR:HG21	2.09	0.52
3:N:169:THR:HG22	3:N:179:SER:N	2.25	0.52
1:A:29:THR:OG1	1:A:30:ASN:N	2.39	0.52
1:B:58:PHE:CE1	1:B:275:PHE:CZ	2.97	0.52
1:B:303:LEU:N	1:B:303:LEU:CD1	2.73	0.52
2:H:135:SER:OG	2:H:158:LYS:O	2.28	0.52
3:L:115:VAL:CG1	3:L:205:GLY:HA2	2.39	0.52
2:J:135:SER:OG	2:J:158:LYS:O	2.28	0.52
3:N:172:ASP:O	3:N:176:SER:CA	2.58	0.52
1:B:558:LYS:O	1:C:43:PHE:CZ	2.63	0.52
1:C:46:SER:OG	1:C:280:ASN:C	2.53	0.52
3:M:120:VAL:O	3:M:212:LYS:HG3	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:53:ILE:HG23	3:N:58:ASN:H	1.75	0.52
1:A:48:LEU:HD21	1:A:276:LEU:HG	1.85	0.51
1:A:73:THR:HG23	1:A:74:ASN:N	2.25	0.51
1:A:811:LYS:CB	1:A:812:PRO:CD	2.88	0.51
1:B:22:THR:O	1:B:23:GLN:HG3	2.10	0.51
1:B:72:GLY:O	1:B:73:THR:HB	2.09	0.51
2:I:141:PRO:HG2	2:I:228:PRO:HA	1.73	0.51
3:M:8:PRO:C	3:M:10:SER:N	2.67	0.51
3:N:115:VAL:CG1	3:N:205:GLY:HA2	2.39	0.51
1:A:111:ASP:OD1	1:A:134:GLN:NE2	2.37	0.51
1:A:161:SER:OG	1:A:162:SER:N	2.44	0.51
1:B:559:PHE:CE1	1:C:43:PHE:HD2	2.25	0.51
1:C:24:LEU:HB3	1:C:25:PRO:CD	2.41	0.51
1:C:470:THR:CG2	1:C:471:GLU:N	2.73	0.51
2:I:161:PHE:N	2:I:162:PRO:CD	2.74	0.51
3:N:120:VAL:CG1	3:N:212:LYS:HB2	2.40	0.51
3:N:120:VAL:O	3:N:212:LYS:HG3	2.10	0.51
1:A:22:THR:O	1:A:23:GLN:HG3	2.10	0.51
1:A:24:LEU:HB3	1:A:25:PRO:CD	2.41	0.51
1:A:72:GLY:O	1:A:73:THR:HB	2.09	0.51
1:C:1138:TYR:OH	1:C:1143:PRO:HG2	2.11	0.51
3:M:153:TRP:HZ2	3:M:182:SER:HB2	1.24	0.51
2:J:160:TYR:O	2:J:191:TYR:HB2	2.11	0.51
1:A:329:PHE:HD2	1:A:528:LYS:HB2	1.75	0.51
1:B:29:THR:OG1	1:B:30:ASN:N	2.39	0.51
1:C:674:TYR:O	1:C:675:GLN:HB3	2.09	0.51
2:H:160:TYR:O	2:H:191:TYR:HB2	2.11	0.51
2:H:161:PHE:N	2:H:162:PRO:CD	2.74	0.51
2:I:160:TYR:O	2:I:191:TYR:HB2	2.11	0.51
2:I:162:PRO:O	2:I:217:PRO:CG	2.59	0.51
3:M:53:ILE:HG23	3:M:58:ASN:H	1.75	0.51
3:M:151:VAL:HG21	3:M:180:LEU:CG	2.27	0.51
3:N:115:VAL:HG12	3:N:205:GLY:CA	2.38	0.51
1:B:1141:LEU:HD23	1:B:1141:LEU:C	2.34	0.51
2:H:167:VAL:C	2:H:169:TRP:H	2.15	0.51
3:L:53:ILE:HG23	3:L:58:ASN:H	1.75	0.51
3:L:118:PRO:HG3	3:L:144:PHE:CD2	2.42	0.51
2:J:162:PRO:O	2:J:217:PRO:CG	2.59	0.51
1:C:457:ARG:H	1:C:457:ARG:CD	1.96	0.51
2:H:162:PRO:O	2:H:217:PRO:CG	2.59	0.51
3:L:118:PRO:CD	3:L:206:LEU:HD21	2.31	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:169:THR:HG22	3:M:179:SER:N	2.25	0.51
1:A:402:ILE:C	1:A:403:ARG:O	2.53	0.51
1:A:1030:SER:HB3	1:C:1041:ASP:HB2	1.93	0.51
1:B:73:THR:HG23	1:B:74:ASN:N	2.25	0.51
1:C:454:ARG:HD2	1:C:458:LYS:HZ1	1.76	0.51
3:L:120:VAL:O	3:L:212:LYS:HG3	2.10	0.51
3:M:2:ILE:CG2	3:M:3:VAL:N	2.74	0.51
3:N:44:ARG:NH1	3:N:86:GLU:O	2.44	0.51
3:N:202:THR:C	3:N:203:HIS:CG	2.89	0.51
1:A:329:PHE:O	1:A:330:PRO:O	2.29	0.51
1:B:33:THR:HG22	1:B:58:PHE:CD2	2.45	0.51
2:H:184:VAL:CG2	2:H:185:LEU:H	2.22	0.51
2:I:142:SER:HB3	3:M:214:PHE:HD2	0.56	0.51
3:M:202:THR:C	3:M:203:HIS:CG	2.89	0.51
3:N:2:ILE:CG2	3:N:3:VAL:N	2.74	0.51
3:N:8:PRO:C	3:N:10:SER:N	2.67	0.51
1:A:38:TYR:CD2	1:C:562:PHE:CZ	2.99	0.51
1:C:161:SER:OG	1:C:162:SER:N	2.44	0.51
1:C:495:TYR:HE2	1:C:507:PRO:HG3	1.76	0.51
3:L:9:LEU:C	3:L:10:SER:HG	2.07	0.51
2:I:160:TYR:CD2	2:I:162:PRO:CG	2.94	0.51
2:I:169:TRP:HD1	2:I:197:VAL:CB	2.24	0.51
1:A:379:CYS:HB3	1:A:432:CYS:HA	1.93	0.51
1:A:453:TYR:CE2	1:A:495:TYR:CZ	2.98	0.51
1:A:503:VAL:C	1:A:505:TYR:H	2.19	0.51
1:A:516:GLU:C	1:A:518:LEU:H	2.19	0.51
1:C:1142:GLN:HB2	1:C:1143:PRO:HD3	1.93	0.51
2:H:178:VAL:HG23	2:H:178:VAL:O	2.11	0.51
2:I:177:GLY:O	2:I:197:VAL:HG13	2.11	0.51
2:J:177:GLY:O	2:J:197:VAL:HG13	2.11	0.51
3:N:31:HIS:HB2	3:N:97:THR:CG2	2.41	0.51
3:N:198:ALA:CA	3:N:213:SER:HB3	2.41	0.51
1:C:457:ARG:NH2	1:C:489:TYR:CD2	2.79	0.50
3:L:31:HIS:HB2	3:L:97:THR:CG2	2.41	0.50
2:I:185:LEU:HD23	2:I:191:TYR:CD1	2.46	0.50
3:M:31:HIS:HB2	3:M:97:THR:CG2	2.41	0.50
3:M:151:VAL:HG21	3:M:180:LEU:CD1	2.39	0.50
3:M:198:ALA:CA	3:M:213:SER:HB3	2.41	0.50
3:N:154:LYS:CG	3:N:157:ASN:HA	2.41	0.50
1:A:78:ARG:CG	1:A:78:ARG:HH11	2.16	0.50
1:A:330:PRO:C	1:A:528:LYS:HE2	2.36	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:457:ARG:O	1:B:458:LYS:HG2	2.10	0.50
3:M:44:ARG:NH1	3:M:86:GLU:O	2.44	0.50
2:J:155:CYS:HB2	2:J:169:TRP:HH2	1.76	0.50
2:J:161:PHE:N	2:J:162:PRO:CD	2.74	0.50
2:J:179:HIS:CG	3:N:179:SER:OG	2.64	0.50
1:A:449:TYR:CB	1:A:497:PHE:HB2	2.40	0.50
1:C:454:ARG:CD	1:C:458:LYS:CE	2.87	0.50
1:C:1142:GLN:OE1	1:C:1142:GLN:HA	2.10	0.50
2:H:160:TYR:CD2	2:H:162:PRO:CG	2.94	0.50
3:M:156:ASP:OD2	3:M:194:HIS:CD2	2.65	0.50
2:J:116:ASP:HA	3:N:51:LEU:HD22	1.94	0.50
1:A:46:SER:OG	1:A:280:ASN:C	2.53	0.50
1:A:337:PRO:HB2	1:A:358:ILE:HD12	1.93	0.50
1:A:515:PHE:N	1:A:515:PHE:CD1	2.79	0.50
3:L:120:VAL:CG1	3:L:212:LYS:HB2	2.40	0.50
3:L:169:THR:HG22	3:L:179:SER:N	2.25	0.50
3:M:172:ASP:O	3:M:176:SER:CA	2.58	0.50
1:B:220:PHE:HE2	1:B:287:ASP:HA	1.67	0.50
1:B:248:TYR:OH	2:I:31:GLU:OE1	2.30	0.50
3:L:216:ARG:HG2	3:L:216:ARG:NH1	2.21	0.50
2:J:160:TYR:CD2	2:J:162:PRO:CG	2.94	0.50
2:J:166:THR:O	2:J:167:VAL:HB	2.12	0.50
1:B:21:ARG:O	1:B:22:THR:O	2.30	0.50
3:M:2:ILE:HG22	3:M:3:VAL:H	1.74	0.50
3:M:154:LYS:HD3	3:M:157:ASN:CA	2.31	0.50
2:J:35:HIS:HA	2:J:50:GLY:HA2	1.94	0.50
1:B:24:LEU:HB3	1:B:25:PRO:CD	2.40	0.50
1:C:21:ARG:O	1:C:22:THR:O	2.30	0.50
2:H:177:GLY:O	2:H:197:VAL:HG13	2.11	0.50
2:H:185:LEU:HD23	2:H:191:TYR:CD1	2.46	0.50
3:L:44:ARG:NH1	3:L:86:GLU:O	2.44	0.50
2:I:179:HIS:CG	3:M:179:SER:OG	2.65	0.50
1:B:22:THR:CG2	1:B:78:ARG:CD	2.75	0.50
1:C:454:ARG:CD	1:C:458:LYS:HZ1	2.22	0.50
3:L:2:ILE:C	3:L:3:VAL:HG13	2.35	0.50
3:L:198:ALA:CA	3:L:213:SER:HB3	2.41	0.50
2:I:178:VAL:O	2:I:178:VAL:HG23	2.11	0.50
3:M:118:PRO:HG3	3:M:144:PHE:CD2	2.42	0.50
1:A:390:LEU:CG	1:A:391:CYS:H	2.19	0.50
1:B:161:SER:OG	1:B:162:SER:N	2.44	0.50
1:C:456:PHE:HD1	1:C:457:ARG:NH1	2.09	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:35:HIS:HA	2:H:50:GLY:HA2	1.94	0.50
2:H:140:ALA:HB1	2:H:141:PRO:HD2	1.94	0.50
2:H:162:PRO:O	2:H:217:PRO:HG3	2.12	0.50
3:L:172:ASP:O	3:L:176:SER:CA	2.58	0.50
2:I:166:THR:O	2:I:167:VAL:HB	2.12	0.50
2:J:162:PRO:O	2:J:217:PRO:HG3	2.12	0.50
2:J:185:LEU:HD23	2:J:191:TYR:CD1	2.46	0.50
1:B:457:ARG:HA	1:B:473:TYR:HE2	1.77	0.49
2:H:142:SER:HB3	3:L:214:PHE:HD2	0.57	0.49
3:L:2:ILE:CG2	3:L:3:VAL:N	2.74	0.49
1:A:248:TYR:O	1:A:250:THR:N	2.43	0.49
1:A:248:TYR:OH	2:H:31:GLU:OE1	2.30	0.49
1:B:1141:LEU:HD23	1:B:1142:GLN:CA	2.42	0.49
2:H:179:HIS:CG	3:L:179:SER:OG	2.65	0.49
3:N:143:ASN:CG	3:N:177:THR:CG2	2.80	0.49
1:A:327:VAL:HG12	1:A:542:ASN:HB3	1.94	0.49
1:A:357:ARG:HH12	1:B:167:THR:CA	2.25	0.49
1:A:453:TYR:CD1	1:A:454:ARG:HB2	2.47	0.49
3:M:143:ASN:CG	3:M:177:THR:CG2	2.80	0.49
3:M:154:LYS:CG	3:M:157:ASN:HA	2.41	0.49
2:J:170:ASN:ND2	2:J:171:SER:H	2.10	0.49
1:A:38:TYR:OH	1:A:284:THR:HG23	2.12	0.49
1:A:43:PHE:CE2	1:C:557:LYS:HB3	2.47	0.49
1:C:456:PHE:CB	1:C:457:ARG:HH11	2.16	0.49
2:H:166:THR:O	2:H:167:VAL:HB	2.12	0.49
2:H:184:VAL:HG22	2:H:185:LEU:H	1.75	0.49
3:L:7:SER:CB	3:L:8:PRO:CD	2.84	0.49
3:L:157:ASN:O	3:L:158:ALA:HB2	2.13	0.49
2:I:35:HIS:HA	2:I:50:GLY:HA2	1.94	0.49
3:M:169:THR:HG23	3:M:179:SER:H	1.77	0.49
2:J:140:ALA:HB1	2:J:141:PRO:HD2	1.94	0.49
3:N:156:ASP:OD2	3:N:194:HIS:CD2	2.65	0.49
3:N:202:THR:O	3:N:203:HIS:CD2	2.65	0.49
1:B:122:ASN:O	1:B:124:THR:N	2.40	0.49
1:C:824:ASN:O	1:C:827:THR:CG2	2.57	0.49
3:L:156:ASP:OD2	3:L:194:HIS:CD2	2.65	0.49
2:J:169:TRP:HD1	2:J:197:VAL:CB	2.24	0.49
2:J:178:VAL:HG23	2:J:178:VAL:O	2.11	0.49
1:C:164:ASN:HD22	4:d:1:NAG:C8	2.26	0.49
2:I:170:ASN:ND2	2:I:171:SER:H	2.10	0.49
1:B:454:ARG:HD2	1:B:456:PHE:CE1	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:277:LEU:N	1:C:277:LEU:CD1	2.75	0.49
3:L:154:LYS:CG	3:L:157:ASN:HA	2.41	0.49
3:N:201:VAL:HB	3:N:203:HIS:CD2	2.44	0.49
1:B:220:PHE:CD2	1:B:287:ASP:HA	2.47	0.49
3:N:150:LYS:O	3:N:203:HIS:NE2	2.46	0.49
1:A:164:ASN:HD22	4:E:1:NAG:C8	2.26	0.49
1:B:417:LYS:NZ	1:B:456:PHE:HZ	2.11	0.49
1:C:182:LYS:HG3	1:C:186:PHE:CE2	2.48	0.49
2:H:116:ASP:HA	3:L:51:LEU:HD22	1.94	0.49
3:L:120:VAL:CB	3:L:210:VAL:CG1	2.85	0.49
3:L:202:THR:C	3:L:203:HIS:CG	2.89	0.49
2:I:116:ASP:HA	3:M:51:LEU:HD22	1.94	0.49
3:M:202:THR:O	3:M:203:HIS:CD2	2.65	0.49
1:A:21:ARG:O	1:A:22:THR:O	2.30	0.49
1:A:277:LEU:N	1:A:277:LEU:CD1	2.75	0.49
1:A:344:ALA:HB3	1:A:347:PHE:HE1	1.77	0.49
2:H:170:ASN:ND2	2:H:171:SER:H	2.10	0.49
3:L:145:TYR:OH	3:L:147:ARG:HD2	2.13	0.49
3:M:119:SER:OG	3:M:142:ASN:HB3	2.13	0.49
3:N:145:TYR:OH	3:N:147:ARG:HD2	2.13	0.49
5:O:2:NAG:C8	5:O:2:NAG:C1	2.91	0.49
1:A:16:VAL:O	1:A:16:VAL:HG23	2.13	0.48
1:B:16:VAL:HG23	1:B:16:VAL:O	2.13	0.48
1:B:457:ARG:CZ	1:B:491:PRO:HA	2.43	0.48
1:C:48:LEU:HD23	1:C:276:LEU:CG	2.36	0.48
1:C:179:LEU:C	1:C:179:LEU:CD2	2.86	0.48
2:I:140:ALA:HB1	2:I:141:PRO:HD2	1.94	0.48
2:I:162:PRO:O	2:I:217:PRO:HG3	2.12	0.48
3:M:8:PRO:O	3:M:10:SER:N	2.46	0.48
2:J:11:VAL:HG11	2:J:161:PHE:CE2	2.47	0.48
1:A:453:TYR:O	1:A:454:ARG:HB3	2.12	0.48
1:C:111:ASP:OD1	1:C:134:GLN:NE2	2.37	0.48
3:N:123:PHE:O	3:N:137:VAL:HG23	2.13	0.48
1:B:50:SER:C	1:B:51:THR:CG2	2.86	0.48
2:H:169:TRP:HD1	2:H:197:VAL:CB	2.24	0.48
3:L:202:THR:O	3:L:203:HIS:CD2	2.65	0.48
3:M:141:LEU:HD22	3:M:201:VAL:CG1	2.25	0.48
3:M:157:ASN:O	3:M:158:ALA:HB2	2.13	0.48
1:C:22:THR:C	1:C:23:GLN:CG	2.85	0.48
1:C:248:TYR:OH	2:J:31:GLU:OE1	2.30	0.48
2:H:63:LYS:HE2	2:H:63:LYS:HB3	1.59	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:138:VAL:C	3:L:153:TRP:HH2	2.21	0.48
2:I:184:VAL:O	2:I:185:LEU:HD23	2.13	0.48
1:A:26:PRO:O	1:A:28:TYR:CD1	2.67	0.48
1:A:276:LEU:O	1:A:289:VAL:HG12	2.13	0.48
1:A:350:VAL:HG13	1:A:453:TYR:HB2	1.95	0.48
1:B:22:THR:C	1:B:23:GLN:CG	2.85	0.48
1:C:26:PRO:O	1:C:28:TYR:CD1	2.67	0.48
1:C:454:ARG:O	1:C:455:LEU:HG	2.13	0.48
3:M:2:ILE:C	3:M:3:VAL:HG13	2.35	0.48
3:M:201:VAL:HB	3:M:203:HIS:CD2	2.44	0.48
1:A:329:PHE:HB3	1:A:528:LYS:HD2	1.95	0.48
1:B:38:TYR:OH	1:B:284:THR:HA	2.12	0.48
1:B:182:LYS:HG3	1:B:186:PHE:CE2	2.48	0.48
1:C:470:THR:C	1:C:471:GLU:CG	2.86	0.48
1:C:1119:ASN:OD1	1:C:1119:ASN:N	2.46	0.48
2:I:11:VAL:HG11	2:I:161:PHE:CE2	2.47	0.48
3:M:14:THR:HA	3:M:112:LYS:HB3	1.96	0.48
3:M:124:PRO:HG3	3:M:214:PHE:CE1	2.49	0.48
3:N:9:LEU:C	3:N:10:SER:HG	2.10	0.48
1:A:182:LYS:HG3	1:A:186:PHE:CE2	2.48	0.48
3:L:14:THR:HA	3:L:112:LYS:HB3	1.96	0.48
3:L:119:SER:OG	3:L:142:ASN:HB3	2.13	0.48
3:M:9:LEU:C	3:M:10:SER:HG	2.15	0.48
3:M:120:VAL:CG2	3:M:210:VAL:HB	2.33	0.48
2:J:186:GLN:OE1	2:J:191:TYR:O	2.32	0.48
3:N:119:SER:OG	3:N:142:ASN:HB3	2.13	0.48
3:N:210:VAL:CG1	3:N:211:THR:N	2.43	0.48
1:A:22:THR:C	1:A:23:GLN:CG	2.85	0.48
1:A:181:GLY:O	1:A:182:LYS:HD3	2.14	0.48
1:A:811:LYS:HB3	1:A:812:PRO:HD2	1.96	0.48
1:C:181:GLY:O	1:C:182:LYS:HD3	2.14	0.48
2:H:169:TRP:CE3	2:H:211:CYS:HA	2.49	0.48
2:H:184:VAL:O	2:H:185:LEU:HD23	2.13	0.48
2:H:185:LEU:HD21	2:H:191:TYR:OH	2.13	0.48
2:H:186:GLN:OE1	2:H:191:TYR:O	2.32	0.48
3:M:118:PRO:CD	3:M:206:LEU:HD21	2.31	0.48
3:M:145:TYR:OH	3:M:147:ARG:HD2	2.13	0.48
3:N:4:MET:O	3:N:5:THR:CG2	2.62	0.48
1:A:563:GLN:HB3	1:B:41:LYS:O	2.13	0.48
1:B:164:ASN:HD22	4:T:1:NAG:C8	2.26	0.48
1:B:181:GLY:O	1:B:182:LYS:HD3	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:16:VAL:HG23	1:C:16:VAL:O	2.13	0.48
1:C:289:VAL:CG2	1:C:306:PHE:CZ	2.93	0.48
3:L:120:VAL:HG22	3:L:201:VAL:HG21	1.96	0.48
3:L:156:ASP:OD1	3:L:197:TYR:CD1	2.67	0.48
2:I:55:ASP:HB3	2:I:57:GLU:CG	2.44	0.48
3:M:201:VAL:CG2	3:M:210:VAL:HB	2.44	0.48
3:N:124:PRO:HG3	3:N:214:PHE:CE1	2.49	0.48
3:N:156:ASP:OD1	3:N:197:TYR:CD1	2.67	0.48
1:A:167:THR:O	1:A:168:PHE:HB2	2.14	0.48
1:B:707:TYR:HB3	1:C:792:PRO:HG2	1.95	0.48
1:C:220:PHE:CZ	1:C:288:ALA:N	2.79	0.48
1:C:567:ARG:HH21	1:C:573:THR:HG22	1.79	0.48
1:C:827:THR:O	1:C:828:LEU:HG	2.14	0.48
2:H:142:SER:CB	2:H:145:SER:HB2	2.44	0.48
3:L:8:PRO:O	3:L:10:SER:N	2.46	0.48
3:L:150:LYS:O	3:L:203:HIS:NE2	2.46	0.48
3:M:156:ASP:OD1	3:M:197:TYR:CD1	2.67	0.48
2:J:184:VAL:O	2:J:185:LEU:HD23	2.13	0.48
3:N:201:VAL:CG2	3:N:210:VAL:HB	2.44	0.48
1:A:1097:SER:C	1:A:1099:GLY:H	2.22	0.47
1:B:75:GLY:O	1:B:76:THR:O	2.32	0.47
1:B:449:TYR:N	1:B:495:TYR:O	2.47	0.47
1:B:746:SER:OG	1:B:748:GLU:OE2	2.31	0.47
1:C:456:PHE:CB	1:C:457:ARG:NH1	2.73	0.47
2:J:169:TRP:CE3	2:J:211:CYS:HA	2.49	0.47
3:N:8:PRO:O	3:N:10:SER:N	2.46	0.47
1:A:449:TYR:CG	1:A:497:PHE:HD2	2.28	0.47
1:B:736:VAL:O	1:B:764:ASN:ND2	2.47	0.47
1:C:122:ASN:O	1:C:124:THR:N	2.40	0.47
1:C:457:ARG:CZ	1:C:489:TYR:CD2	2.97	0.47
3:L:123:PHE:O	3:L:137:VAL:HG23	2.13	0.47
3:L:143:ASN:CG	3:L:177:THR:CG2	2.80	0.47
3:M:196:VAL:O	3:M:196:VAL:HG12	2.14	0.47
2:J:142:SER:CB	2:J:145:SER:HB2	2.44	0.47
2:J:185:LEU:HD21	2:J:191:TYR:OH	2.13	0.47
1:B:722:VAL:HG12	1:B:1065:VAL:HG22	1.96	0.47
1:C:179:LEU:HD23	1:C:180:GLU:C	2.40	0.47
2:I:169:TRP:CE3	2:I:211:CYS:HA	2.49	0.47
3:M:123:PHE:O	3:M:137:VAL:HG23	2.13	0.47
1:A:858:LEU:HD13	1:A:959:LEU:HD22	1.95	0.47
1:B:430:THR:OG1	1:B:431:GLY:N	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:55:ASP:HB3	2:H:57:GLU:CG	2.44	0.47
3:L:201:VAL:CG2	3:L:210:VAL:HB	2.44	0.47
1:B:24:LEU:N	1:B:24:LEU:CD1	2.73	0.47
1:B:51:THR:O	1:B:274:THR:HG23	2.14	0.47
1:B:179:LEU:C	1:B:179:LEU:CD2	2.86	0.47
1:C:470:THR:CG2	1:C:471:GLU:H	2.27	0.47
1:C:578:ASP:OD1	1:C:578:ASP:N	2.47	0.47
3:L:56:ILE:CG2	3:L:57:SER:N	2.40	0.47
2:J:53:PRO:HD2	2:J:113:TYR:CE1	2.49	0.47
3:N:10:SER:C	3:N:11:SER:HG	2.02	0.47
3:N:56:ILE:CG2	3:N:57:SER:N	2.40	0.47
1:A:23:GLN:CD	1:A:24:LEU:N	2.73	0.47
1:A:122:ASN:O	1:A:124:THR:N	2.40	0.47
1:A:605:SER:OG	1:A:606:ASN:N	2.47	0.47
1:A:808:ASP:OD2	1:A:810:SER:OG	2.33	0.47
1:A:825:LYS:HZ1	1:A:944:ALA:CB	2.24	0.47
1:B:26:PRO:O	1:B:28:TYR:CD1	2.67	0.47
1:B:248:TYR:O	1:B:250:THR:N	2.43	0.47
1:B:289:VAL:CG2	1:B:306:PHE:CE2	2.97	0.47
1:B:457:ARG:C	1:B:458:LYS:CG	2.86	0.47
2:H:11:VAL:HG11	2:H:161:PHE:CE2	2.47	0.47
2:J:52:ASP:CB	3:N:99:PHE:HE1	2.25	0.47
2:J:55:ASP:HB3	2:J:57:GLU:CG	2.44	0.47
2:J:141:PRO:HG2	2:J:228:PRO:CB	2.44	0.47
3:N:120:VAL:HG22	3:N:201:VAL:HG21	1.96	0.47
1:A:75:GLY:O	1:A:76:THR:O	2.32	0.47
1:A:318:PHE:HZ	1:A:620:VAL:O	1.90	0.47
1:A:358:ILE:HB	1:A:395:VAL:HB	1.95	0.47
1:A:389:ASP:OD1	1:A:389:ASP:N	2.46	0.47
1:B:23:GLN:CD	1:B:24:LEU:N	2.73	0.47
1:B:179:LEU:HD23	1:B:180:GLU:C	2.40	0.47
1:B:272:PRO:O	1:B:273:ARG:HG3	2.15	0.47
1:B:457:ARG:HA	1:B:473:TYR:CE2	2.49	0.47
1:B:867:ASP:OD1	1:B:867:ASP:N	2.48	0.47
1:C:616:ASN:C	1:C:618:THR:N	2.73	0.47
2:H:227:GLU:OE1	2:H:227:GLU:N	2.46	0.47
3:L:124:PRO:HG3	3:L:214:PHE:CE1	2.49	0.47
3:L:196:VAL:O	3:L:196:VAL:HG12	2.14	0.47
2:I:52:ASP:CB	3:M:99:PHE:HE1	2.25	0.47
2:I:142:SER:CB	2:I:145:SER:HB2	2.44	0.47
2:I:186:GLN:OE1	2:I:191:TYR:O	2.32	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:120:VAL:HG22	3:M:201:VAL:HG21	1.96	0.47
3:M:122:ILE:HG22	3:M:213:SER:CA	2.42	0.47
3:M:150:LYS:O	3:M:203:HIS:NE2	2.46	0.47
3:N:14:THR:HA	3:N:112:LYS:HB3	1.96	0.47
3:N:157:ASN:O	3:N:158:ALA:HB2	2.13	0.47
1:B:167:THR:O	1:B:168:PHE:HB2	2.14	0.47
1:B:220:PHE:HZ	1:B:288:ALA:H	1.49	0.47
1:C:23:GLN:CD	1:C:24:LEU:N	2.73	0.47
1:C:24:LEU:N	1:C:24:LEU:CD1	2.73	0.47
3:N:144:PHE:CE2	3:N:203:HIS:CD2	3.00	0.47
3:N:169:THR:HG23	3:N:179:SER:H	1.77	0.47
1:A:333:THR:O	1:A:334:ASN:HB2	2.14	0.47
1:A:335:LEU:O	1:A:336:CYS:HB3	2.15	0.47
1:B:277:LEU:HB3	1:B:285:ILE:HG12	1.97	0.47
1:C:293:LEU:C	1:C:293:LEU:HD12	2.40	0.47
3:L:144:PHE:CZ	3:L:203:HIS:HB3	2.40	0.47
3:L:144:PHE:CE2	3:L:203:HIS:CD2	3.00	0.47
3:M:203:HIS:CD2	3:M:203:HIS:N	2.83	0.47
3:N:138:VAL:C	3:N:153:TRP:HH2	2.21	0.47
1:A:703:ASN:ND2	1:B:787:GLN:OE1	2.48	0.47
1:A:812:PRO:C	1:A:814:LYS:H	2.22	0.47
1:B:57:PRO:HG3	1:B:271:GLN:NE2	2.30	0.47
3:L:122:ILE:HG22	3:L:213:SER:CA	2.42	0.47
3:M:4:MET:O	3:M:5:THR:CG2	2.62	0.47
1:A:22:THR:CB	1:A:78:ARG:CZ	2.93	0.46
1:A:813:SER:O	1:A:814:LYS:HB2	2.15	0.46
1:A:916:LEU:HD12	1:A:923:ILE:HD13	1.97	0.46
1:C:22:THR:CB	1:C:78:ARG:CZ	2.93	0.46
2:H:52:ASP:CB	3:L:99:PHE:HE1	2.25	0.46
2:H:53:PRO:HD2	2:H:113:TYR:CE1	2.49	0.46
2:H:141:PRO:HG2	2:H:228:PRO:CB	2.45	0.46
2:I:167:VAL:C	2:I:169:TRP:N	2.73	0.46
2:I:181:PHE:HD2	3:M:167:SER:O	1.89	0.46
2:I:227:GLU:OE1	2:I:227:GLU:N	2.46	0.46
2:J:167:VAL:C	2:J:169:TRP:N	2.73	0.46
3:N:6:GLN:HG2	3:N:105:GLN:HB3	1.97	0.46
3:N:196:VAL:O	3:N:196:VAL:HG12	2.14	0.46
4:d:1:NAG:H61	4:d:2:NAG:H82	1.98	0.46
1:A:48:LEU:HD23	1:A:276:LEU:HG	1.96	0.46
1:B:393:THR:O	1:B:523:THR:OG1	2.32	0.46
1:C:22:THR:C	1:C:23:GLN:HG3	2.40	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:167:THR:O	1:C:168:PHE:HB2	2.14	0.46
1:C:856:ASN:N	1:C:856:ASN:OD1	2.48	0.46
2:H:169:TRP:CE3	2:H:169:TRP:CA	2.97	0.46
3:L:25:SER:HB3	3:L:74:THR:HG23	1.96	0.46
2:I:52:ASP:C	2:I:54:GLU:N	2.73	0.46
2:I:53:PRO:HD2	2:I:113:TYR:CE1	2.49	0.46
2:I:169:TRP:CE3	2:I:169:TRP:CA	2.97	0.46
3:M:25:SER:HB3	3:M:74:THR:HG23	1.96	0.46
3:M:144:PHE:CE1	3:M:203:HIS:CB	2.94	0.46
1:A:517:LEU:CD2	1:A:519:HIS:CB	2.85	0.46
1:A:642:VAL:HG22	1:A:651:ILE:HG12	1.96	0.46
1:B:282:ASN:CG	5:V:1:NAG:C1	2.72	0.46
2:I:185:LEU:HD21	2:I:191:TYR:OH	2.13	0.46
1:A:179:LEU:HD23	1:A:180:GLU:C	2.40	0.46
1:A:299:THR:O	1:A:303:LEU:HD13	2.15	0.46
1:A:900:MET:HB3	1:A:900:MET:HE2	1.82	0.46
1:B:312:ILE:HG23	1:B:312:ILE:O	2.15	0.46
1:C:20:THR:OG1	1:C:21:ARG:N	2.48	0.46
1:C:75:GLY:O	1:C:76:THR:O	2.32	0.46
1:C:674:TYR:HE1	1:C:691:SER:N	2.12	0.46
3:L:4:MET:O	3:L:5:THR:CG2	2.62	0.46
2:J:141:PRO:HG2	2:J:228:PRO:HB3	1.96	0.46
1:A:516:GLU:C	1:A:518:LEU:N	2.73	0.46
1:B:57:PRO:CB	1:B:273:ARG:NH2	2.78	0.46
1:B:293:LEU:C	1:B:293:LEU:HD12	2.40	0.46
1:C:19:THR:C	1:C:20:THR:HG1	2.05	0.46
1:C:662:CYS:HB3	1:C:697:MET:HG2	1.98	0.46
2:J:164:PRO:O	2:J:165:VAL:HB	2.15	0.46
1:A:220:PHE:CE2	1:A:287:ASP:OD1	2.69	0.46
1:A:276:LEU:HD22	1:A:289:VAL:HG11	1.92	0.46
1:A:517:LEU:C	1:A:519:HIS:N	2.73	0.46
1:B:415:THR:OG1	1:B:416:GLY:N	2.47	0.46
1:C:457:ARG:C	1:C:459:SER:N	2.73	0.46
1:C:560:LEU:O	1:C:562:PHE:N	2.46	0.46
1:C:605:SER:OG	1:C:606:ASN:N	2.49	0.46
2:H:161:PHE:C	2:H:163:GLU:N	2.74	0.46
3:L:66:ARG:NH1	3:L:87:ASP:OD2	2.39	0.46
3:L:203:HIS:CD2	3:L:203:HIS:N	2.83	0.46
2:I:181:PHE:HB3	2:I:182:PRO:CD	2.45	0.46
3:N:7:SER:CB	3:N:8:PRO:CD	2.84	0.46
3:N:25:SER:HB3	3:N:74:THR:HG23	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:66:ARG:NH1	3:N:84:GLU:OE1	2.49	0.46
3:N:156:ASP:CG	3:N:194:HIS:CE1	2.94	0.46
1:B:20:THR:OG1	1:B:21:ARG:N	2.48	0.46
1:B:111:ASP:OD1	1:B:134:GLN:NE2	2.37	0.46
1:C:662:CYS:HB2	1:C:671:CYS:HB3	1.80	0.46
3:L:142:ASN:O	3:L:143:ASN:HB2	2.16	0.46
2:I:141:PRO:HG3	2:I:228:PRO:CG	2.46	0.46
2:I:164:PRO:O	2:I:165:VAL:HB	2.15	0.46
3:M:144:PHE:CE2	3:M:203:HIS:CD2	3.00	0.46
2:J:63:LYS:HB3	2:J:63:LYS:HE2	1.60	0.46
3:N:2:ILE:HG21	3:N:4:MET:HE2	1.80	0.46
3:N:142:ASN:O	3:N:143:ASN:HB2	2.16	0.46
1:A:20:THR:OG1	1:A:21:ARG:N	2.48	0.46
1:A:22:THR:C	1:A:23:GLN:HG3	2.41	0.46
1:A:392:PHE:HD2	1:A:515:PHE:CB	2.29	0.46
1:A:707:TYR:HB3	1:B:792:PRO:HG3	1.98	0.46
1:B:22:THR:CB	1:B:78:ARG:CZ	2.93	0.46
1:B:50:SER:O	1:B:51:THR:HG22	2.15	0.46
2:H:73:ASP:OD1	2:H:76:THR:OG1	2.31	0.46
2:H:164:PRO:O	2:H:165:VAL:HB	2.15	0.46
3:L:118:PRO:CD	3:L:206:LEU:CD2	2.73	0.46
3:M:6:GLN:HG2	3:M:105:GLN:HB3	1.97	0.46
2:J:52:ASP:C	2:J:54:GLU:N	2.74	0.46
2:J:161:PHE:C	2:J:163:GLU:H	2.24	0.46
4:E:1:NAG:H61	4:E:2:NAG:H82	1.98	0.46
1:B:391:CYS:HB3	1:B:525:CYS:HB2	1.41	0.46
1:C:23:GLN:CD	1:C:23:GLN:N	2.73	0.46
1:C:280:ASN:N	1:C:284:THR:O	2.49	0.46
2:H:141:PRO:C	2:H:142:SER:OG	2.59	0.46
3:L:156:ASP:CG	3:L:194:HIS:CE1	2.94	0.46
2:I:170:ASN:O	2:I:212:ASN:ND2	2.49	0.46
2:I:183:ALA:O	2:I:184:VAL:HB	2.16	0.46
3:M:66:ARG:NH1	3:M:84:GLU:OE1	2.49	0.46
1:A:23:GLN:CD	1:A:23:GLN:N	2.73	0.46
1:A:826:VAL:C	1:A:828:LEU:N	2.73	0.46
1:B:23:GLN:CD	1:B:23:GLN:N	2.73	0.46
2:H:140:ALA:HB1	2:H:229:LYS:CG	2.46	0.46
1:A:293:LEU:C	1:A:293:LEU:HD12	2.40	0.45
1:A:392:PHE:CE1	1:A:518:LEU:CD2	2.95	0.45
1:B:22:THR:C	1:B:23:GLN:HG3	2.41	0.45
1:B:313:TYR:N	1:B:313:TYR:CD1	2.83	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:452:LEU:HD21	1:B:494:SER:OG	2.16	0.45
1:C:720:ILE:HD11	1:C:927:PHE:HB2	1.98	0.45
2:I:140:ALA:CB	2:I:229:LYS:HD2	2.16	0.45
2:J:170:ASN:O	2:J:212:ASN:ND2	2.49	0.45
3:N:8:PRO:C	3:N:10:SER:H	2.24	0.45
3:N:66:ARG:NH1	3:N:87:ASP:OD2	2.39	0.45
3:N:118:PRO:CD	3:N:206:LEU:HD21	2.31	0.45
1:A:393:THR:HG23	1:A:518:LEU:CB	2.39	0.45
1:A:812:PRO:C	1:A:814:LYS:N	2.73	0.45
1:B:50:SER:C	1:B:51:THR:HG23	2.42	0.45
1:C:44:ARG:O	1:C:283:GLY:HA2	2.17	0.45
1:C:58:PHE:CE2	1:C:290:ASP:HB2	2.50	0.45
3:L:5:THR:C	3:L:6:GLN:HG2	2.42	0.45
3:L:104:GLY:C	3:L:106:GLY:N	2.75	0.45
3:M:156:ASP:CG	3:M:194:HIS:CE1	2.94	0.45
2:J:45:LEU:HD23	3:N:103:PHE:HE2	1.80	0.45
2:J:141:PRO:HG3	2:J:228:PRO:CG	2.46	0.45
2:J:179:HIS:CB	3:N:179:SER:OG	2.65	0.45
2:J:181:PHE:HB3	2:J:182:PRO:CD	2.45	0.45
3:N:122:ILE:HG22	3:N:213:SER:CA	2.42	0.45
1:A:390:LEU:CG	1:A:391:CYS:N	2.73	0.45
1:A:1144:GLU:C	1:A:1146:ASP:N	2.73	0.45
2:H:170:ASN:O	2:H:212:ASN:ND2	2.49	0.45
2:I:141:PRO:C	2:I:142:SER:OG	2.59	0.45
3:M:139:CYS:HB3	3:M:153:TRP:CZ2	2.52	0.45
2:J:55:ASP:C	2:J:57:GLU:N	2.74	0.45
3:N:118:PRO:CB	3:N:144:PHE:CE2	2.97	0.45
3:N:144:PHE:CZ	3:N:203:HIS:HB3	2.40	0.45
1:A:565:PHE:O	1:B:42:VAL:HA	2.17	0.45
1:B:277:LEU:N	1:B:277:LEU:HD22	2.32	0.45
1:C:248:TYR:O	1:C:250:THR:N	2.43	0.45
2:H:183:ALA:O	2:H:184:VAL:HB	2.16	0.45
2:I:134:PRO:HB2	2:I:136:VAL:HG23	1.99	0.45
2:I:166:THR:C	2:I:167:VAL:CG2	2.81	0.45
3:N:5:THR:C	3:N:6:GLN:HG2	2.42	0.45
3:N:216:ARG:NH1	3:N:216:ARG:CG	2.80	0.45
1:A:143:VAL:HG12	1:A:152:TRP:HE3	1.82	0.45
1:B:46:SER:C	1:B:47:VAL:HG13	2.42	0.45
2:H:161:PHE:C	2:H:163:GLU:H	2.24	0.45
3:L:66:ARG:NH1	3:L:84:GLU:OE1	2.49	0.45
3:L:150:LYS:O	3:L:202:THR:O	2.35	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:150:LYS:O	3:M:202:THR:O	2.35	0.45
3:M:170:GLU:C	3:M:178:TYR:CD1	2.95	0.45
2:J:184:VAL:H	2:J:191:TYR:HD1	1.64	0.45
3:N:118:PRO:CD	3:N:206:LEU:CD2	2.73	0.45
3:N:139:CYS:HB3	3:N:153:TRP:CZ2	2.52	0.45
3:N:170:GLU:C	3:N:178:TYR:CE1	2.95	0.45
1:B:73:THR:CG2	1:B:74:ASN:N	2.80	0.45
1:B:182:LYS:HD3	1:B:182:LYS:HA	1.85	0.45
1:B:276:LEU:CD1	1:B:289:VAL:HG21	2.12	0.45
3:L:4:MET:C	3:L:5:THR:HG23	2.42	0.45
3:L:6:GLN:HG2	3:L:105:GLN:HB3	1.97	0.45
3:L:8:PRO:C	3:L:10:SER:H	2.24	0.45
2:I:7:SER:OG	2:I:21:SER:O	2.33	0.45
2:I:161:PHE:C	2:I:163:GLU:H	2.24	0.45
2:I:210:ILE:HD12	2:I:225:LYS:HD2	1.99	0.45
3:M:216:ARG:HH11	3:M:216:ARG:CG	2.23	0.45
2:J:169:TRP:CE3	2:J:169:TRP:CA	2.97	0.45
1:A:303:LEU:HD12	1:A:303:LEU:N	2.31	0.45
1:A:393:THR:HG21	1:A:518:LEU:C	2.42	0.45
1:A:1141:LEU:HA	1:A:1141:LEU:HD23	1.81	0.45
1:B:776:LYS:HE3	1:B:776:LYS:HB3	1.80	0.45
2:H:134:PRO:HB2	2:H:136:VAL:HG23	1.99	0.45
3:L:170:GLU:C	3:L:178:TYR:CE1	2.95	0.45
2:I:55:ASP:C	2:I:57:GLU:N	2.74	0.45
2:I:161:PHE:C	2:I:163:GLU:N	2.74	0.45
3:M:169:THR:OG1	3:M:170:GLU:N	2.50	0.45
3:M:170:GLU:C	3:M:178:TYR:CE1	2.95	0.45
2:J:161:PHE:C	2:J:163:GLU:N	2.74	0.45
4:T:1:NAG:H61	4:T:2:NAG:H82	1.98	0.45
1:A:38:TYR:HD2	1:C:562:PHE:CZ	2.35	0.45
1:A:43:PHE:CD2	1:C:559:PHE:CD1	3.04	0.45
1:B:310:LYS:HB2	1:B:310:LYS:HE3	1.68	0.45
1:C:597:VAL:HG12	1:C:610:VAL:HG22	1.99	0.45
1:C:827:THR:O	1:C:828:LEU:HD12	2.14	0.45
2:H:179:HIS:CB	3:L:179:SER:OG	2.65	0.45
3:L:156:ASP:CB	3:L:194:HIS:ND1	2.80	0.45
2:I:141:PRO:HG2	2:I:229:LYS:N	2.32	0.45
3:M:138:VAL:C	3:M:153:TRP:HH2	2.21	0.45
2:J:141:PRO:C	2:J:142:SER:OG	2.59	0.45
3:N:31:HIS:HB2	3:N:97:THR:HG21	1.99	0.45
3:N:203:HIS:CD2	3:N:203:HIS:N	2.83	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:143:VAL:HG12	1:B:152:TRP:HE3	1.82	0.45
1:B:280:ASN:N	1:B:284:THR:O	2.49	0.45
1:C:456:PHE:HD2	1:C:491:PRO:CA	2.19	0.45
2:H:141:PRO:HG2	2:H:229:LYS:H	1.82	0.45
2:H:151:ALA:HB3	2:H:199:VAL:HG23	1.99	0.45
3:L:118:PRO:HG2	3:L:206:LEU:HD12	1.91	0.45
3:L:170:GLU:C	3:L:178:TYR:CD1	2.95	0.45
2:I:179:HIS:CB	3:M:179:SER:OG	2.65	0.45
3:M:171:GLN:N	3:M:178:TYR:CE1	2.85	0.45
2:J:134:PRO:HB2	2:J:136:VAL:HG23	1.99	0.45
2:J:140:ALA:HB1	2:J:229:LYS:CG	2.46	0.45
2:J:183:ALA:O	2:J:184:VAL:HB	2.16	0.45
3:N:104:GLY:C	3:N:106:GLY:N	2.75	0.45
1:A:22:THR:CG2	1:A:78:ARG:HG2	2.31	0.45
1:A:179:LEU:C	1:A:179:LEU:CD2	2.86	0.45
1:A:422:ASN:HD21	1:A:454:ARG:HA	1.81	0.45
2:H:52:ASP:C	2:H:54:GLU:N	2.74	0.45
2:H:210:ILE:HD12	2:H:225:LYS:HD2	1.99	0.45
2:I:140:ALA:HB1	2:I:229:LYS:CG	2.46	0.45
2:I:165:VAL:CG1	2:I:166:THR:N	2.73	0.45
3:M:120:VAL:CG2	3:M:201:VAL:CG2	2.95	0.45
3:N:150:LYS:O	3:N:202:THR:O	2.35	0.45
3:N:170:GLU:C	3:N:178:TYR:CD1	2.95	0.45
1:A:73:THR:CG2	1:A:74:ASN:N	2.80	0.44
1:A:403:ARG:NH2	1:A:505:TYR:CE1	2.85	0.44
1:B:86:PHE:O	1:B:86:PHE:CD1	2.70	0.44
1:B:425:LEU:HD23	1:B:425:LEU:HA	1.86	0.44
1:C:143:VAL:HG12	1:C:152:TRP:HE3	1.82	0.44
1:C:182:LYS:O	1:C:183:GLN:C	2.60	0.44
1:C:248:TYR:HD1	1:C:248:TYR:HA	1.68	0.44
1:C:558:LYS:CG	5:G:1:NAG:O7	2.55	0.44
3:L:99:PHE:O	3:L:101:TYR:CD1	2.70	0.44
2:I:45:LEU:HD23	3:M:103:PHE:HE2	1.80	0.44
3:M:56:ILE:CG2	3:M:57:SER:N	2.40	0.44
1:A:182:LYS:O	1:A:183:GLN:C	2.60	0.44
1:C:73:THR:CG2	1:C:74:ASN:N	2.80	0.44
1:C:614:ASP:C	1:C:615:VAL:HG23	2.42	0.44
1:C:900:MET:HE2	1:C:900:MET:HB3	1.73	0.44
2:H:184:VAL:H	2:H:191:TYR:HD1	1.64	0.44
3:L:105:GLN:HB3	3:L:105:GLN:HE21	1.62	0.44
3:L:139:CYS:HB3	3:L:153:TRP:CZ2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:210:VAL:CG1	3:L:211:THR:N	2.43	0.44
2:I:169:TRP:HE3	2:I:211:CYS:HA	1.82	0.44
3:M:5:THR:C	3:M:6:GLN:HG2	2.42	0.44
3:M:139:CYS:HB3	3:M:153:TRP:CH2	2.52	0.44
3:M:201:VAL:HG22	3:M:210:VAL:HB	2.00	0.44
3:N:120:VAL:CG2	3:N:201:VAL:CG2	2.95	0.44
1:A:86:PHE:CD1	1:A:86:PHE:O	2.70	0.44
1:A:303:LEU:N	1:A:303:LEU:CD1	2.79	0.44
1:C:455:LEU:O	1:C:456:PHE:CG	2.70	0.44
2:H:141:PRO:HG3	2:H:228:PRO:CG	2.46	0.44
3:L:2:ILE:CG2	3:L:3:VAL:H	2.30	0.44
3:L:6:GLN:HE21	3:L:106:GLY:N	2.15	0.44
2:I:141:PRO:HG2	2:I:229:LYS:H	1.82	0.44
2:I:160:TYR:CG	2:I:162:PRO:HD3	2.51	0.44
2:I:161:PHE:CD2	2:I:161:PHE:O	2.70	0.44
2:J:141:PRO:HG2	2:J:229:LYS:H	1.82	0.44
2:J:141:PRO:HG2	2:J:229:LYS:N	2.32	0.44
2:J:161:PHE:CD2	2:J:161:PHE:O	2.71	0.44
3:N:118:PRO:HG2	3:N:206:LEU:HD12	1.91	0.44
3:N:156:ASP:CB	3:N:194:HIS:ND1	2.80	0.44
3:N:171:GLN:N	3:N:178:TYR:CE1	2.85	0.44
1:A:80:ASP:C	1:A:82:PRO:HD3	2.36	0.44
1:A:453:TYR:HE2	1:A:495:TYR:OH	2.01	0.44
1:B:182:LYS:O	1:B:183:GLN:C	2.60	0.44
1:C:455:LEU:O	1:C:456:PHE:CD1	2.70	0.44
2:H:161:PHE:O	2:H:161:PHE:CG	2.70	0.44
2:I:161:PHE:O	2:I:161:PHE:CG	2.70	0.44
2:I:184:VAL:H	2:I:191:TYR:HD1	1.64	0.44
3:M:142:ASN:O	3:M:143:ASN:HB2	2.16	0.44
3:M:156:ASP:CB	3:M:194:HIS:ND1	2.80	0.44
3:N:120:VAL:CB	3:N:210:VAL:CG1	2.85	0.44
1:B:179:LEU:CD2	1:B:180:GLU:N	2.79	0.44
2:H:161:PHE:O	2:H:161:PHE:CD2	2.70	0.44
2:H:185:LEU:O	2:H:186:GLN:O	2.36	0.44
1:A:170:TYR:CE1	1:A:172:SER:HB2	2.53	0.44
1:B:379:CYS:HA	1:B:432:CYS:HA	2.00	0.44
1:B:453:TYR:O	1:B:453:TYR:CD1	2.70	0.44
1:C:48:LEU:HD23	1:C:276:LEU:HG	1.96	0.44
2:H:182:PRO:O	2:H:183:ALA:C	2.60	0.44
3:L:201:VAL:HG22	3:L:210:VAL:HB	2.00	0.44
3:M:6:GLN:HE21	3:M:106:GLY:N	2.15	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:37:TYR:HB3	3:M:96:ALA:HB3	1.99	0.44
3:N:2:ILE:CG2	3:N:3:VAL:H	2.30	0.44
3:N:6:GLN:HE21	3:N:106:GLY:N	2.15	0.44
1:A:23:GLN:O	1:A:24:LEU:HD22	2.16	0.44
2:H:132:LYS:HG2	2:H:133:GLY:N	2.33	0.44
3:L:31:HIS:HB2	3:L:97:THR:HG21	1.99	0.44
3:L:169:THR:HG23	3:L:179:SER:H	1.77	0.44
3:M:2:ILE:CG2	3:M:3:VAL:H	2.30	0.44
3:M:99:PHE:O	3:M:101:TYR:CD1	2.70	0.44
2:J:210:ILE:HD12	2:J:225:LYS:HD2	1.99	0.44
3:N:11:SER:O	3:N:13:VAL:N	2.51	0.44
1:A:717:ASN:HD22	1:A:1071:GLN:HE21	1.66	0.44
1:A:856:ASN:OD1	1:A:856:ASN:N	2.51	0.44
1:B:1116:THR:OG1	1:B:1118:ASP:OD1	2.23	0.44
2:H:141:PRO:HG2	2:H:229:LYS:N	2.32	0.44
2:I:142:SER:OG	2:I:145:SER:HB2	2.18	0.44
2:I:181:PHE:CD2	3:M:181:SER:OG	2.63	0.44
3:M:11:SER:O	3:M:13:VAL:N	2.51	0.44
2:J:54:GLU:OE2	2:J:111:TYR:CE2	2.71	0.44
2:J:161:PHE:O	2:J:161:PHE:CG	2.70	0.44
3:N:99:PHE:O	3:N:101:TYR:CD1	2.70	0.44
1:A:99:ASN:N	1:A:99:ASN:OD1	2.51	0.44
1:A:187:LYS:HA	1:A:187:LYS:HD3	1.83	0.44
1:B:164:ASN:O	1:B:165:ASN:HB2	2.18	0.44
1:C:86:PHE:CD1	1:C:86:PHE:O	2.71	0.44
1:C:164:ASN:O	1:C:165:ASN:HB2	2.18	0.44
2:H:210:ILE:HB	2:H:225:LYS:HD2	2.00	0.44
3:L:10:SER:C	3:L:11:SER:HG	2.05	0.44
3:L:11:SER:O	3:L:13:VAL:N	2.51	0.44
3:L:169:THR:OG1	3:L:170:GLU:N	2.50	0.44
3:L:171:GLN:N	3:L:178:TYR:CE1	2.85	0.44
3:L:201:VAL:HB	3:L:203:HIS:CD2	2.44	0.44
3:M:122:ILE:HG13	3:M:123:PHE:N	2.33	0.44
2:J:142:SER:OG	2:J:145:SER:HB2	2.18	0.44
2:J:151:ALA:HB3	2:J:199:VAL:HG23	1.99	0.44
2:J:185:LEU:O	2:J:186:GLN:O	2.36	0.44
3:N:122:ILE:HG13	3:N:123:PHE:N	2.33	0.44
1:A:21:ARG:HE	1:A:21:ARG:HB3	1.65	0.43
1:A:106:PHE:HD2	1:A:117:LEU:HD23	1.83	0.43
1:A:334:ASN:O	1:A:335:LEU:HB2	2.17	0.43
1:B:22:THR:CG2	1:B:78:ARG:HG2	2.31	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:289:VAL:CG2	1:B:306:PHE:CZ	3.00	0.43
1:C:457:ARG:NH2	1:C:489:TYR:CD1	2.79	0.43
1:C:675:GLN:HG3	1:C:675:GLN:O	2.17	0.43
2:H:55:ASP:HB3	2:H:57:GLU:HG3	2.00	0.43
3:L:120:VAL:CG2	3:L:201:VAL:CG2	2.95	0.43
2:I:141:PRO:HG2	2:I:228:PRO:HB3	1.96	0.43
3:M:4:MET:C	3:M:5:THR:HG23	2.42	0.43
3:M:31:HIS:HB2	3:M:97:THR:HG21	1.99	0.43
2:J:160:TYR:CG	2:J:162:PRO:HD3	2.51	0.43
3:N:37:TYR:HB3	3:N:96:ALA:HB3	1.99	0.43
1:A:357:ARG:HH12	1:B:167:THR:HB	1.83	0.43
2:H:154:GLY:HA3	2:H:196:VAL:HA	2.00	0.43
2:H:169:TRP:HE3	2:H:211:CYS:HA	1.82	0.43
3:L:37:TYR:HB3	3:L:96:ALA:HB3	1.99	0.43
3:L:122:ILE:HG13	3:L:123:PHE:N	2.33	0.43
2:I:132:LYS:HG2	2:I:133:GLY:N	2.33	0.43
2:I:154:GLY:HA3	2:I:196:VAL:HA	2.00	0.43
3:M:118:PRO:HG2	3:M:206:LEU:HD12	1.91	0.43
2:J:184:VAL:HG22	2:J:185:LEU:H	1.75	0.43
3:N:169:THR:OG1	3:N:170:GLU:N	2.50	0.43
3:N:195:LYS:O	3:N:197:TYR:CD2	2.71	0.43
1:A:438:SER:O	1:A:507:PRO:HG2	2.18	0.43
1:B:170:TYR:CE1	1:B:172:SER:HB2	2.53	0.43
1:B:300:LYS:CE	1:B:306:PHE:O	2.67	0.43
2:H:52:ASP:CG	3:L:99:PHE:HE1	2.26	0.43
3:M:8:PRO:C	3:M:10:SER:H	2.24	0.43
3:M:104:GLY:C	3:M:106:GLY:N	2.75	0.43
2:J:141:PRO:HB2	2:J:142:SER:H	1.72	0.43
3:N:2:ILE:C	3:N:3:VAL:HG13	2.35	0.43
1:A:334:ASN:C	1:A:336:CYS:N	2.75	0.43
1:A:574:ASP:O	1:A:587:ILE:N	2.50	0.43
1:A:1142:GLN:NE2	1:A:1142:GLN:CA	2.73	0.43
1:B:106:PHE:HD2	1:B:117:LEU:HD23	1.83	0.43
1:B:900:MET:HE2	1:B:900:MET:HB3	1.88	0.43
3:L:118:PRO:CB	3:L:144:PHE:CE2	2.97	0.43
2:I:210:ILE:HB	2:I:225:LYS:HD2	2.00	0.43
3:M:144:PHE:CZ	3:M:203:HIS:HB3	2.40	0.43
2:J:169:TRP:HE3	2:J:211:CYS:HA	1.82	0.43
3:N:177:THR:HB	3:N:178:TYR:H	1.68	0.43
1:B:23:GLN:O	1:B:24:LEU:HD22	2.16	0.43
1:B:418:ILE:HD12	1:B:422:ASN:HD22	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:106:PHE:HD2	1:C:117:LEU:HD23	1.83	0.43
2:H:141:PRO:HG2	2:H:228:PRO:HB3	1.96	0.43
3:L:177:THR:HB	3:L:178:TYR:H	1.68	0.43
2:J:59:MET:CB	3:N:99:PHE:CD2	2.98	0.43
2:J:182:PRO:O	2:J:183:ALA:C	2.60	0.43
3:N:139:CYS:CB	3:N:153:TRP:CZ2	3.01	0.43
1:C:170:TYR:CE1	1:C:172:SER:HB2	2.53	0.43
3:L:13:VAL:C	3:L:112:LYS:HB2	2.43	0.43
3:L:120:VAL:CG2	3:L:210:VAL:HB	2.33	0.43
2:I:54:GLU:OE2	2:I:111:TYR:CE2	2.71	0.43
2:I:184:VAL:HG22	2:I:185:LEU:H	1.75	0.43
3:M:112:LYS:HG3	3:M:112:LYS:O	2.18	0.43
3:M:139:CYS:CB	3:M:153:TRP:CZ2	3.01	0.43
1:B:21:ARG:HG2	1:B:22:THR:H	1.83	0.43
1:B:21:ARG:HE	1:B:21:ARG:HB3	1.65	0.43
1:B:70:VAL:HG22	1:B:71:SER:N	2.33	0.43
1:B:111:ASP:OD2	1:B:113:LYS:NZ	2.52	0.43
1:B:113:LYS:HE2	1:B:113:LYS:HB2	1.90	0.43
1:C:70:VAL:HG22	1:C:71:SER:N	2.33	0.43
3:L:139:CYS:HB3	3:L:153:TRP:CH2	2.52	0.43
2:I:151:ALA:HB3	2:I:199:VAL:HG23	1.99	0.43
2:J:52:ASP:CG	3:N:99:PHE:HE1	2.26	0.43
2:J:204:LEU:CD1	2:J:228:PRO:HG3	2.41	0.43
2:J:227:GLU:OE1	2:J:227:GLU:N	2.46	0.43
1:A:164:ASN:O	1:A:165:ASN:HB2	2.18	0.43
1:A:574:ASP:OD1	1:A:574:ASP:N	2.43	0.43
1:C:285:ILE:O	1:C:285:ILE:HG22	2.19	0.43
3:L:50:ARG:HB2	3:L:51:LEU:H	1.68	0.43
3:L:99:PHE:CB	3:L:100:PRO:CD	2.97	0.43
3:L:143:ASN:ND2	3:L:177:THR:HG21	2.33	0.43
2:I:52:ASP:CG	3:M:99:PHE:HE1	2.26	0.43
2:I:182:PRO:O	2:I:183:ALA:C	2.60	0.43
2:I:185:LEU:O	2:I:186:GLN:O	2.36	0.43
3:M:143:ASN:ND2	3:M:177:THR:HG21	2.33	0.43
2:J:210:ILE:HB	2:J:225:LYS:HD2	2.00	0.43
3:N:13:VAL:C	3:N:112:LYS:HB2	2.43	0.43
1:A:126:VAL:HB	1:A:174:PRO:HA	2.01	0.43
1:A:410:ILE:HG21	1:A:433:VAL:HG11	2.01	0.43
1:B:557:LYS:HD3	1:C:43:PHE:CE2	2.50	0.43
1:B:1128:VAL:HG13	1:B:1129:VAL:N	2.34	0.43
1:C:758:SER:HB2	1:C:761:THR:HB	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:54:GLU:OE2	2:H:111:TYR:CE2	2.71	0.43
2:H:220:THR:O	2:H:220:THR:OG1	2.34	0.43
2:I:55:ASP:HB3	2:I:57:GLU:HG3	2.00	0.43
3:M:13:VAL:C	3:M:112:LYS:HB2	2.43	0.43
3:N:4:MET:C	3:N:5:THR:HG23	2.42	0.43
3:N:112:LYS:HG3	3:N:112:LYS:O	2.18	0.43
1:A:50:SER:HA	1:A:276:LEU:HA	2.00	0.43
1:A:392:PHE:CD2	1:A:515:PHE:CB	3.01	0.43
1:A:403:ARG:HD3	1:A:505:TYR:CD1	2.37	0.43
1:C:21:ARG:HG2	1:C:22:THR:H	1.84	0.43
3:L:112:LYS:HG3	3:L:112:LYS:O	2.18	0.43
3:L:195:LYS:O	3:L:197:TYR:CD2	2.71	0.43
3:M:120:VAL:HG21	3:M:201:VAL:HG22	2.01	0.43
2:J:132:LYS:HG2	2:J:133:GLY:N	2.33	0.43
3:N:201:VAL:HG22	3:N:210:VAL:HB	2.00	0.43
1:B:149:ASN:O	1:B:150:LYS:C	2.62	0.42
1:B:961:THR:HG22	1:C:762:GLN:HE21	1.80	0.42
1:C:501:ASN:O	1:C:505:TYR:CB	2.56	0.42
1:C:1139:ASP:OD1	1:C:1140:PRO:HD2	2.18	0.42
2:H:186:GLN:N	2:H:190:LEU:O	2.47	0.42
3:L:2:ILE:CD1	3:L:98:GLN:CG	2.94	0.42
3:L:149:ALA:HB1	3:L:203:HIS:HD1	1.84	0.42
2:I:163:GLU:CB	2:I:164:PRO:CD	2.86	0.42
3:M:133:GLY:H	3:M:188:LYS:HE3	1.84	0.42
2:J:55:ASP:HB3	2:J:57:GLU:HG3	2.00	0.42
2:J:73:ASP:OD1	2:J:76:THR:OG1	2.31	0.42
3:N:2:ILE:CD1	3:N:98:GLN:CG	2.94	0.42
3:N:198:ALA:HB2	3:N:213:SER:HB3	2.00	0.42
1:A:449:TYR:CG	1:A:497:PHE:HB2	2.53	0.42
1:A:517:LEU:C	1:A:519:HIS:H	2.26	0.42
1:B:21:ARG:O	1:B:22:THR:C	2.61	0.42
1:B:26:PRO:O	1:B:28:TYR:HD1	2.02	0.42
1:C:310:LYS:HB2	1:C:310:LYS:HE3	1.73	0.42
2:H:167:VAL:C	2:H:169:TRP:N	2.73	0.42
3:L:198:ALA:HB2	3:L:213:SER:HB3	2.00	0.42
3:M:120:VAL:CB	3:M:210:VAL:CG1	2.85	0.42
3:N:149:ALA:HB1	3:N:203:HIS:HD1	1.84	0.42
1:A:21:ARG:HG2	1:A:22:THR:H	1.83	0.42
1:A:43:PHE:CZ	1:C:557:LYS:HB3	2.55	0.42
1:A:70:VAL:HG22	1:A:71:SER:N	2.33	0.42
1:A:179:LEU:CD2	1:A:180:GLU:N	2.79	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:705:VAL:HB	1:B:883:THR:HG21	2.00	0.42
1:C:111:ASP:OD2	1:C:113:LYS:NZ	2.52	0.42
1:C:126:VAL:HG12	1:C:172:SER:C	2.41	0.42
3:M:195:LYS:O	3:M:197:TYR:CD2	2.71	0.42
2:J:184:VAL:C	2:J:185:LEU:HD23	2.44	0.42
3:N:133:GLY:H	3:N:188:LYS:HE3	1.84	0.42
1:A:21:ARG:O	1:A:22:THR:C	2.61	0.42
1:C:496:GLY:O	1:C:501:ASN:ND2	2.53	0.42
1:C:658:ASN:ND2	1:C:660:TYR:OH	2.47	0.42
2:J:154:GLY:HA3	2:J:196:VAL:HA	2.00	0.42
2:J:166:THR:C	2:J:167:VAL:CG2	2.81	0.42
1:A:111:ASP:OD2	1:A:113:LYS:NZ	2.52	0.42
1:A:126:VAL:HG12	1:A:172:SER:C	2.41	0.42
1:A:418:ILE:HG22	1:A:453:TYR:CD1	2.55	0.42
1:A:497:PHE:C	1:A:498:GLN:HG2	2.44	0.42
1:A:813:SER:HB2	1:A:868:GLU:HA	2.02	0.42
1:B:34:ARG:NH2	1:B:217:PRO:HG2	2.35	0.42
1:B:52:GLN:HE21	1:B:52:GLN:HB2	1.60	0.42
1:B:452:LEU:HD23	1:B:494:SER:HA	1.78	0.42
1:C:26:PRO:O	1:C:28:TYR:HD1	2.02	0.42
1:C:182:LYS:HD3	1:C:182:LYS:HA	1.85	0.42
1:C:353:TRP:CD1	1:C:353:TRP:H	2.37	0.42
1:C:1101:HIS:HD2	5:k:1:NAG:H5	1.83	0.42
2:H:142:SER:OG	2:H:145:SER:HB2	2.18	0.42
2:I:186:GLN:N	2:I:190:LEU:O	2.47	0.42
3:M:118:PRO:CB	3:M:144:PHE:CE2	2.97	0.42
3:M:210:VAL:CG1	3:M:211:THR:N	2.43	0.42
3:N:139:CYS:HB3	3:N:153:TRP:CH2	2.52	0.42
1:A:149:ASN:O	1:A:150:LYS:C	2.62	0.42
1:B:473:TYR:HB2	1:B:489:TYR:HB3	2.00	0.42
1:B:676:THR:HA	1:B:690:GLN:HA	2.01	0.42
1:C:34:ARG:NH2	1:C:217:PRO:HG2	2.35	0.42
1:C:149:ASN:O	1:C:150:LYS:C	2.62	0.42
3:L:167:SER:O	3:L:181:SER:OG	2.34	0.42
2:I:155:CYS:HB2	2:I:169:TRP:HH2	1.76	0.42
3:M:149:ALA:HB1	3:M:203:HIS:HD1	1.84	0.42
3:N:171:GLN:CG	3:N:178:TYR:CZ	2.96	0.42
1:A:391:CYS:HB2	1:A:524:VAL:C	2.45	0.42
1:A:395:VAL:HG23	1:A:524:VAL:HG21	2.02	0.42
1:A:1053:PRO:O	1:A:1054:GLN:NE2	2.52	0.42
1:A:1138:TYR:OH	1:A:1143:PRO:HG3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:21:ARG:C	1:B:22:THR:O	2.63	0.42
1:B:645:THR:OG1	1:B:646:ARG:N	2.53	0.42
1:C:50:SER:HA	1:C:276:LEU:HA	2.01	0.42
1:C:187:LYS:HA	1:C:187:LYS:HD3	1.83	0.42
3:L:216:ARG:NH1	3:L:216:ARG:CG	2.80	0.42
2:I:179:HIS:CG	3:M:179:SER:HG	2.38	0.42
1:A:48:LEU:HD23	1:A:276:LEU:CG	2.36	0.42
1:A:179:LEU:O	1:A:181:GLY:N	2.53	0.42
1:B:642:VAL:HG12	1:B:651:ILE:HG12	2.02	0.42
1:C:23:GLN:O	1:C:24:LEU:HD22	2.16	0.42
1:C:329:PHE:HD1	1:C:329:PHE:HA	1.72	0.42
3:M:198:ALA:HB2	3:M:213:SER:HB3	2.00	0.42
1:A:26:PRO:O	1:A:28:TYR:HD1	2.02	0.42
1:A:102:ARG:HA	1:A:102:ARG:HD3	1.87	0.42
1:A:517:LEU:O	1:A:519:HIS:N	2.53	0.42
1:B:126:VAL:HG12	1:B:172:SER:C	2.41	0.42
3:L:133:GLY:H	3:L:188:LYS:HE3	1.84	0.42
2:I:88:SER:OG	2:I:89:GLU:OE1	2.32	0.42
3:M:66:ARG:NH1	3:M:87:ASP:OD2	2.39	0.42
3:N:154:LYS:HD2	3:N:157:ASN:HA	1.95	0.42
1:A:454:ARG:HD3	1:A:454:ARG:C	2.45	0.42
1:B:474:GLN:HA	1:B:489:TYR:HB2	2.01	0.42
1:C:21:ARG:O	1:C:22:THR:C	2.61	0.42
1:C:441:LEU:HD23	1:C:441:LEU:HA	1.92	0.42
1:C:500:THR:HB	1:C:501:ASN:H	1.69	0.42
1:C:567:ARG:HE	1:C:567:ARG:HB3	1.68	0.42
3:L:139:CYS:CB	3:L:153:TRP:CZ2	3.01	0.42
3:L:144:PHE:CE1	3:L:203:HIS:CB	2.94	0.42
2:I:184:VAL:C	2:I:185:LEU:HD23	2.44	0.42
3:N:118:PRO:CG	3:N:144:PHE:CD2	2.98	0.42
3:N:167:SER:O	3:N:181:SER:OG	2.34	0.42
1:B:1105:THR:HG23	1:B:1111:GLU:H	1.85	0.41
1:C:179:LEU:O	1:C:181:GLY:N	2.53	0.41
3:L:98:GLN:N	3:L:98:GLN:CD	2.73	0.41
3:M:1:GLU:OE1	3:M:1:GLU:N	2.48	0.41
2:J:186:GLN:N	2:J:190:LEU:O	2.47	0.41
3:N:99:PHE:CB	3:N:100:PRO:CD	2.97	0.41
1:A:34:ARG:NH2	1:A:217:PRO:HG2	2.35	0.41
1:A:248:TYR:HD1	1:A:248:TYR:HA	1.68	0.41
1:B:943:SER:O	1:B:943:SER:OG	2.32	0.41
3:N:202:THR:O	3:N:203:HIS:CG	2.73	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:19:THR:C	1:B:20:THR:HG1	2.07	0.41
1:B:330:PRO:HD3	1:B:544:ASN:HD21	1.85	0.41
1:B:422:ASN:HB2	1:B:423:TYR:H	1.66	0.41
1:C:24:LEU:HB2	1:C:25:PRO:HD2	2.01	0.41
1:C:179:LEU:CD2	1:C:180:GLU:N	2.79	0.41
3:M:99:PHE:CB	3:M:100:PRO:CD	2.97	0.41
2:J:181:PHE:CD2	3:N:181:SER:OG	2.63	0.41
1:A:522:ALA:C	1:A:523:THR:HG23	2.45	0.41
1:A:886:TRP:H	1:A:886:TRP:HE3	1.68	0.41
2:H:155:CYS:HB2	2:H:169:TRP:HH2	1.76	0.41
3:L:202:THR:O	3:L:203:HIS:CG	2.73	0.41
2:I:174:LEU:HD23	2:I:174:LEU:HA	1.91	0.41
2:J:7:SER:OG	2:J:21:SER:O	2.33	0.41
3:N:120:VAL:HG21	3:N:201:VAL:HG22	2.01	0.41
1:A:777:ASN:OD1	1:A:1019:ARG:NH1	2.53	0.41
1:B:49:HIS:CD2	1:B:51:THR:CG2	3.02	0.41
1:B:126:VAL:HB	1:B:174:PRO:HA	2.01	0.41
1:B:179:LEU:O	1:B:181:GLY:N	2.53	0.41
1:B:403:ARG:HE	1:B:406:GLU:HG2	1.85	0.41
1:B:600:PRO:HD3	1:B:692:ILE:HD11	2.01	0.41
1:C:21:ARG:C	1:C:22:THR:O	2.63	0.41
1:C:80:ASP:C	1:C:82:PRO:HD3	2.36	0.41
1:C:981:LEU:HD23	1:C:981:LEU:HA	1.84	0.41
2:H:45:LEU:HD23	3:L:103:PHE:HE2	1.80	0.41
2:H:54:GLU:O	2:H:55:ASP:CB	2.68	0.41
3:L:5:THR:O	3:L:6:GLN:OE1	2.39	0.41
2:I:73:ASP:OD1	2:I:76:THR:OG1	2.31	0.41
3:M:139:CYS:CA	3:M:153:TRP:CH2	3.03	0.41
1:A:959:LEU:HD23	1:A:959:LEU:HA	1.96	0.41
1:B:275:PHE:HA	1:B:289:VAL:O	2.20	0.41
1:B:452:LEU:HD21	1:B:494:SER:CB	2.51	0.41
1:C:29:THR:OG1	1:C:30:ASN:N	2.39	0.41
1:C:312:ILE:O	1:C:312:ILE:HG23	2.21	0.41
1:C:826:VAL:HB	1:C:1057:PRO:HG2	2.03	0.41
2:H:184:VAL:C	2:H:185:LEU:HD23	2.44	0.41
2:I:142:SER:HB2	2:I:145:SER:HB2	2.03	0.41
3:M:198:ALA:HA	3:M:213:SER:CB	2.49	0.41
3:M:202:THR:O	3:M:203:HIS:CG	2.73	0.41
3:N:6:GLN:HE21	3:N:106:GLY:H	1.69	0.41
3:N:143:ASN:ND2	3:N:177:THR:HG21	2.33	0.41
1:A:14:GLN:HE21	1:A:158:ARG:CZ	2.33	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:345:THR:OG1	1:A:346:ARG:N	2.53	0.41
1:B:443:SER:HB2	1:B:497:PHE:HB2	2.02	0.41
1:B:981:LEU:HD12	1:B:981:LEU:HA	1.92	0.41
2:H:55:ASP:C	2:H:57:GLU:N	2.74	0.41
2:H:160:TYR:O	2:H:160:TYR:CD1	2.74	0.41
2:H:163:GLU:CB	2:H:164:PRO:CD	2.85	0.41
2:H:181:PHE:HB3	2:H:182:PRO:CD	2.45	0.41
2:I:63:LYS:HB3	2:I:63:LYS:HE2	1.59	0.41
2:I:150:THR:OG1	2:I:199:VAL:O	2.38	0.41
3:M:124:PRO:HB2	3:M:125:PRO:CD	2.51	0.41
3:N:5:THR:O	3:N:6:GLN:OE1	2.39	0.41
1:A:329:PHE:CB	1:A:330:PRO:HD2	2.48	0.41
1:A:403:ARG:NH1	1:A:496:GLY:O	2.54	0.41
1:B:14:GLN:HE21	1:B:158:ARG:CZ	2.33	0.41
1:B:455:LEU:HD12	1:B:455:LEU:HA	1.81	0.41
1:C:14:GLN:HE21	1:C:158:ARG:CZ	2.33	0.41
1:C:355:ARG:NH1	1:C:398:ASP:OD2	2.54	0.41
1:C:642:VAL:HG22	1:C:651:ILE:HG22	2.02	0.41
1:C:714:ILE:HA	1:C:715:PRO:HD3	1.94	0.41
2:H:38:ARG:HH11	2:H:38:ARG:HD3	1.71	0.41
2:H:166:THR:C	2:H:167:VAL:CG2	2.81	0.41
2:I:141:PRO:HG2	2:I:228:PRO:CB	2.45	0.41
3:M:216:ARG:NH1	3:M:216:ARG:CG	2.80	0.41
2:J:54:GLU:O	2:J:55:ASP:CB	2.68	0.41
1:A:328:ARG:HA	1:A:328:ARG:HD2	1.86	0.41
1:A:403:ARG:CD	1:A:505:TYR:HD1	2.23	0.41
1:B:80:ASP:C	1:B:82:PRO:HD3	2.36	0.41
1:B:99:ASN:OD1	1:B:99:ASN:N	2.51	0.41
1:B:289:VAL:HG23	1:B:306:PHE:CE2	2.55	0.41
1:B:408:ARG:O	1:B:414:GLN:NE2	2.54	0.41
1:C:294:ASP:HB2	1:C:295:PRO:CD	2.51	0.41
3:L:124:PRO:HB2	3:L:125:PRO:CD	2.51	0.41
3:M:118:PRO:CD	3:M:206:LEU:CD2	2.73	0.41
3:M:167:SER:O	3:M:181:SER:OG	2.34	0.41
2:J:142:SER:HB2	2:J:145:SER:HB2	2.03	0.41
3:N:139:CYS:CA	3:N:153:TRP:CH2	3.03	0.41
1:A:248:TYR:HE1	2:H:27:TYR:HE2	1.69	0.41
1:B:22:THR:CG2	1:B:78:ARG:CZ	2.99	0.41
1:B:290:ASP:OD1	1:B:291:CYS:N	2.54	0.41
1:C:126:VAL:HB	1:C:174:PRO:HA	2.01	0.41
1:C:454:ARG:HD3	1:C:458:LYS:CD	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:103:ALA:HB3	2:H:110:ASP:HB2	2.03	0.41
2:I:159:ASP:HA	2:I:190:LEU:HB3	2.03	0.41
2:J:88:SER:OG	2:J:89:GLU:OE1	2.32	0.41
2:J:159:ASP:HA	2:J:190:LEU:HB3	2.03	0.41
2:J:179:HIS:CE1	3:N:142:ASN:ND2	2.89	0.41
2:J:229:LYS:O	3:N:218:GLU:O	2.39	0.41
1:C:22:THR:CG2	1:C:78:ARG:CD	2.75	0.40
1:C:977:LEU:HD11	1:C:993:ILE:HG12	2.04	0.40
2:H:150:THR:OG1	2:H:199:VAL:O	2.38	0.40
2:H:165:VAL:CG1	2:H:166:THR:H	2.30	0.40
3:L:120:VAL:HG21	3:L:201:VAL:HG22	2.01	0.40
2:I:54:GLU:O	2:I:55:ASP:CB	2.68	0.40
3:N:31:HIS:HB2	3:N:97:THR:HG23	2.04	0.40
3:N:59:ARG:HG2	3:N:63:VAL:HB	2.04	0.40
1:A:21:ARG:C	1:A:22:THR:O	2.63	0.40
1:A:280:ASN:HB2	1:A:284:THR:O	2.21	0.40
1:A:663:ASP:OD2	1:A:673:SER:HB2	2.21	0.40
1:A:811:LYS:HD3	1:A:820:ASP:CG	2.36	0.40
1:B:246:ARG:HD2	1:B:246:ARG:HA	1.85	0.40
1:C:282:ASN:CG	5:f:1:NAG:C1	2.72	0.40
1:C:456:PHE:CE2	1:C:490:PHE:O	2.74	0.40
2:H:59:MET:SD	3:L:99:PHE:HE2	2.44	0.40
2:I:153:LEU:O	2:I:197:VAL:N	2.54	0.40
3:M:31:HIS:HB2	3:M:97:THR:HG23	2.04	0.40
3:M:155:VAL:HB	3:M:160:GLN:CD	2.47	0.40
2:J:59:MET:SD	3:N:99:PHE:HE2	2.44	0.40
3:N:144:PHE:CE1	3:N:203:HIS:CB	2.94	0.40
3:N:151:VAL:HG22	3:N:180:LEU:HD22	1.91	0.40
3:N:155:VAL:HB	3:N:160:GLN:CD	2.47	0.40
1:A:24:LEU:N	1:A:24:LEU:CD1	2.73	0.40
1:A:44:ARG:O	1:A:283:GLY:HA2	2.21	0.40
1:A:357:ARG:NH1	1:B:167:THR:HB	2.35	0.40
1:A:883:THR:HG21	1:C:705:VAL:HB	2.01	0.40
1:B:567:ARG:HE	1:B:567:ARG:HB3	1.67	0.40
1:C:455:LEU:HD12	1:C:493:GLN:HB2	2.03	0.40
1:C:1101:HIS:CD2	5:k:1:NAG:H5	2.57	0.40
2:H:159:ASP:HA	2:H:190:LEU:HB3	2.03	0.40
2:H:179:HIS:CE1	3:L:142:ASN:ND2	2.89	0.40
3:L:6:GLN:HE21	3:L:106:GLY:H	1.69	0.40
3:L:8:PRO:O	3:L:9:LEU:C	2.65	0.40
2:I:156:LEU:HD13	3:M:129:GLN:HE22	1.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:5:THR:O	3:M:6:GLN:OE1	2.39	0.40
3:M:97:THR:C	3:M:98:GLN:CG	2.94	0.40
2:J:160:TYR:O	2:J:160:TYR:CD1	2.74	0.40
3:N:8:PRO:O	3:N:9:LEU:C	2.65	0.40
1:A:328:ARG:HH22	1:A:533:LEU:HD22	1.86	0.40
1:B:308:VAL:HG22	1:B:602:THR:HG23	2.04	0.40
3:L:55:LYS:O	3:L:55:LYS:HG2	2.22	0.40
2:I:160:TYR:O	2:I:160:TYR:CD1	2.74	0.40
2:I:179:HIS:CE1	3:M:142:ASN:ND2	2.89	0.40
3:M:5:THR:O	3:M:6:GLN:CD	2.64	0.40
3:M:6:GLN:HE21	3:M:106:GLY:H	1.69	0.40
2:J:140:ALA:C	2:J:141:PRO:O	2.64	0.40
2:J:142:SER:HB3	3:N:214:PHE:HD2	0.56	0.40
3:N:198:ALA:HA	3:N:213:SER:CB	2.49	0.40
1:B:451:TYR:O	1:B:452:LEU:HD23	2.21	0.40
1:C:457:ARG:O	1:C:459:SER:N	2.53	0.40
3:L:5:THR:O	3:L:6:GLN:CD	2.64	0.40
3:L:68:SER:OG	3:L:79:LYS:O	2.40	0.40
2:J:156:LEU:HD13	3:N:129:GLN:HE22	1.87	0.40
3:N:124:PRO:HB2	3:N:125:PRO:CD	2.51	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 PDB entries followed by that with respect to all EM entries.

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	1017/1283 (79%)	864 (85%)	121 (12%)	32 (3%)	3	18
1	B	1039/1283 (81%)	901 (87%)	110 (11%)	28 (3%)	4	20
1	C	1035/1283 (81%)	884 (85%)	125 (12%)	26 (2%)	4	21
2	H	227/458 (50%)	184 (81%)	29 (13%)	14 (6%)	1	7

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	I	227/458 (50%)	184 (81%)	29 (13%)	14 (6%)	1	7
2	J	227/458 (50%)	182 (80%)	31 (14%)	14 (6%)	1	7
3	L	217/219 (99%)	149 (69%)	46 (21%)	22 (10%)	0	3
3	M	217/219 (99%)	149 (69%)	46 (21%)	22 (10%)	0	3
3	N	217/219 (99%)	149 (69%)	46 (21%)	22 (10%)	0	3
All	All	4423/5880 (75%)	3646 (82%)	583 (13%)	194 (4%)	3	12

All (194) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	22	THR
1	A	23	GLN
1	A	76	THR
1	A	285	ILE
1	A	330	PRO
1	A	810	SER
1	A	811	LYS
1	B	22	THR
1	B	23	GLN
1	B	76	THR
1	B	270	LEU
1	B	271	GLN
1	B	428	ASP
1	B	455	LEU
1	B	459	SER
1	B	1126	CYS
1	C	22	THR
1	C	23	GLN
1	C	76	THR
1	C	286	THR
1	C	457	ARG
1	C	460	ASN
1	C	617	CYS
1	C	827	THR
2	H	141	PRO
2	H	163	GLU
2	H	165	VAL
2	H	167	VAL
3	L	3	VAL
3	L	10	SER

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Mol	Chain	Res	Type
3	L	99	PHE
3	L	147	ARG
3	L	155	VAL
3	L	158	ALA
3	L	159	LEU
3	L	211	THR
2	I	141	PRO
2	I	163	GLU
2	I	165	VAL
2	I	167	VAL
3	M	3	VAL
3	M	10	SER
3	M	99	PHE
3	M	147	ARG
3	M	155	VAL
3	M	158	ALA
3	M	159	LEU
3	M	211	THR
2	J	141	PRO
2	J	163	GLU
2	J	165	VAL
2	J	167	VAL
3	N	3	VAL
3	N	10	SER
3	N	99	PHE
3	N	147	ARG
3	N	155	VAL
3	N	158	ALA
3	N	159	LEU
3	N	211	THR
1	A	19	THR
1	A	21	ARG
1	A	24	LEU
1	A	73	THR
1	A	74	ASN
1	A	286	THR
1	A	292	ALA
1	A	334	ASN
1	A	442	ASP
1	A	519	HIS
1	A	827	THR
1	B	19	THR

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Mol	Chain	Res	Type
1	B	21	ARG
1	B	24	LEU
1	B	73	THR
1	B	74	ASN
1	B	456	PHE
1	C	19	THR
1	C	21	ARG
1	C	24	LEU
1	C	73	THR
1	C	74	ASN
1	C	292	ALA
1	C	614	ASP
2	H	56	GLY
2	H	183	ALA
2	H	184	VAL
2	H	186	GLN
3	L	56	ILE
2	I	56	GLY
2	I	183	ALA
2	I	184	VAL
2	I	186	GLN
3	M	56	ILE
2	J	56	GLY
2	J	183	ALA
2	J	184	VAL
2	J	186	GLN
3	N	56	ILE
1	A	20	THR
1	A	81	ASN
1	A	87	ASN
1	A	180	GLU
1	A	337	PRO
1	A	503	VAL
1	A	522	ALA
1	B	20	THR
1	B	40	ASP
1	B	81	ASN
1	B	87	ASN
1	B	180	GLU
1	B	454	ARG
1	B	458	LYS
1	C	20	THR

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Mol	Chain	Res	Type
1	C	81	ASN
1	C	87	ASN
1	C	180	GLU
2	H	166	THR
2	H	170	ASN
3	L	7	SER
3	L	9	LEU
3	L	100	PRO
3	L	101	TYR
3	L	126	SER
3	L	195	LYS
3	L	210	VAL
2	I	166	THR
2	I	170	ASN
3	M	7	SER
3	M	9	LEU
3	M	100	PRO
3	M	101	TYR
3	M	126	SER
3	M	195	LYS
3	M	210	VAL
2	J	166	THR
2	J	170	ASN
3	N	7	SER
3	N	9	LEU
3	N	100	PRO
3	N	101	TYR
3	N	126	SER
3	N	195	LYS
3	N	210	VAL
1	A	67	ALA
1	A	544	ASN
1	B	67	ALA
1	B	273	ARG
1	B	491	PRO
1	C	67	ALA
1	C	500	THR
1	C	691	SER
1	C	1138	TYR
2	H	175	THR
3	L	4	MET
3	L	194	HIS

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Mol	Chain	Res	Type
3	L	196	VAL
2	I	175	THR
3	M	4	MET
3	M	194	HIS
3	M	196	VAL
2	J	175	THR
3	N	4	MET
3	N	194	HIS
1	A	518	LEU
1	A	520	ALA
2	H	57	GLU
2	H	164	PRO
2	H	182	PRO
3	L	5	THR
2	I	57	GLU
2	I	164	PRO
2	I	182	PRO
3	M	5	THR
2	J	57	GLU
2	J	164	PRO
2	J	182	PRO
3	N	5	THR
3	N	196	VAL
1	A	249	LEU
1	A	336	CYS
1	B	249	LEU
1	B	488	CYS
1	C	249	LEU
1	A	75	GLY
1	B	75	GLY
1	C	75	GLY
3	L	2	ILE
3	M	2	ILE
3	N	2	ILE
3	L	12	PRO
3	M	12	PRO
3	N	12	PRO
1	C	502	GLY

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 PDB entries followed by that with respect to all EM entries.

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	902/1122 (80%)	863 (96%)	39 (4%)	26	57
1	B	924/1122 (82%)	877 (95%)	47 (5%)	21	52
1	C	920/1122 (82%)	880 (96%)	40 (4%)	26	57
2	H	193/405 (48%)	176 (91%)	17 (9%)	9	33
2	I	193/405 (48%)	176 (91%)	17 (9%)	9	33
2	J	193/405 (48%)	176 (91%)	17 (9%)	9	33
3	L	194/194 (100%)	170 (88%)	24 (12%)	4	19
3	M	194/194 (100%)	170 (88%)	24 (12%)	4	19
3	N	194/194 (100%)	170 (88%)	24 (12%)	4	19
All	All	3907/5163 (76%)	3658 (94%)	249 (6%)	18	44

All (249) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	LEU
1	A	19	THR
1	A	21	ARG
1	A	22	THR
1	A	23	GLN
1	A	24	LEU
1	A	48	LEU
1	A	71	SER
1	A	76	THR
1	A	77	LYS
1	A	78	ARG
1	A	88	ASP
1	A	138	ASP
1	A	150	LYS
1	A	166	CYS
1	A	169	GLU
1	A	170	TYR
1	A	277	LEU

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Mol	Chain	Res	Type
1	A	296	LEU
1	A	312	ILE
1	A	379	CYS
1	A	495	TYR
1	A	500	THR
1	A	506	GLN
1	A	515	PHE
1	A	516	GLU
1	A	524	VAL
1	A	595	VAL
1	A	617	CYS
1	A	675	GLN
1	A	729	VAL
1	A	794	ILE
1	A	811	LYS
1	A	814	LYS
1	A	878	LEU
1	A	976	VAL
1	A	1057	PRO
1	A	1130	ILE
1	A	1141	LEU
1	B	18	LEU
1	B	19	THR
1	B	21	ARG
1	B	22	THR
1	B	23	GLN
1	B	24	LEU
1	B	44	ARG
1	B	46	SER
1	B	52	GLN
1	B	54	LEU
1	B	71	SER
1	B	76	THR
1	B	77	LYS
1	B	78	ARG
1	B	88	ASP
1	B	138	ASP
1	B	150	LYS
1	B	166	CYS
1	B	169	GLU
1	B	170	TYR
1	B	273	ARG

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Mol	Chain	Res	Type
1	B	276	LEU
1	B	277	LEU
1	B	287	ASP
1	B	296	LEU
1	B	300	LYS
1	B	303	LEU
1	B	309	GLU
1	B	422	ASN
1	B	424	LYS
1	B	425	LEU
1	B	457	ARG
1	B	458	LYS
1	B	487	ASN
1	B	524	VAL
1	B	525	CYS
1	B	534	VAL
1	B	588	THR
1	B	597	VAL
1	B	608	VAL
1	B	615	VAL
1	B	692	ILE
1	B	720	ILE
1	B	976	VAL
1	B	1141	LEU
1	B	1142	GLN
1	B	1146	ASP
1	C	18	LEU
1	C	19	THR
1	C	21	ARG
1	C	22	THR
1	C	23	GLN
1	C	24	LEU
1	C	48	LEU
1	C	71	SER
1	C	76	THR
1	C	77	LYS
1	C	78	ARG
1	C	88	ASP
1	C	138	ASP
1	C	150	LYS
1	C	166	CYS
1	C	169	GLU

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Mol	Chain	Res	Type
1	C	170	TYR
1	C	277	LEU
1	C	287	ASP
1	C	296	LEU
1	C	309	GLU
1	C	310	LYS
1	C	333	THR
1	C	455	LEU
1	C	457	ARG
1	C	458	LYS
1	C	471	GLU
1	C	500	THR
1	C	558	LYS
1	C	611	LEU
1	C	613	GLN
1	C	617	CYS
1	C	619	GLU
1	C	720	ILE
1	C	729	VAL
1	C	976	VAL
1	C	1043	CYS
1	C	1045	LYS
1	C	1129	VAL
1	C	1145	LEU
2	H	54	GLU
2	H	55	ASP
2	H	57	GLU
2	H	59	MET
2	H	63	LYS
2	H	91	THR
2	H	124	VAL
2	H	130	SER
2	H	142	SER
2	H	145	SER
2	H	146	THR
2	H	160	TYR
2	H	163	GLU
2	H	169	TRP
2	H	170	ASN
2	H	179	HIS
2	H	195	SER
3	L	2	ILE

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Mol	Chain	Res	Type
3	L	4	MET
3	L	5	THR
3	L	9	LEU
3	L	23	CYS
3	L	56	ILE
3	L	88	VAL
3	L	97	THR
3	L	98	GLN
3	L	99	PHE
3	L	102	THR
3	L	105	GLN
3	L	112	LYS
3	L	144	PHE
3	L	148	GLU
3	L	154	LYS
3	L	157	ASN
3	L	177	THR
3	L	178	TYR
3	L	192	GLU
3	L	193	LYS
3	L	195	LYS
3	L	203	HIS
3	L	212	LYS
2	I	54	GLU
2	I	55	ASP
2	I	57	GLU
2	I	59	MET
2	I	63	LYS
2	I	91	THR
2	I	124	VAL
2	I	130	SER
2	I	142	SER
2	I	145	SER
2	I	146	THR
2	I	160	TYR
2	I	163	GLU
2	I	169	TRP
2	I	170	ASN
2	I	179	HIS
2	I	195	SER
3	M	2	ILE
3	M	4	MET

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Mol	Chain	Res	Type
3	M	5	THR
3	M	9	LEU
3	M	23	CYS
3	M	56	ILE
3	M	88	VAL
3	M	97	THR
3	M	98	GLN
3	M	99	PHE
3	M	102	THR
3	M	105	GLN
3	M	112	LYS
3	M	144	PHE
3	M	148	GLU
3	M	154	LYS
3	M	157	ASN
3	M	177	THR
3	M	178	TYR
3	M	192	GLU
3	M	193	LYS
3	M	195	LYS
3	M	203	HIS
3	M	212	LYS
2	J	54	GLU
2	J	55	ASP
2	J	57	GLU
2	J	59	MET
2	J	63	LYS
2	J	91	THR
2	J	124	VAL
2	J	130	SER
2	J	142	SER
2	J	145	SER
2	J	146	THR
2	J	160	TYR
2	J	163	GLU
2	J	169	TRP
2	J	170	ASN
2	J	179	HIS
2	J	195	SER
3	N	2	ILE
3	N	4	MET
3	N	5	THR

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Mol	Chain	Res	Type
3	N	9	LEU
3	N	23	CYS
3	N	56	ILE
3	N	88	VAL
3	N	97	THR
3	N	98	GLN
3	N	99	PHE
3	N	102	THR
3	N	105	GLN
3	N	112	LYS
3	N	144	PHE
3	N	148	GLU
3	N	154	LYS
3	N	157	ASN
3	N	177	THR
3	N	178	TYR
3	N	192	GLU
3	N	193	LYS
3	N	195	LYS
3	N	203	HIS
3	N	212	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (101) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	14	GLN
1	A	23	GLN
1	A	30	ASN
1	A	69	HIS
1	A	115	GLN
1	A	211	ASN
1	A	271	GLN
1	A	334	ASN
1	A	409	GLN
1	A	414	GLN
1	A	422	ASN
1	A	542	ASN
1	A	564	GLN
1	A	641	ASN
1	A	675	GLN
1	A	751	ASN
1	A	755	GLN

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Mol	Chain	Res	Type
1	A	762	GLN
1	A	764	ASN
1	A	914	ASN
1	A	919	ASN
1	A	949	GLN
1	A	978	ASN
1	A	1083	HIS
1	A	1101	HIS
1	A	1142	GLN
1	B	14	GLN
1	B	23	GLN
1	B	30	ASN
1	B	52	GLN
1	B	69	HIS
1	B	115	GLN
1	B	211	ASN
1	B	271	GLN
1	B	360	ASN
1	B	422	ASN
1	B	498	GLN
1	B	542	ASN
1	B	544	ASN
1	B	564	GLN
1	B	580	GLN
1	B	644	GLN
1	B	655	HIS
1	B	764	ASN
1	B	914	ASN
1	B	926	GLN
1	B	1011	GLN
1	B	1054	GLN
1	B	1113	GLN
1	C	14	GLN
1	C	23	GLN
1	C	30	ASN
1	C	69	HIS
1	C	115	GLN
1	C	211	ASN
1	C	271	GLN
1	C	321	GLN
1	C	370	ASN
1	C	388	ASN

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Mol	Chain	Res	Type
1	C	394	ASN
1	C	414	GLN
1	C	498	GLN
1	C	501	ASN
1	C	564	GLN
1	C	613	GLN
1	C	658	ASN
1	C	762	GLN
1	C	804	GLN
1	C	907	ASN
1	C	914	ASN
1	C	955	ASN
1	C	965	GLN
1	C	969	ASN
1	C	1010	GLN
1	C	1101	HIS
2	H	170	ASN
2	H	214	ASN
2	H	219	ASN
3	L	42	GLN
3	L	43	GLN
3	L	58	ASN
3	L	105	GLN
3	L	171	GLN
3	L	194	HIS
2	I	170	ASN
2	I	214	ASN
2	I	219	ASN
3	M	42	GLN
3	M	43	GLN
3	M	58	ASN
3	M	105	GLN
3	M	171	GLN
3	M	194	HIS
2	J	170	ASN
2	J	219	ASN
3	N	42	GLN
3	N	43	GLN
3	N	58	ASN
3	N	105	GLN
3	N	171	GLN
3	N	194	HIS

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 ⓘ

64 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	$\# Z > 2$
4	NAG	D	1	1,4	14,14,15	0.69	1 (7%)	17,19,21	0.73	0
4	NAG	D	2	4	14,14,15	0.36	0	17,19,21	0.89	1 (5%)
4	NAG	D	3	4	14,14,15	0.52	0	17,19,21	0.81	1 (5%)
4	NAG	E	1	1,4	14,14,15	0.75	1 (7%)	17,19,21	0.98	0
4	NAG	E	2	4	14,14,15	0.37	0	17,19,21	1.00	1 (5%)
4	NAG	E	3	4	14,14,15	0.36	0	17,19,21	0.53	0
5	NAG	F	1	1,5	14,14,15	0.82	1 (7%)	17,19,21	1.05	2 (11%)
5	NAG	F	2	5	14,14,15	0.75	1 (7%)	17,19,21	0.55	0
5	NAG	G	1	1,5	14,14,15	1.63	1 (7%)	17,19,21	2.72	4 (23%)
5	NAG	G	2	5	14,14,15	0.25	0	17,19,21	0.62	0
5	NAG	K	1	1,5	14,14,15	0.30	0	17,19,21	0.77	1 (5%)
5	NAG	K	2	5	14,14,15	0.22	0	17,19,21	0.48	0
5	NAG	O	1	1,5	14,14,15	0.42	0	17,19,21	1.15	2 (11%)
5	NAG	O	2	5	14,14,15	0.29	0	17,19,21	0.55	0
5	NAG	P	1	1,5	14,14,15	0.32	0	17,19,21	0.60	0
5	NAG	P	2	5	14,14,15	0.64	0	17,19,21	2.51	4 (23%)
5	NAG	Q	1	1,5	14,14,15	0.34	0	17,19,21	0.61	0
5	NAG	Q	2	5	14,14,15	0.39	0	17,19,21	1.01	1 (5%)
5	NAG	R	1	1,5	14,14,15	0.19	0	17,19,21	0.55	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	R	2	5	14,14,15	0.18	0	17,19,21	0.64	1 (5%)
4	NAG	S	1	1,4	14,14,15	0.70	1 (7%)	17,19,21	0.73	0
4	NAG	S	2	4	14,14,15	0.35	0	17,19,21	0.89	1 (5%)
4	NAG	S	3	4	14,14,15	0.52	0	17,19,21	0.80	1 (5%)
4	NAG	T	1	1,4	14,14,15	0.74	1 (7%)	17,19,21	0.98	0
4	NAG	T	2	4	14,14,15	0.38	0	17,19,21	1.00	1 (5%)
4	NAG	T	3	4	14,14,15	0.35	0	17,19,21	0.53	0
5	NAG	U	1	1,5	14,14,15	0.82	1 (7%)	17,19,21	1.05	2 (11%)
5	NAG	U	2	5	14,14,15	0.76	1 (7%)	17,19,21	0.55	0
5	NAG	V	1	5	14,14,15	1.62	1 (7%)	17,19,21	2.73	4 (23%)
5	NAG	V	2	5	14,14,15	0.24	0	17,19,21	0.62	0
5	NAG	W	1	1,5	14,14,15	0.29	0	17,19,21	0.39	0
5	NAG	W	2	5	14,14,15	0.33	0	17,19,21	0.63	1 (5%)
5	NAG	X	1	1,5	14,14,15	0.20	0	17,19,21	1.31	3 (17%)
5	NAG	X	2	5	14,14,15	0.20	0	17,19,21	0.71	1 (5%)
5	NAG	Y	1	1,5	14,14,15	0.41	0	17,19,21	0.74	1 (5%)
5	NAG	Y	2	5	14,14,15	0.17	0	17,19,21	0.64	0
5	NAG	Z	1	1,5	14,14,15	0.30	0	17,19,21	0.55	0
5	NAG	Z	2	5	14,14,15	0.18	0	17,19,21	0.78	1 (5%)
5	NAG	a	1	1,5	14,14,15	0.39	0	17,19,21	0.86	1 (5%)
5	NAG	a	2	5	14,14,15	0.56	0	17,19,21	1.38	2 (11%)
5	NAG	b	1	1,5	14,14,15	0.34	0	17,19,21	0.91	1 (5%)
5	NAG	b	2	5	14,14,15	0.29	0	17,19,21	0.64	0
4	NAG	c	1	1,4	14,14,15	0.68	1 (7%)	17,19,21	0.74	0
4	NAG	c	2	4	14,14,15	0.36	0	17,19,21	0.89	1 (5%)
4	NAG	c	3	4	14,14,15	0.52	0	17,19,21	0.80	1 (5%)
4	NAG	d	1	1,4	14,14,15	0.75	1 (7%)	17,19,21	0.98	0
4	NAG	d	2	4	14,14,15	0.38	0	17,19,21	1.00	1 (5%)
4	NAG	d	3	4	14,14,15	0.36	0	17,19,21	0.52	0
5	NAG	e	1	1,5	14,14,15	0.82	1 (7%)	17,19,21	1.05	2 (11%)
5	NAG	e	2	5	14,14,15	0.76	1 (7%)	17,19,21	0.55	0
5	NAG	f	1	5	14,14,15	1.63	1 (7%)	17,19,21	2.72	4 (23%)
5	NAG	f	2	5	14,14,15	0.25	0	17,19,21	0.61	0
5	NAG	g	1	1,5	14,14,15	0.62	0	17,19,21	2.39	3 (17%)
5	NAG	g	2	5	14,14,15	0.34	0	17,19,21	0.62	1 (5%)
5	NAG	h	1	1,5	14,14,15	0.43	0	17,19,21	0.62	0
5	NAG	h	2	5	14,14,15	0.42	0	17,19,21	0.47	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	i	1	1,5	14,14,15	0.32	0	17,19,21	0.55	0
5	NAG	i	2	5	14,14,15	0.39	0	17,19,21	1.00	1 (5%)
5	NAG	j	1	1,5	14,14,15	0.34	0	17,19,21	0.66	0
5	NAG	j	2	5	14,14,15	0.92	1 (7%)	17,19,21	2.45	4 (23%)
5	NAG	k	1	1,5	14,14,15	0.44	0	17,19,21	0.60	0
5	NAG	k	2	5	14,14,15	0.87	1 (7%)	17,19,21	2.36	3 (17%)
5	NAG	l	1	1,5	14,14,15	0.25	0	17,19,21	0.74	1 (5%)
5	NAG	l	2	5	14,14,15	0.31	0	17,19,21	0.72	1 (5%)

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
4	NAG	D	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	D	2	4	-	2/6/23/26	0/1/1/1
4	NAG	D	3	4	-	2/6/23/26	0/1/1/1
4	NAG	E	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	E	2	4	-	0/6/23/26	0/1/1/1
4	NAG	E	3	4	-	2/6/23/26	0/1/1/1
5	NAG	F	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	F	2	5	-	0/6/23/26	0/1/1/1
5	NAG	G	1	1,5	-	6/6/23/26	0/1/1/1
5	NAG	G	2	5	-	3/6/23/26	0/1/1/1
5	NAG	K	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	K	2	5	-	2/6/23/26	0/1/1/1
5	NAG	O	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	O	2	5	-	3/6/23/26	0/1/1/1
5	NAG	P	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	P	2	5	-	4/6/23/26	0/1/1/1
5	NAG	Q	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	Q	2	5	-	3/6/23/26	0/1/1/1
5	NAG	R	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	R	2	5	-	0/6/23/26	0/1/1/1
4	NAG	S	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	S	2	4	-	2/6/23/26	0/1/1/1
4	NAG	S	3	4	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	T	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	T	2	4	-	0/6/23/26	0/1/1/1
4	NAG	T	3	4	-	2/6/23/26	0/1/1/1
5	NAG	U	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	U	2	5	-	0/6/23/26	0/1/1/1
5	NAG	V	1	5	-	6/6/23/26	0/1/1/1
5	NAG	V	2	5	-	3/6/23/26	0/1/1/1
5	NAG	W	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	W	2	5	-	2/6/23/26	0/1/1/1
5	NAG	X	1	1,5	-	4/6/23/26	0/1/1/1
5	NAG	X	2	5	-	2/6/23/26	0/1/1/1
5	NAG	Y	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	Y	2	5	-	4/6/23/26	0/1/1/1
5	NAG	Z	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	Z	2	5	-	2/6/23/26	0/1/1/1
5	NAG	a	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	a	2	5	-	2/6/23/26	0/1/1/1
5	NAG	b	1	1,5	-	1/6/23/26	0/1/1/1
5	NAG	b	2	5	-	0/6/23/26	0/1/1/1
4	NAG	c	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	c	2	4	-	2/6/23/26	0/1/1/1
4	NAG	c	3	4	-	2/6/23/26	0/1/1/1
4	NAG	d	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	d	2	4	-	0/6/23/26	0/1/1/1
4	NAG	d	3	4	-	2/6/23/26	0/1/1/1
5	NAG	e	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	e	2	5	-	0/6/23/26	0/1/1/1
5	NAG	f	1	5	-	6/6/23/26	0/1/1/1
5	NAG	f	2	5	-	3/6/23/26	0/1/1/1
5	NAG	g	1	1,5	-	6/6/23/26	0/1/1/1
5	NAG	g	2	5	-	2/6/23/26	0/1/1/1
5	NAG	h	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	h	2	5	-	2/6/23/26	0/1/1/1
5	NAG	i	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	i	2	5	-	4/6/23/26	0/1/1/1
5	NAG	j	1	1,5	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	j	2	5	-	6/6/23/26	0/1/1/1
5	NAG	k	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	k	2	5	-	6/6/23/26	0/1/1/1
5	NAG	l	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	l	2	5	-	0/6/23/26	0/1/1/1

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	f	1	NAG	O5-C1	-5.67	1.34	1.43
5	G	1	NAG	O5-C1	-5.67	1.34	1.43
5	V	1	NAG	O5-C1	-5.64	1.34	1.43
5	j	2	NAG	C1-C2	2.88	1.56	1.52
4	E	1	NAG	O5-C1	-2.68	1.39	1.43
4	d	1	NAG	O5-C1	-2.67	1.39	1.43
4	T	1	NAG	O5-C1	-2.66	1.39	1.43
5	k	2	NAG	C1-C2	2.59	1.55	1.52
5	e	2	NAG	C1-C2	2.56	1.55	1.52
5	U	2	NAG	C1-C2	2.55	1.55	1.52
5	F	2	NAG	C1-C2	2.52	1.55	1.52
5	F	1	NAG	O5-C1	-2.34	1.39	1.43
5	e	1	NAG	O5-C1	-2.31	1.39	1.43
5	U	1	NAG	O5-C1	-2.30	1.39	1.43
4	S	1	NAG	O5-C1	-2.15	1.40	1.43
4	D	1	NAG	O5-C1	-2.13	1.40	1.43
4	c	1	NAG	O5-C1	-2.10	1.40	1.43

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	V	1	NAG	C2-N2-C7	8.56	134.37	122.90
5	G	1	NAG	C2-N2-C7	8.55	134.35	122.90
5	f	1	NAG	C2-N2-C7	8.53	134.33	122.90
5	g	1	NAG	C2-N2-C7	8.47	134.26	122.90
5	j	2	NAG	C2-N2-C7	8.31	134.04	122.90
5	k	2	NAG	C2-N2-C7	8.29	134.00	122.90
5	P	2	NAG	C2-N2-C7	8.26	133.97	122.90
5	P	2	NAG	C1-C2-N2	4.73	117.89	110.43
5	j	2	NAG	C1-C2-N2	4.24	117.12	110.43
5	k	2	NAG	C1-C2-N2	4.13	116.94	110.43
5	a	2	NAG	C1-O5-C5	3.95	117.48	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	f	1	NAG	C3-C4-C5	3.93	117.36	110.23
5	V	1	NAG	C3-C4-C5	3.92	117.34	110.23
5	G	1	NAG	C3-C4-C5	3.91	117.33	110.23
5	G	1	NAG	C1-C2-N2	3.87	116.53	110.43
5	V	1	NAG	C1-C2-N2	3.85	116.50	110.43
5	f	1	NAG	C1-C2-N2	3.84	116.49	110.43
5	g	1	NAG	C1-C2-N2	3.81	116.44	110.43
5	X	1	NAG	C2-N2-C7	3.38	127.43	122.90
5	a	2	NAG	C2-N2-C7	3.21	127.20	122.90
5	Q	2	NAG	C2-N2-C7	3.19	127.17	122.90
5	b	1	NAG	C1-O5-C5	3.12	116.36	112.19
5	i	2	NAG	C2-N2-C7	3.09	127.03	122.90
5	X	1	NAG	C1-O5-C5	2.90	116.07	112.19
5	Z	2	NAG	C1-O5-C5	2.79	115.92	112.19
4	D	3	NAG	C1-O5-C5	2.62	115.70	112.19
5	K	1	NAG	C1-O5-C5	2.62	115.70	112.19
4	c	3	NAG	C1-O5-C5	2.61	115.68	112.19
4	S	3	NAG	C1-O5-C5	2.60	115.67	112.19
5	j	2	NAG	C1-O5-C5	2.57	115.63	112.19
5	l	2	NAG	C1-O5-C5	2.56	115.62	112.19
5	a	1	NAG	O4-C4-C5	-2.50	103.18	109.32
5	P	2	NAG	C1-O5-C5	2.49	115.52	112.19
4	S	2	NAG	C1-O5-C5	2.48	115.51	112.19
4	c	2	NAG	C1-O5-C5	2.47	115.50	112.19
4	D	2	NAG	C1-O5-C5	2.47	115.50	112.19
4	d	2	NAG	O3-C3-C2	-2.45	104.32	109.40
4	E	2	NAG	O3-C3-C2	-2.44	104.33	109.40
4	T	2	NAG	O3-C3-C2	-2.44	104.34	109.40
5	X	2	NAG	C1-O5-C5	2.42	115.43	112.19
5	O	1	NAG	C8-C7-N2	2.35	120.02	116.12
5	f	1	NAG	C8-C7-N2	2.35	120.02	116.12
5	V	1	NAG	C8-C7-N2	2.35	120.01	116.12
5	G	1	NAG	C8-C7-N2	2.34	120.00	116.12
5	l	1	NAG	C1-O5-C5	2.25	115.21	112.19
5	g	1	NAG	C8-C7-N2	2.19	119.75	116.12
5	Y	1	NAG	C1-O5-C5	2.16	115.08	112.19
5	X	1	NAG	C1-C2-N2	2.15	113.82	110.43
5	O	1	NAG	C2-N2-C7	-2.15	120.02	122.90
5	g	2	NAG	C1-O5-C5	2.15	115.06	112.19
5	F	1	NAG	O4-C4-C3	-2.13	105.34	110.38
5	e	1	NAG	O4-C4-C3	-2.13	105.35	110.38
5	U	1	NAG	O4-C4-C3	-2.12	105.38	110.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	R	2	NAG	C1-O5-C5	2.12	115.02	112.19
5	j	2	NAG	C8-C7-N2	2.11	119.62	116.12
5	W	2	NAG	C1-O5-C5	2.11	115.01	112.19
5	k	2	NAG	C8-C7-N2	2.08	119.57	116.12
5	P	2	NAG	C8-C7-N2	2.07	119.56	116.12
5	F	1	NAG	C1-O5-C5	2.04	114.92	112.19
5	U	1	NAG	C1-O5-C5	2.03	114.91	112.19
5	e	1	NAG	C1-O5-C5	2.03	114.91	112.19

There are no chirality outliers.

All (132) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	O	2	NAG	C3-C2-N2-C7
5	O	2	NAG	C8-C7-N2-C2
5	O	2	NAG	O7-C7-N2-C2
5	f	2	NAG	O5-C5-C6-O6
5	G	2	NAG	O5-C5-C6-O6
5	V	2	NAG	O5-C5-C6-O6
4	E	3	NAG	O5-C5-C6-O6
4	T	3	NAG	O5-C5-C6-O6
4	d	3	NAG	O5-C5-C6-O6
5	X	1	NAG	O5-C5-C6-O6
4	S	3	NAG	O5-C5-C6-O6
5	G	1	NAG	O5-C5-C6-O6
5	V	1	NAG	O5-C5-C6-O6
5	Z	2	NAG	O5-C5-C6-O6
5	f	1	NAG	O5-C5-C6-O6
5	g	2	NAG	O5-C5-C6-O6
5	l	1	NAG	O5-C5-C6-O6
4	E	1	NAG	C4-C5-C6-O6
4	T	1	NAG	C4-C5-C6-O6
4	d	1	NAG	C4-C5-C6-O6
4	D	3	NAG	O5-C5-C6-O6
4	c	3	NAG	O5-C5-C6-O6
5	R	1	NAG	O5-C5-C6-O6
5	Y	1	NAG	C4-C5-C6-O6
4	E	3	NAG	C4-C5-C6-O6
4	T	3	NAG	C4-C5-C6-O6
4	d	3	NAG	C4-C5-C6-O6
5	W	1	NAG	O5-C5-C6-O6
5	Y	1	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
5	k	2	NAG	O5-C5-C6-O6
5	G	1	NAG	C4-C5-C6-O6
5	V	1	NAG	C4-C5-C6-O6
5	W	1	NAG	C4-C5-C6-O6
5	X	1	NAG	C4-C5-C6-O6
5	f	1	NAG	C4-C5-C6-O6
5	Q	1	NAG	O5-C5-C6-O6
5	G	2	NAG	C4-C5-C6-O6
5	V	2	NAG	C4-C5-C6-O6
5	f	2	NAG	C4-C5-C6-O6
5	F	1	NAG	C4-C5-C6-O6
5	U	1	NAG	C4-C5-C6-O6
5	e	1	NAG	C4-C5-C6-O6
5	j	2	NAG	C4-C5-C6-O6
5	K	1	NAG	C4-C5-C6-O6
4	D	2	NAG	O5-C5-C6-O6
4	S	2	NAG	O5-C5-C6-O6
4	c	2	NAG	O5-C5-C6-O6
5	Q	1	NAG	C4-C5-C6-O6
5	Z	2	NAG	C4-C5-C6-O6
5	g	2	NAG	C4-C5-C6-O6
4	E	1	NAG	O5-C5-C6-O6
4	T	1	NAG	O5-C5-C6-O6
4	d	1	NAG	O5-C5-C6-O6
5	j	2	NAG	O5-C5-C6-O6
5	k	2	NAG	C4-C5-C6-O6
5	R	1	NAG	C4-C5-C6-O6
5	l	1	NAG	C4-C5-C6-O6
5	W	2	NAG	O5-C5-C6-O6
5	G	1	NAG	C8-C7-N2-C2
5	G	1	NAG	O7-C7-N2-C2
5	P	2	NAG	C8-C7-N2-C2
5	P	2	NAG	O7-C7-N2-C2
5	V	1	NAG	C8-C7-N2-C2
5	V	1	NAG	O7-C7-N2-C2
5	Y	2	NAG	C8-C7-N2-C2
5	Y	2	NAG	O7-C7-N2-C2
5	f	1	NAG	C8-C7-N2-C2
5	f	1	NAG	O7-C7-N2-C2
5	g	1	NAG	C8-C7-N2-C2
5	g	1	NAG	O7-C7-N2-C2
5	j	2	NAG	C8-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
5	j	2	NAG	O7-C7-N2-C2
5	k	2	NAG	C8-C7-N2-C2
5	k	2	NAG	O7-C7-N2-C2
4	D	3	NAG	C4-C5-C6-O6
4	S	3	NAG	C4-C5-C6-O6
4	c	3	NAG	C4-C5-C6-O6
5	K	1	NAG	O5-C5-C6-O6
5	Y	2	NAG	C4-C5-C6-O6
5	a	1	NAG	O5-C5-C6-O6
5	h	1	NAG	C4-C5-C6-O6
5	h	2	NAG	C4-C5-C6-O6
5	F	1	NAG	O5-C5-C6-O6
5	U	1	NAG	O5-C5-C6-O6
5	e	1	NAG	O5-C5-C6-O6
4	D	2	NAG	C4-C5-C6-O6
4	S	2	NAG	C4-C5-C6-O6
4	c	2	NAG	C4-C5-C6-O6
5	Y	2	NAG	O5-C5-C6-O6
5	X	2	NAG	O5-C5-C6-O6
5	X	2	NAG	C4-C5-C6-O6
5	h	1	NAG	O5-C5-C6-O6
5	W	2	NAG	C4-C5-C6-O6
5	h	2	NAG	O5-C5-C6-O6
5	i	1	NAG	C4-C5-C6-O6
5	b	1	NAG	O5-C5-C6-O6
5	i	1	NAG	O5-C5-C6-O6
5	j	1	NAG	C4-C5-C6-O6
5	j	1	NAG	O5-C5-C6-O6
5	i	2	NAG	C4-C5-C6-O6
5	g	1	NAG	C4-C5-C6-O6
5	i	2	NAG	O5-C5-C6-O6
5	G	1	NAG	C3-C2-N2-C7
5	Q	2	NAG	C3-C2-N2-C7
5	V	1	NAG	C3-C2-N2-C7
5	a	2	NAG	C3-C2-N2-C7
5	f	1	NAG	C3-C2-N2-C7
5	i	2	NAG	C3-C2-N2-C7
5	Q	2	NAG	O5-C5-C6-O6
5	K	2	NAG	C4-C5-C6-O6
5	g	1	NAG	O5-C5-C6-O6
5	K	2	NAG	O5-C5-C6-O6
5	G	1	NAG	C1-C2-N2-C7

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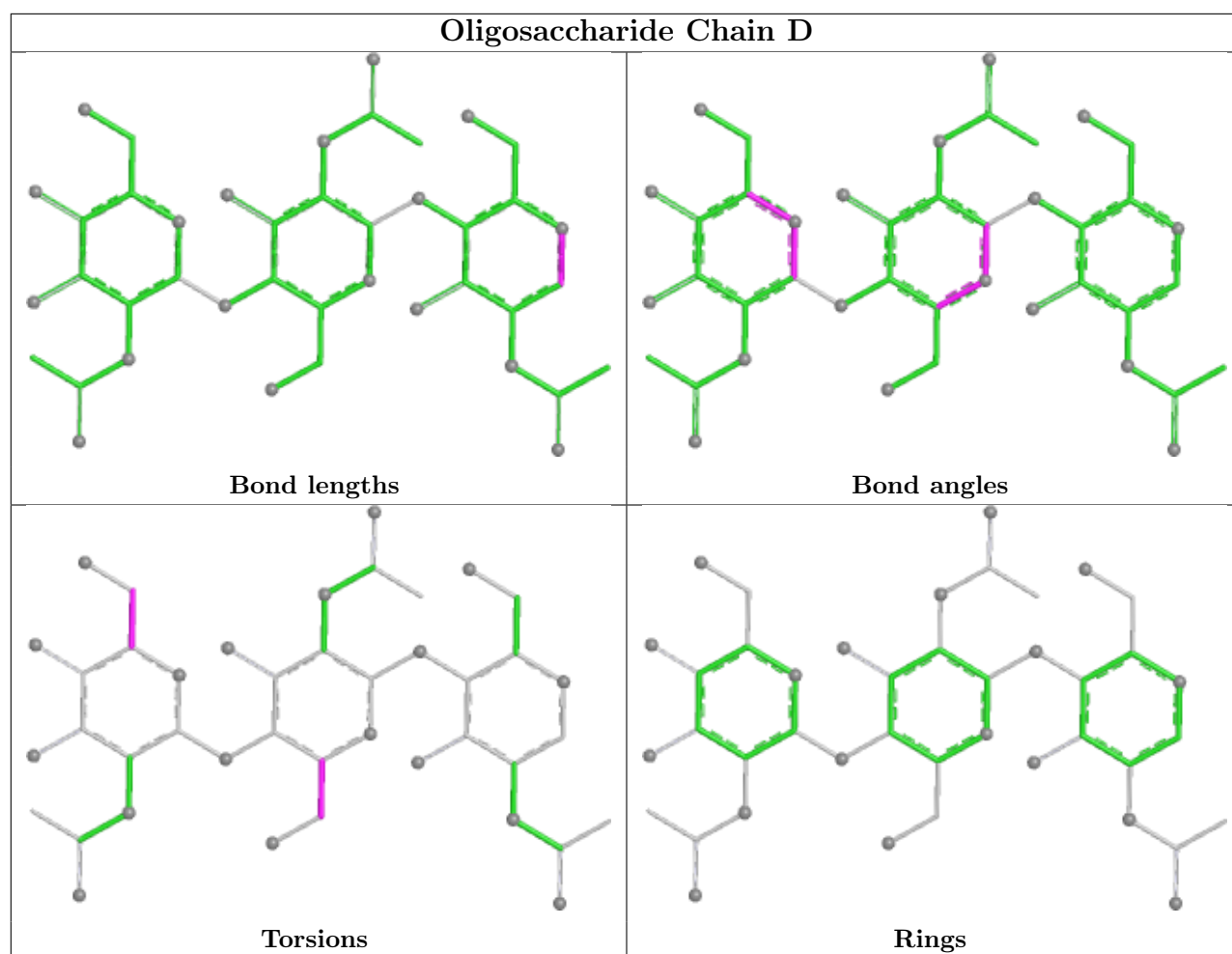
Mol	Chain	Res	Type	Atoms
5	G	2	NAG	C1-C2-N2-C7
5	P	2	NAG	C1-C2-N2-C7
5	Q	2	NAG	C1-C2-N2-C7
5	V	1	NAG	C1-C2-N2-C7
5	V	2	NAG	C1-C2-N2-C7
5	X	1	NAG	C1-C2-N2-C7
5	a	2	NAG	C1-C2-N2-C7
5	f	1	NAG	C1-C2-N2-C7
5	f	2	NAG	C1-C2-N2-C7
5	g	1	NAG	C1-C2-N2-C7
5	i	2	NAG	C1-C2-N2-C7
5	j	2	NAG	C1-C2-N2-C7
5	k	2	NAG	C1-C2-N2-C7
5	P	2	NAG	C3-C2-N2-C7
5	X	1	NAG	C3-C2-N2-C7
5	g	1	NAG	C3-C2-N2-C7
5	j	2	NAG	C3-C2-N2-C7
5	k	2	NAG	C3-C2-N2-C7
5	a	1	NAG	C4-C5-C6-O6

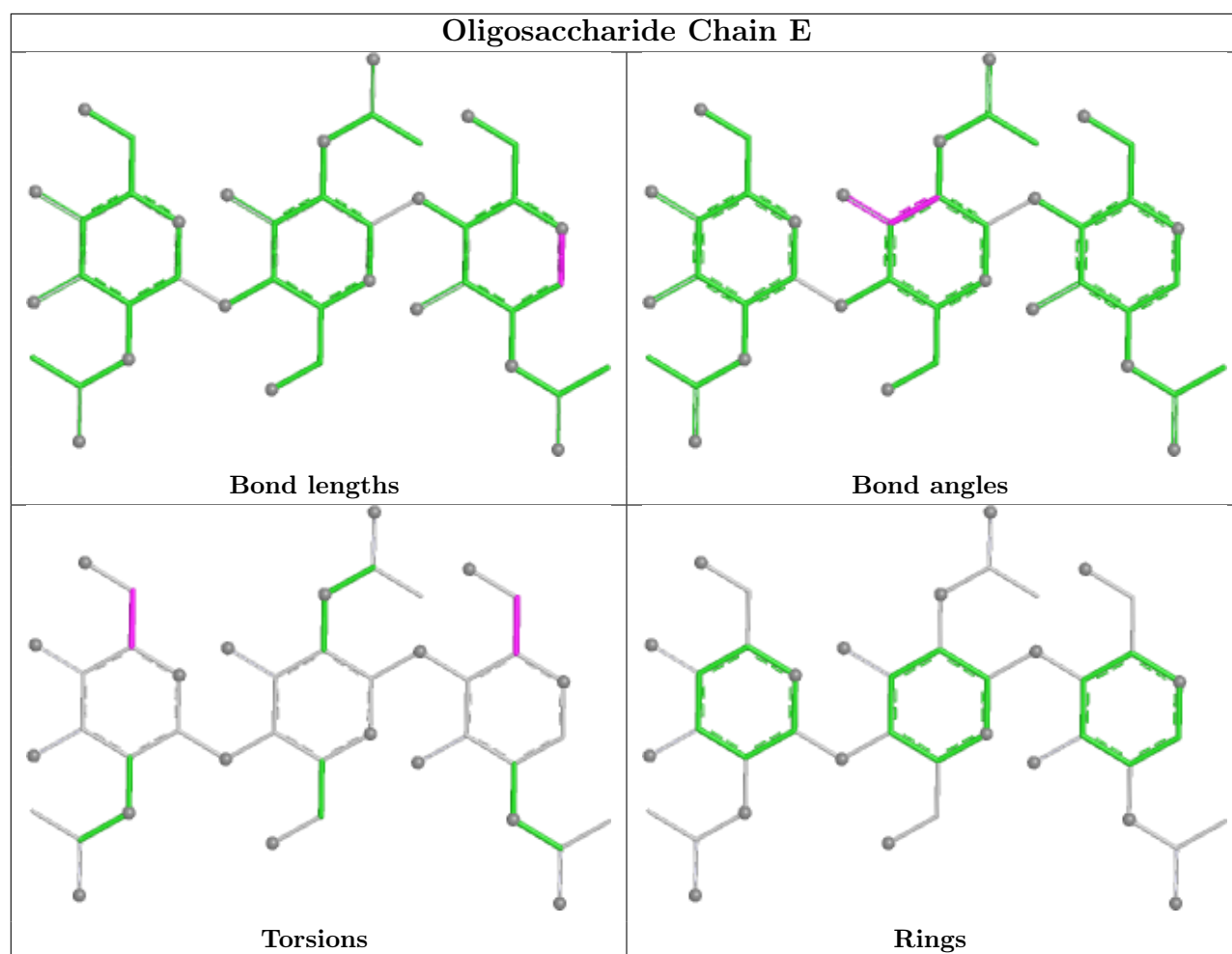
There are no ring outliers.

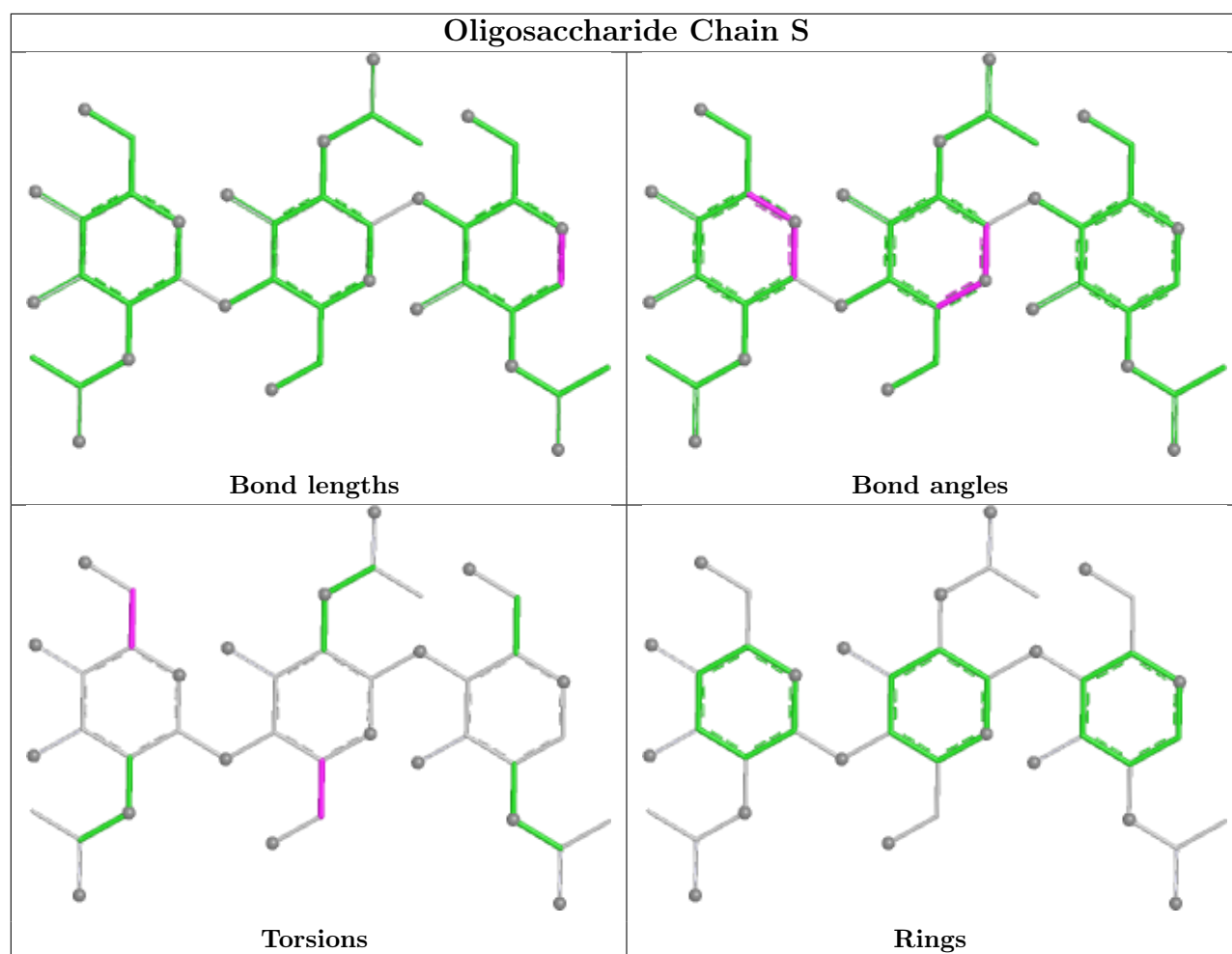
11 monomers are involved in 25 short contacts:

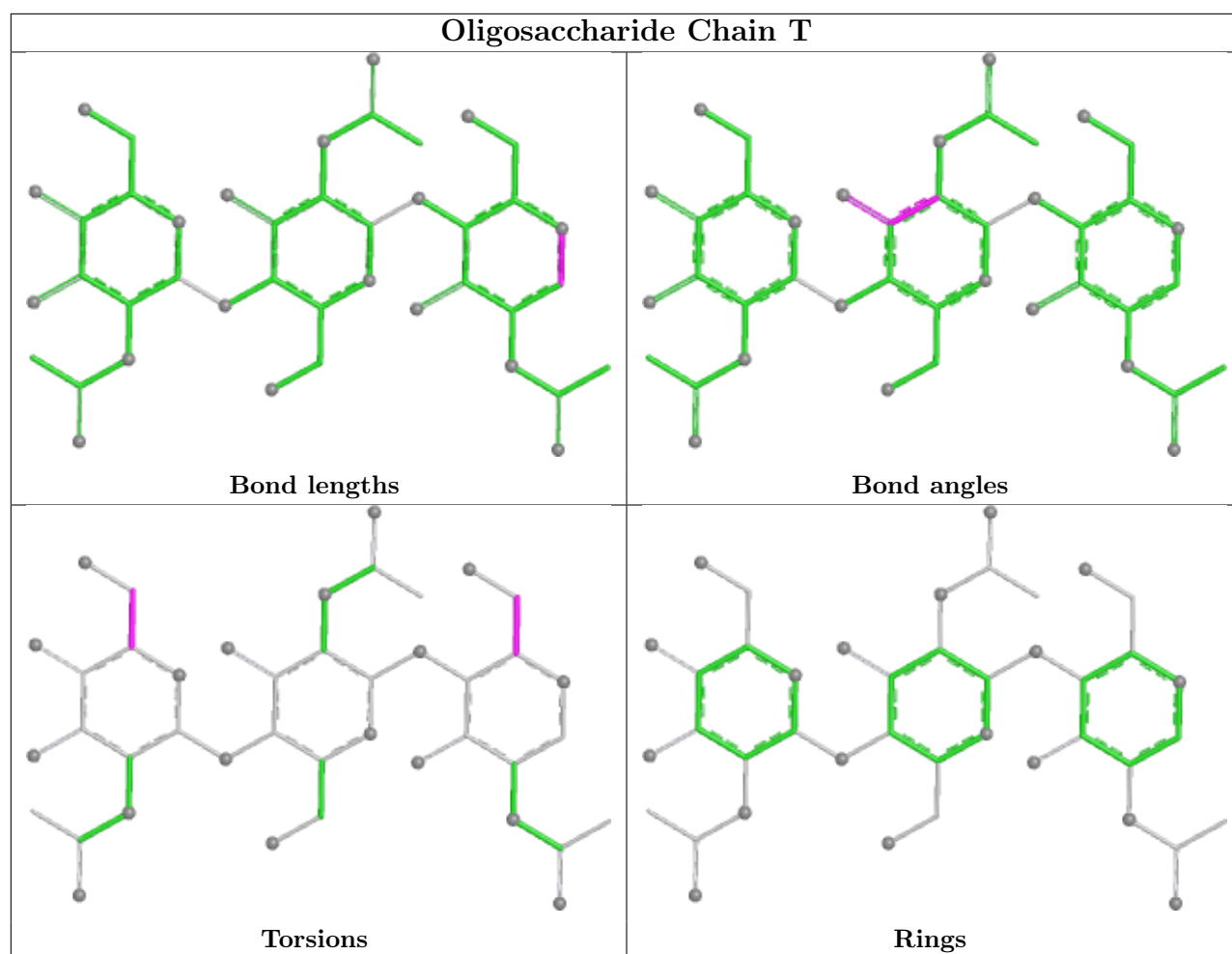
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	d	2	NAG	1	0
5	V	1	NAG	2	0
4	T	2	NAG	1	0
5	f	1	NAG	2	0
5	k	1	NAG	2	0
4	E	2	NAG	1	0
5	O	2	NAG	2	0
5	G	1	NAG	2	0
4	T	1	NAG	5	0
4	E	1	NAG	5	0
4	d	1	NAG	5	0

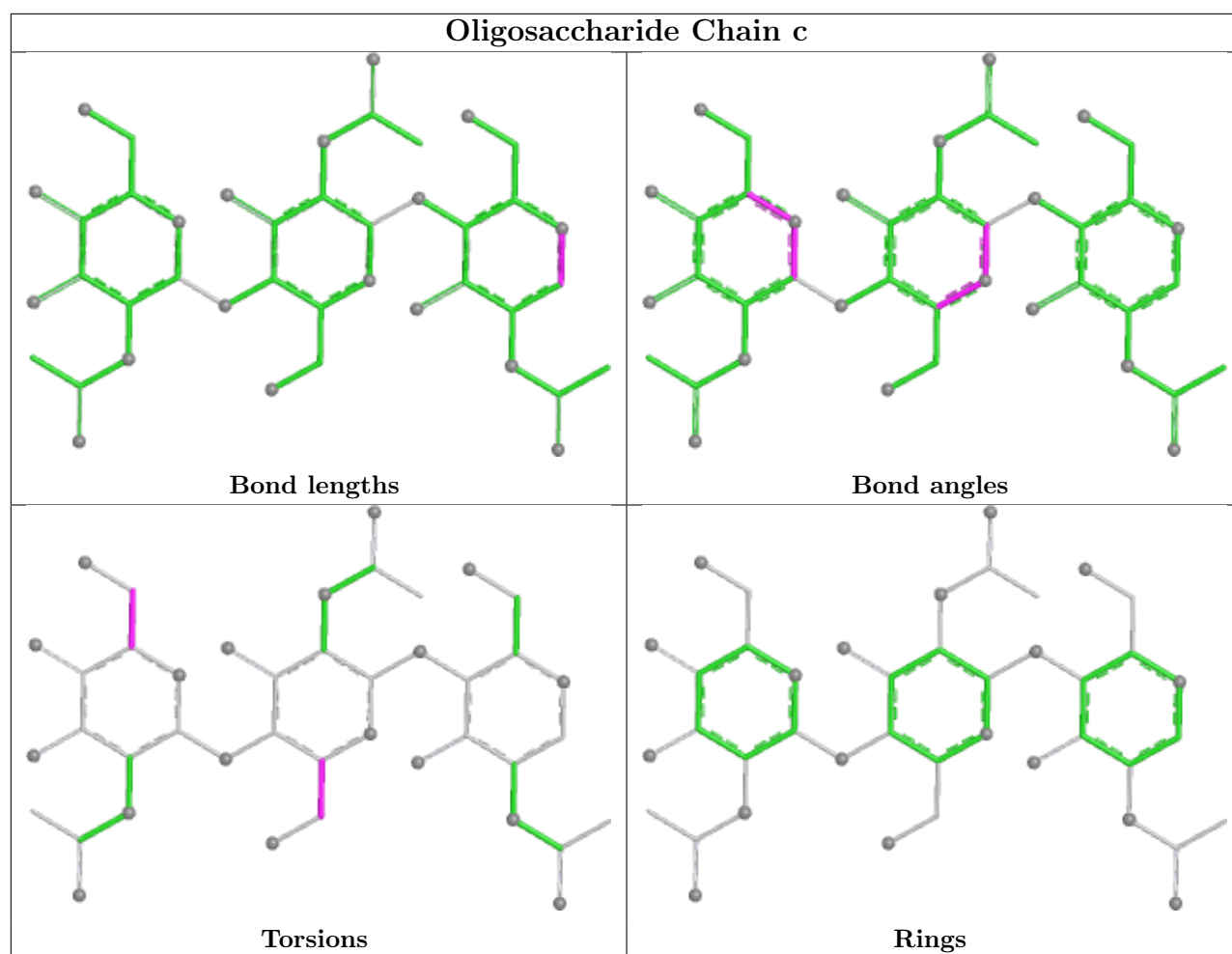
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

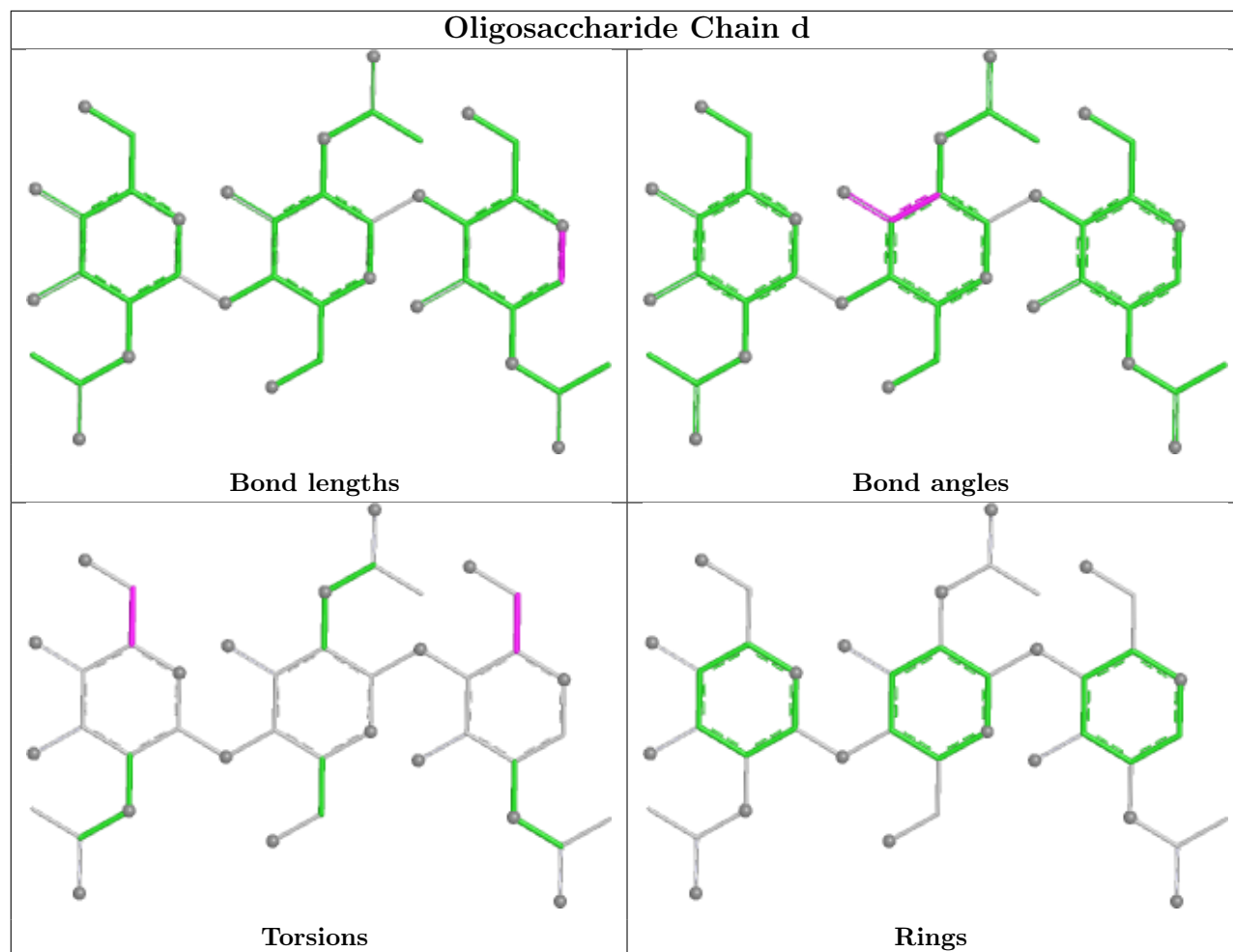


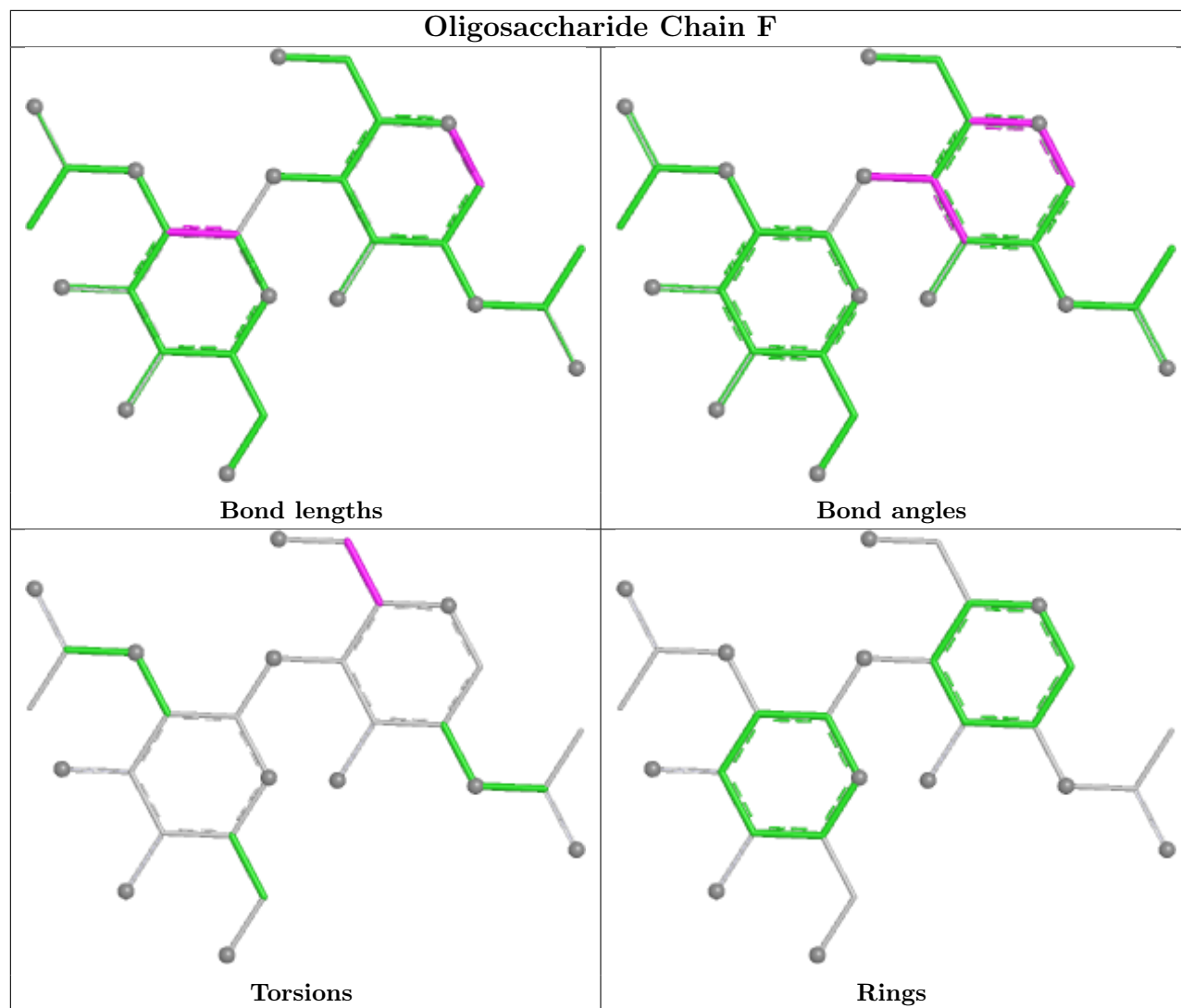


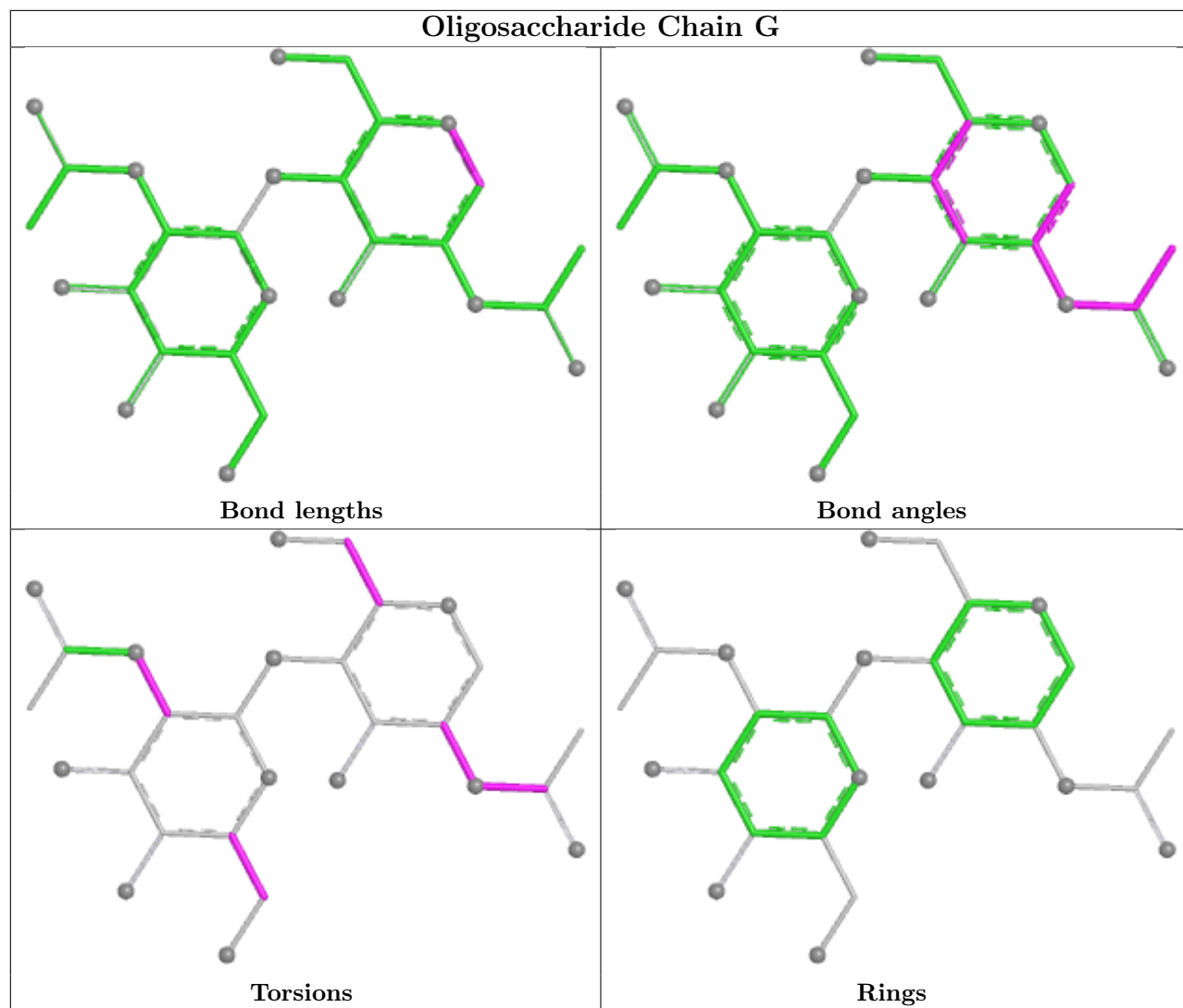


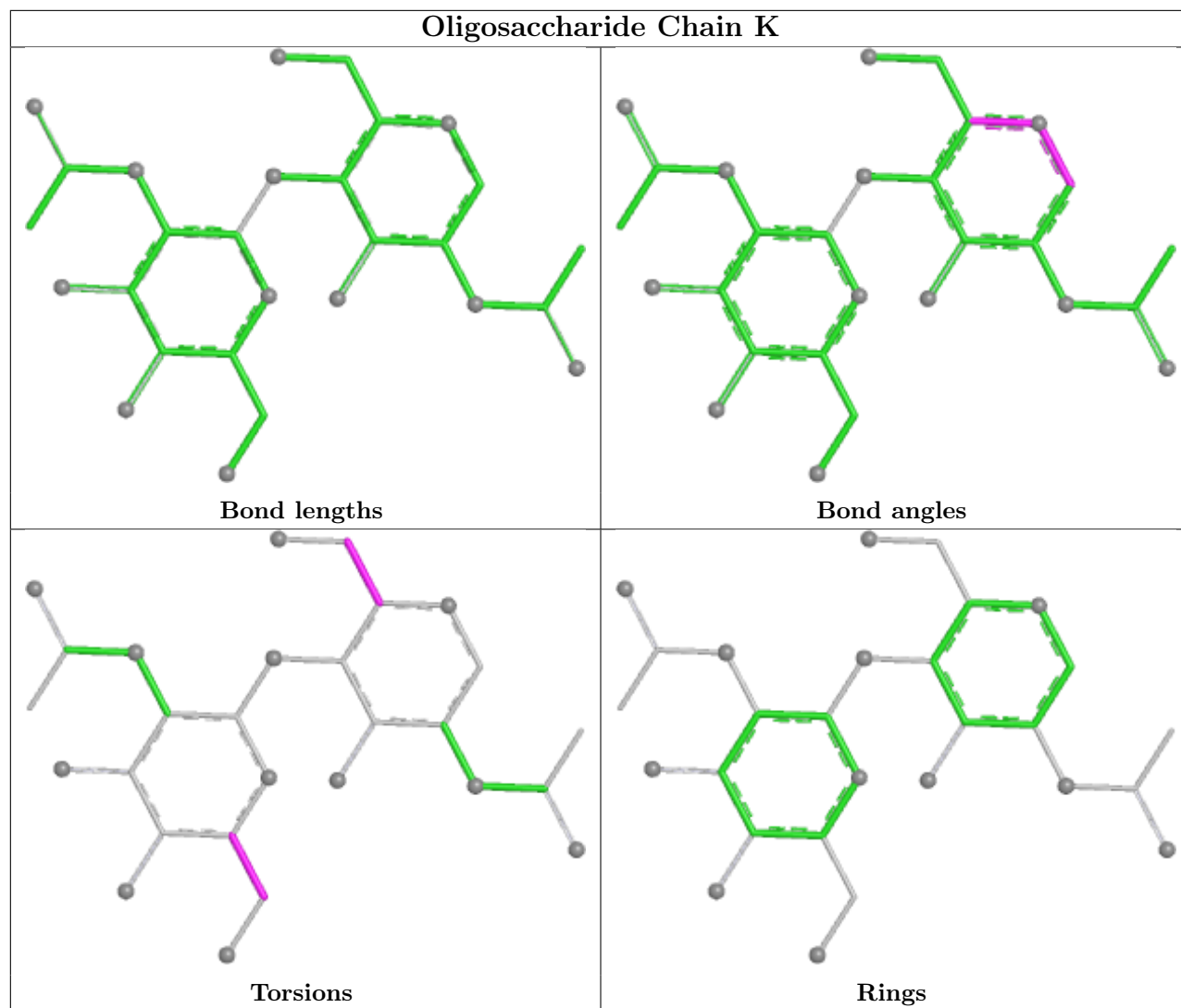


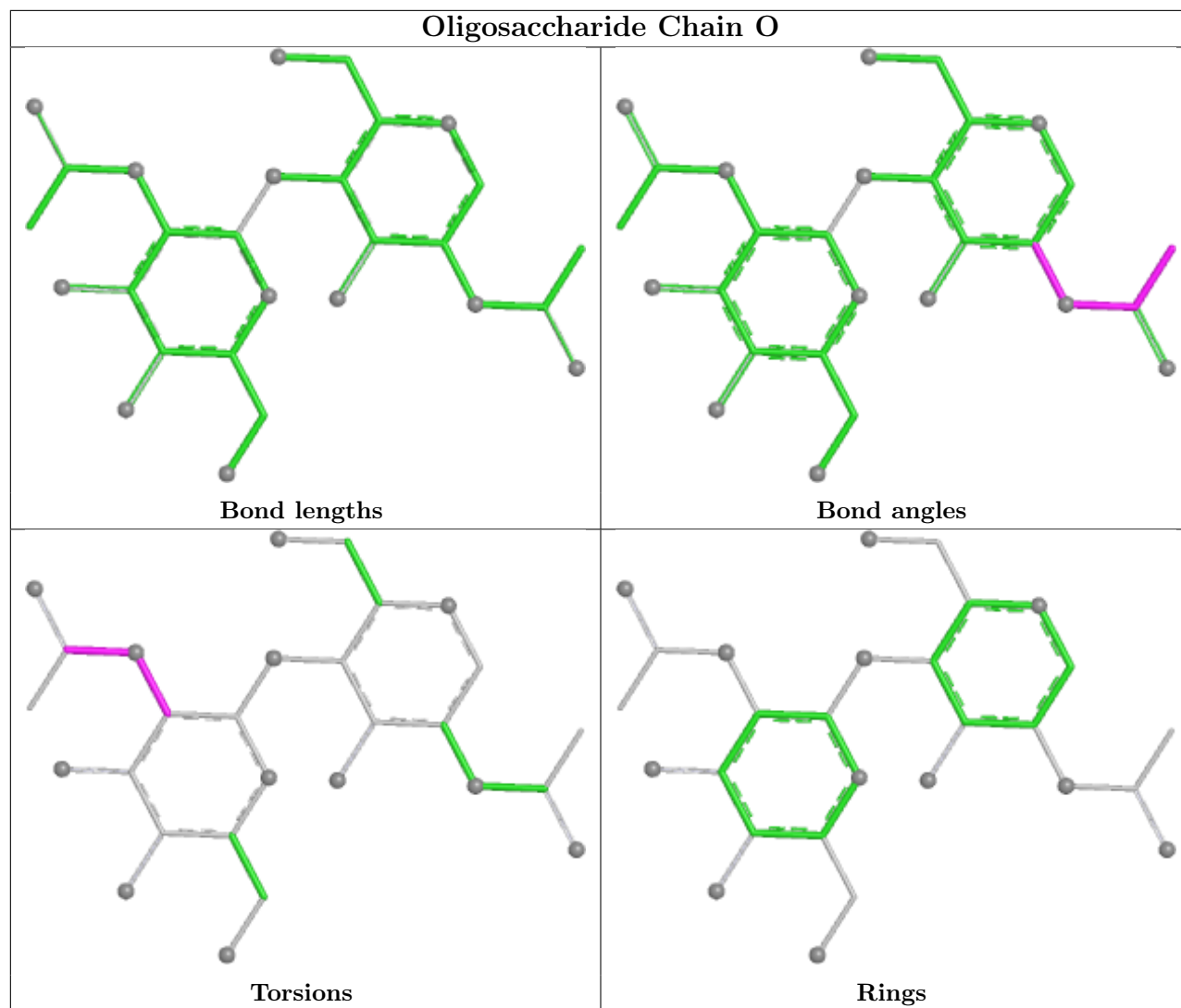


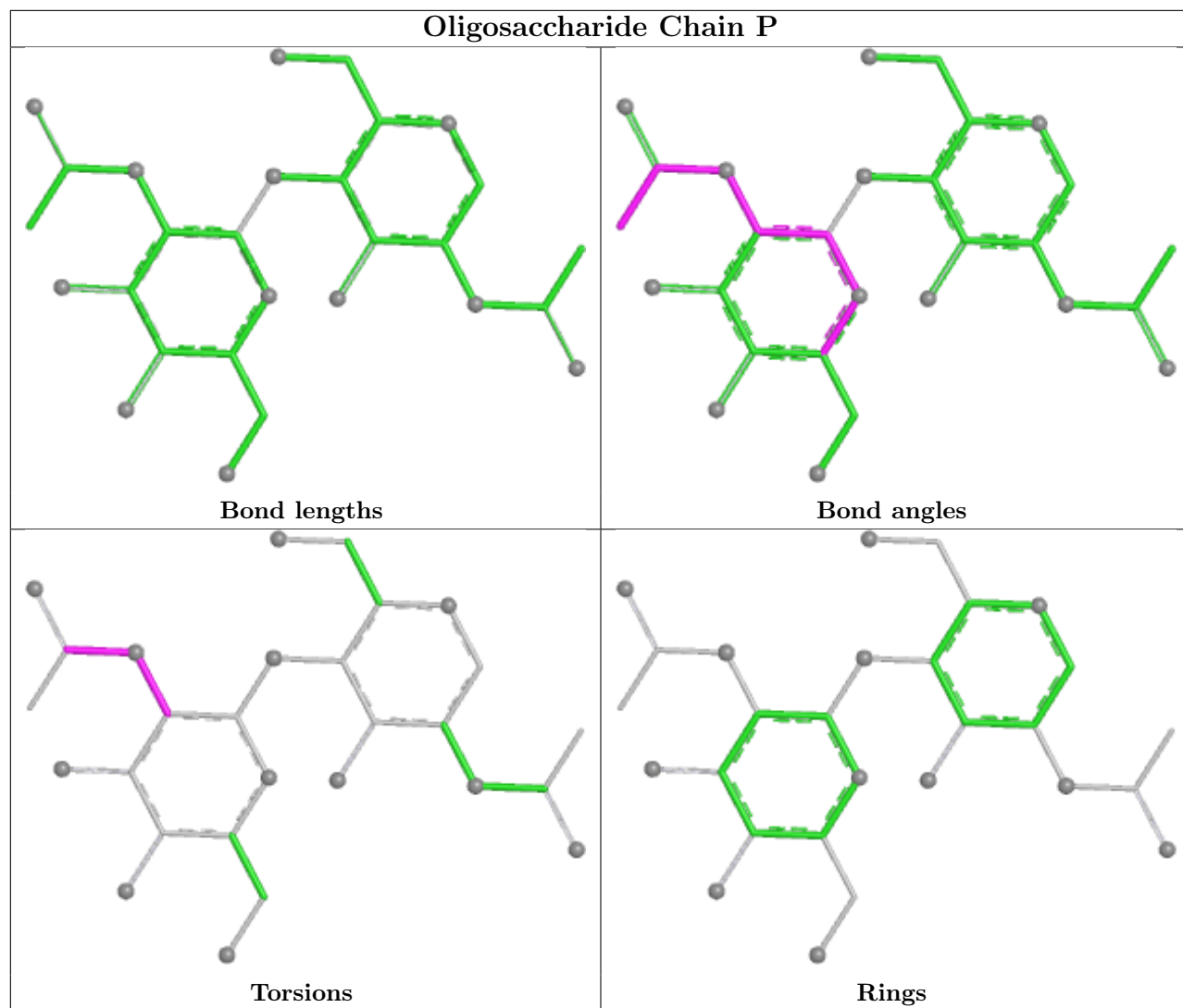


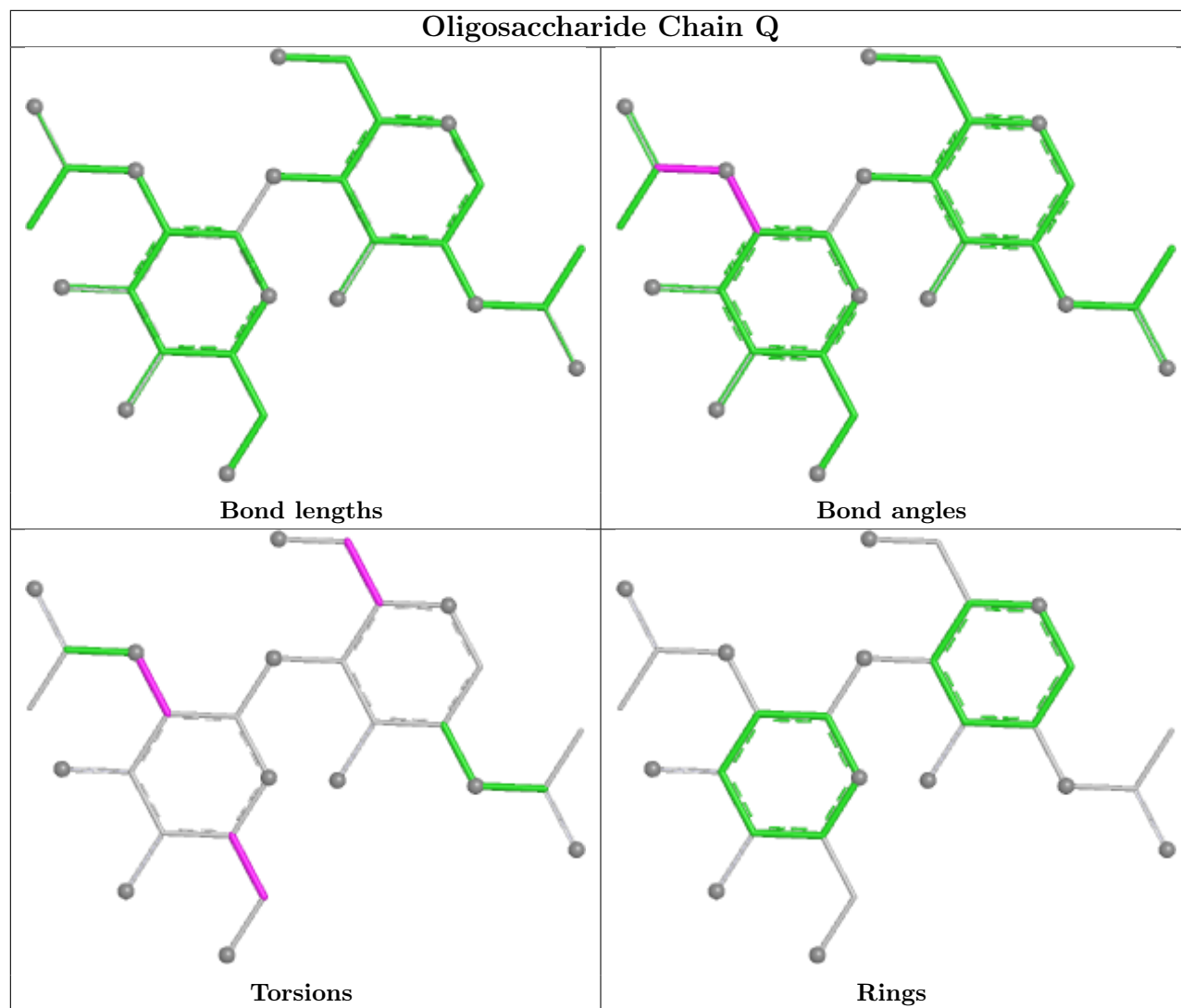


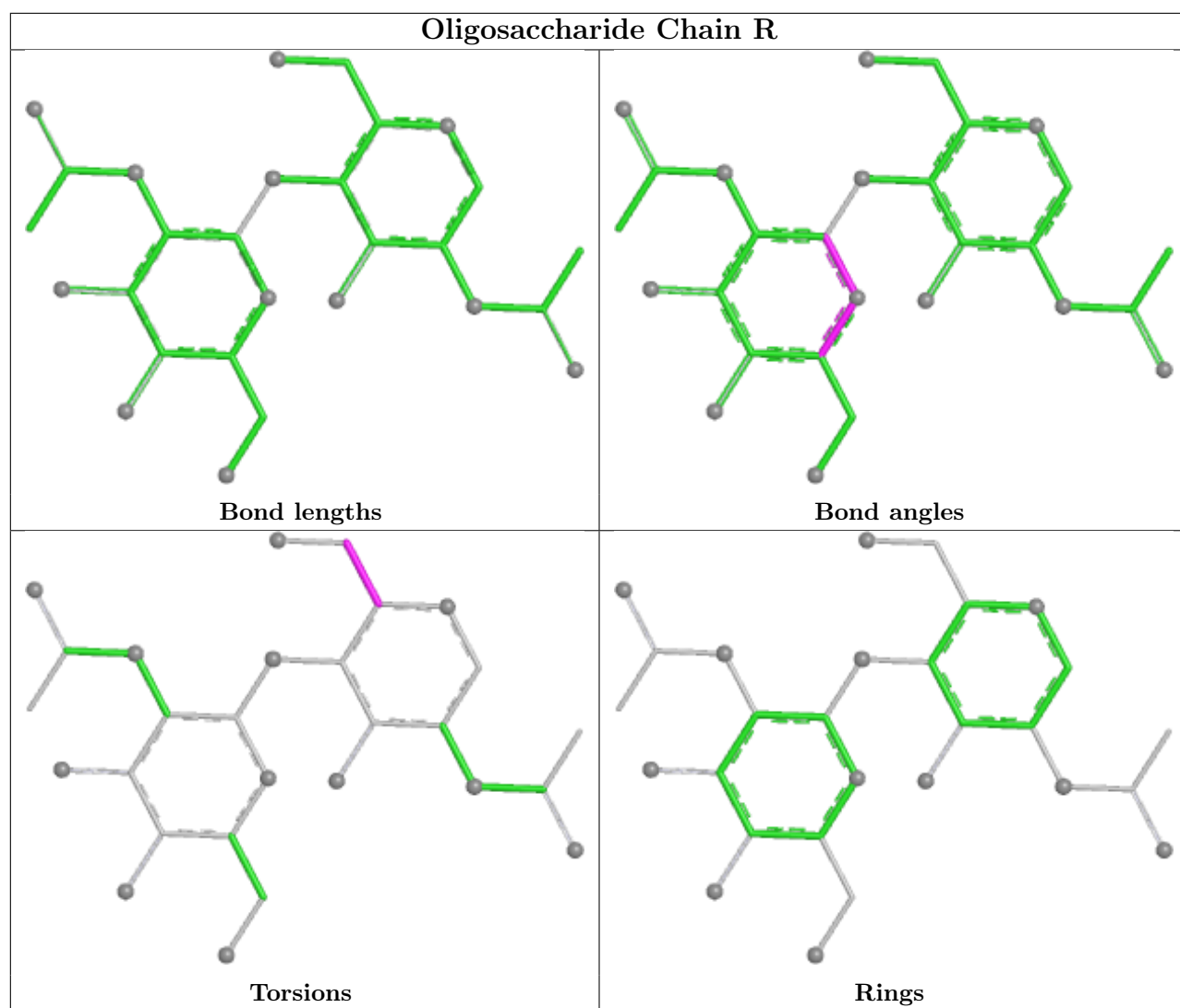


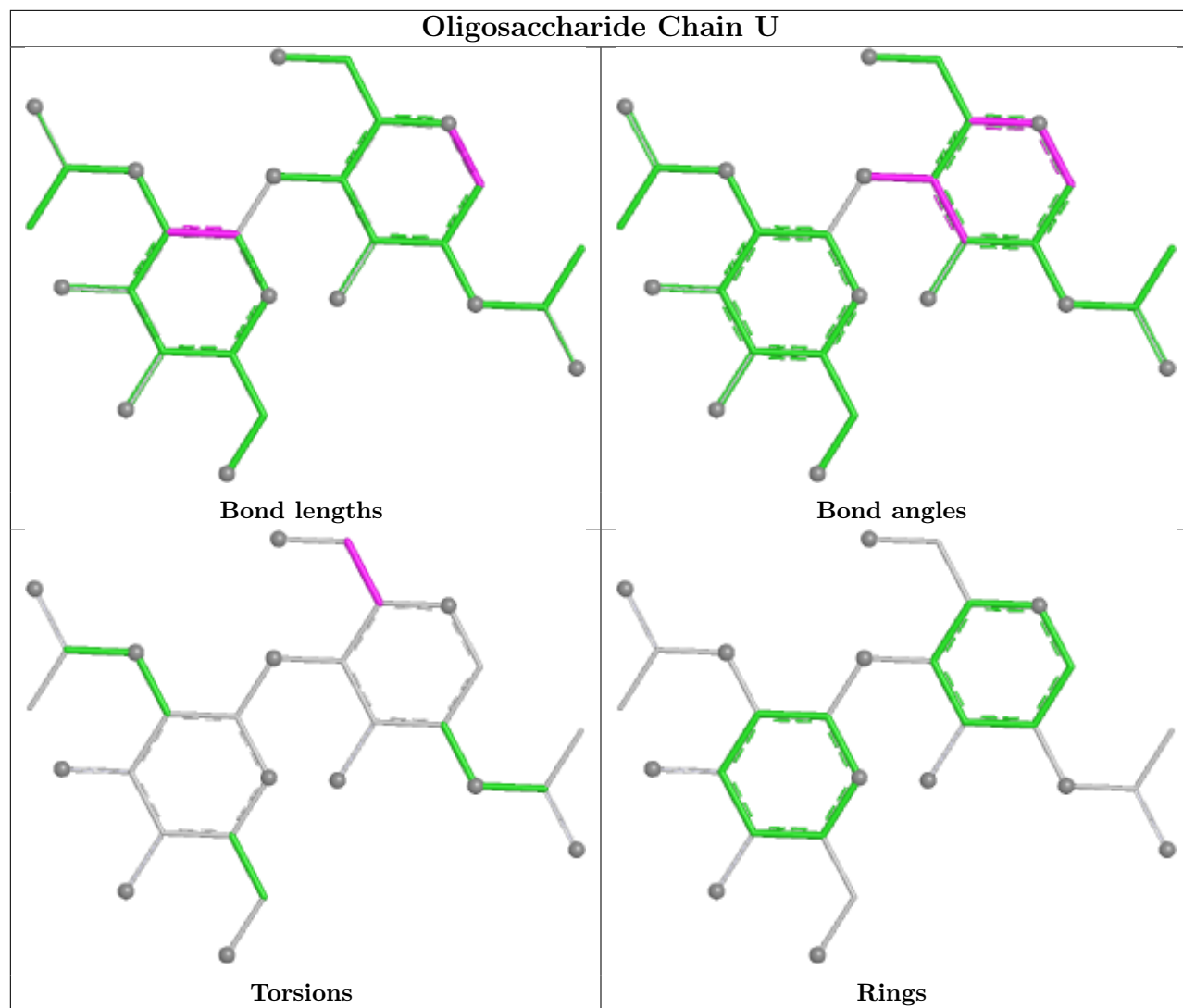


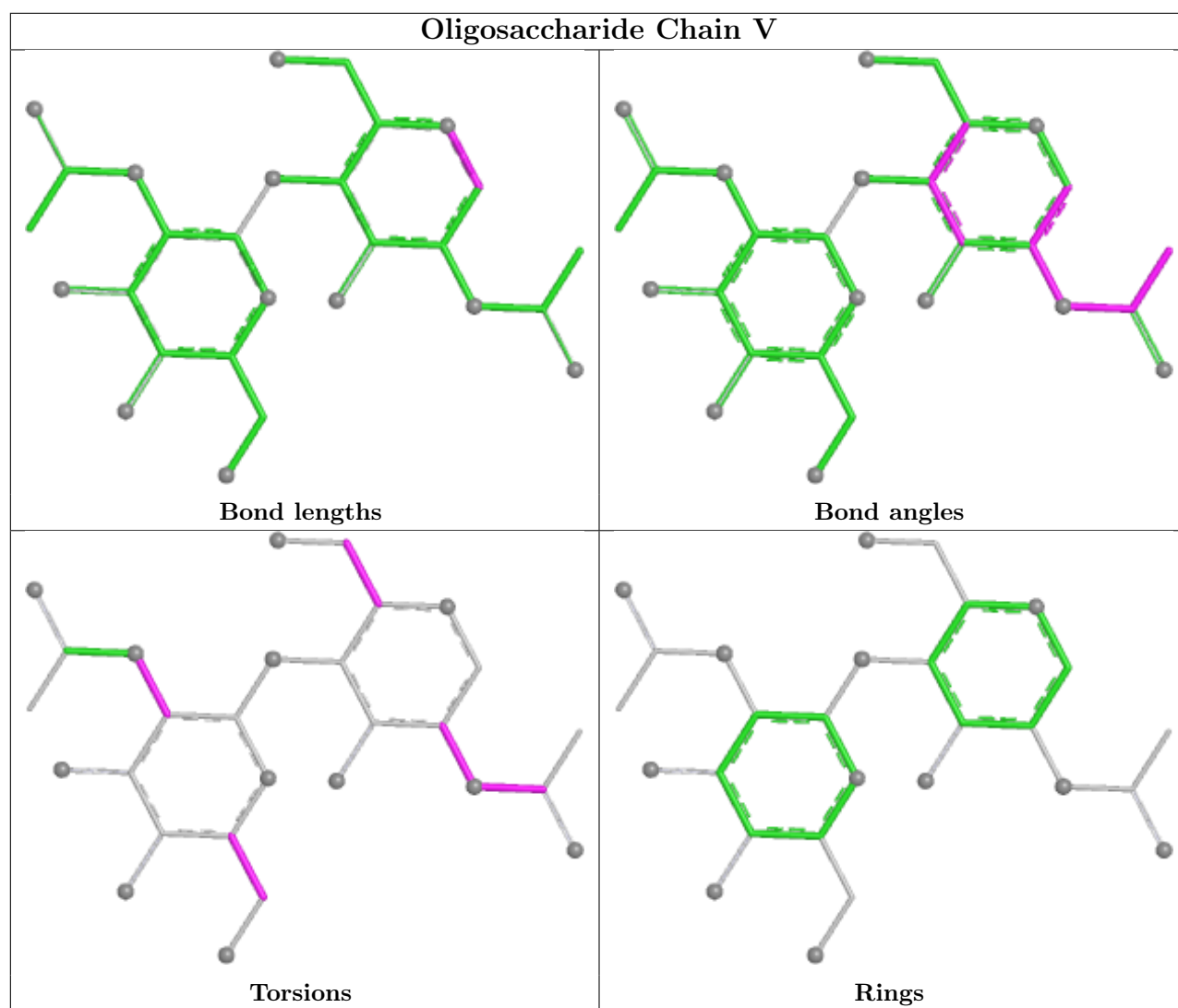


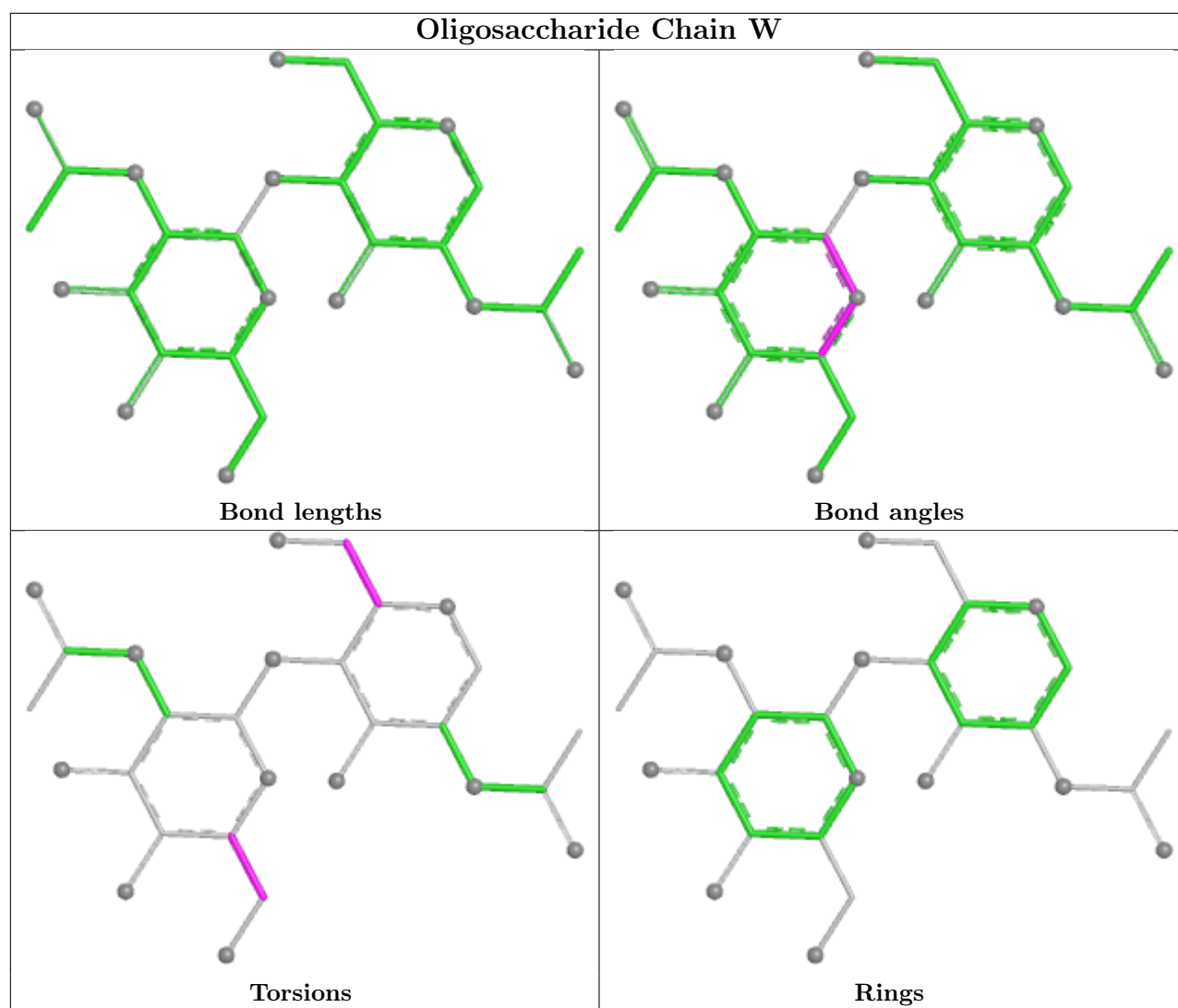


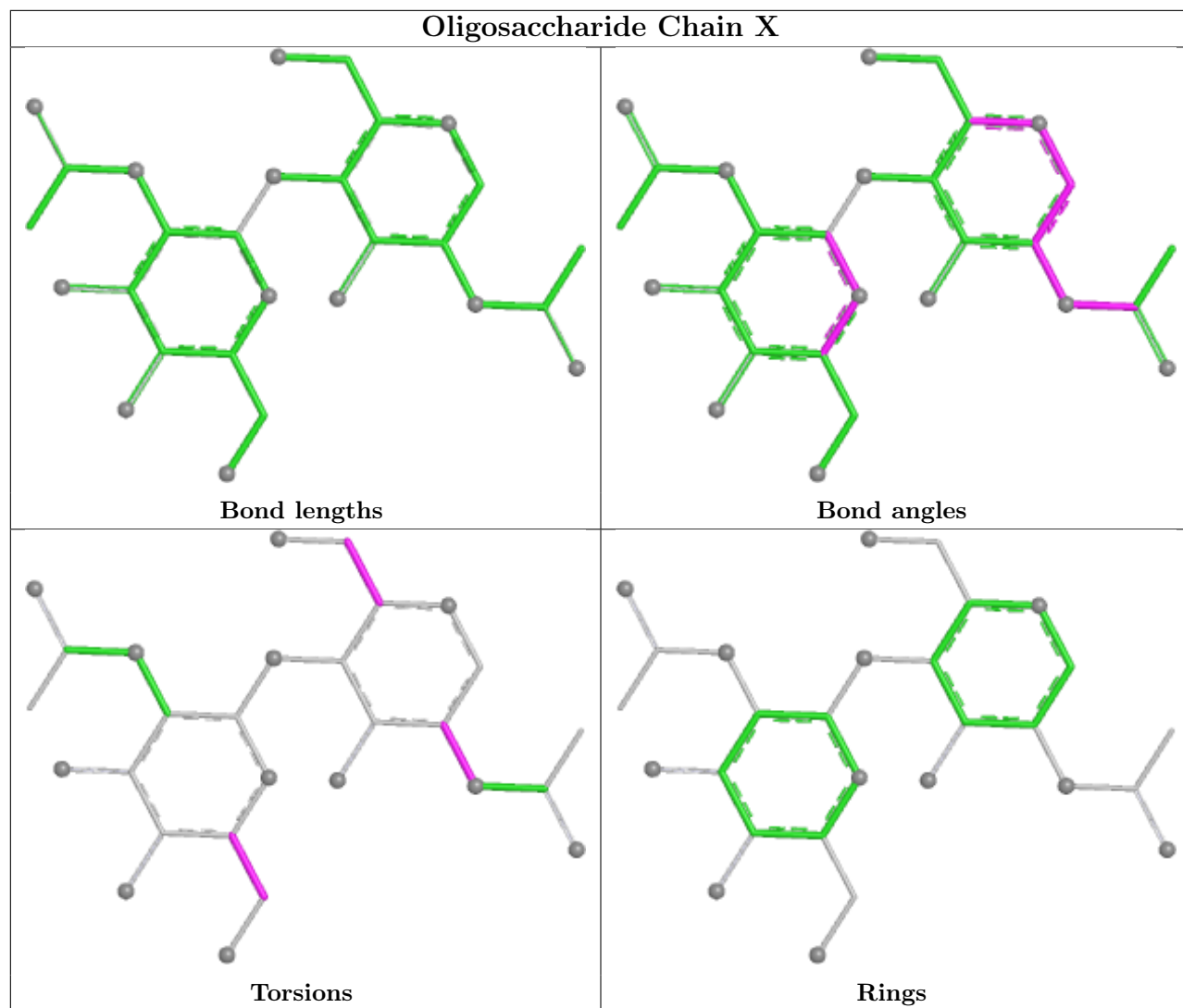


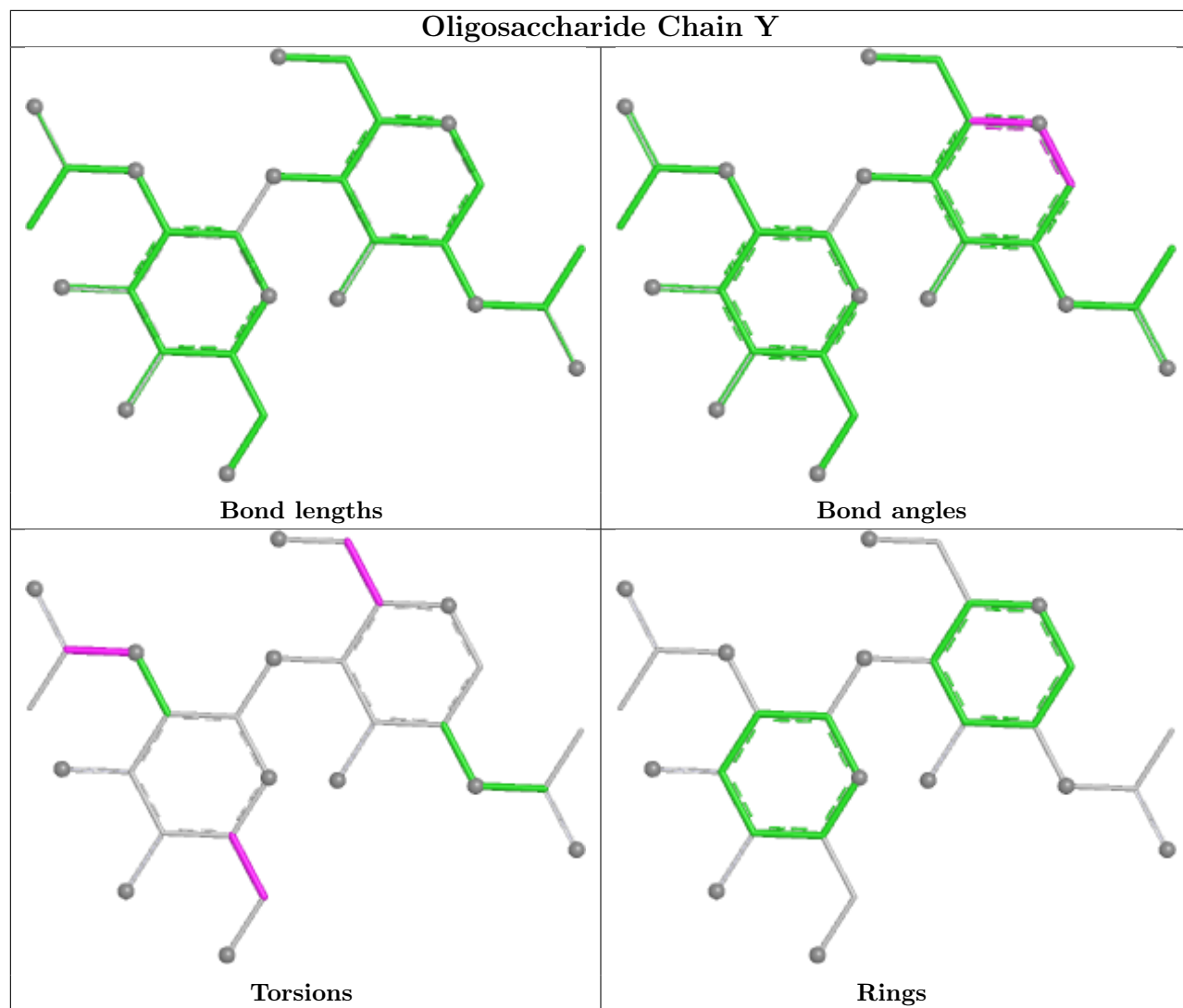


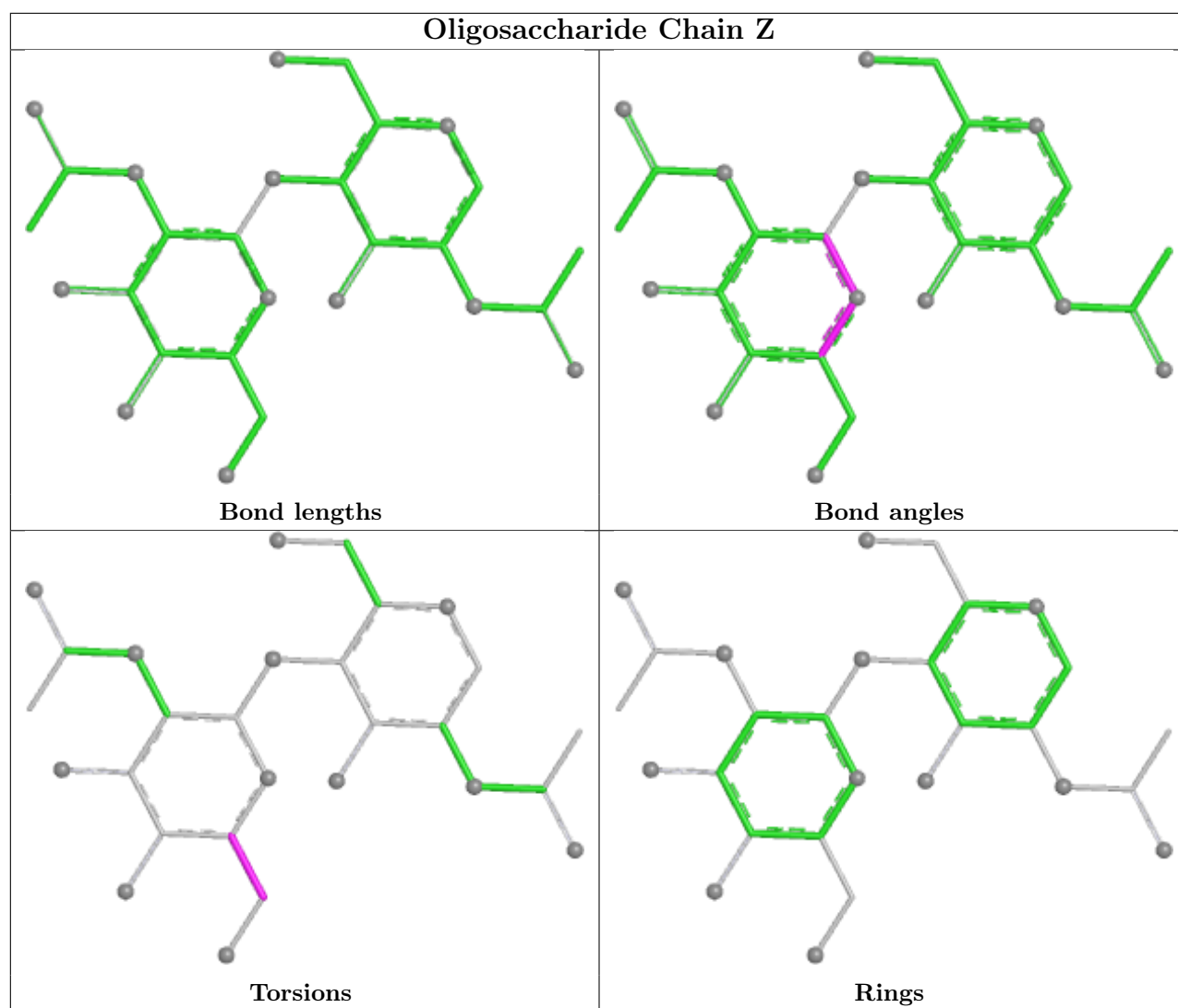


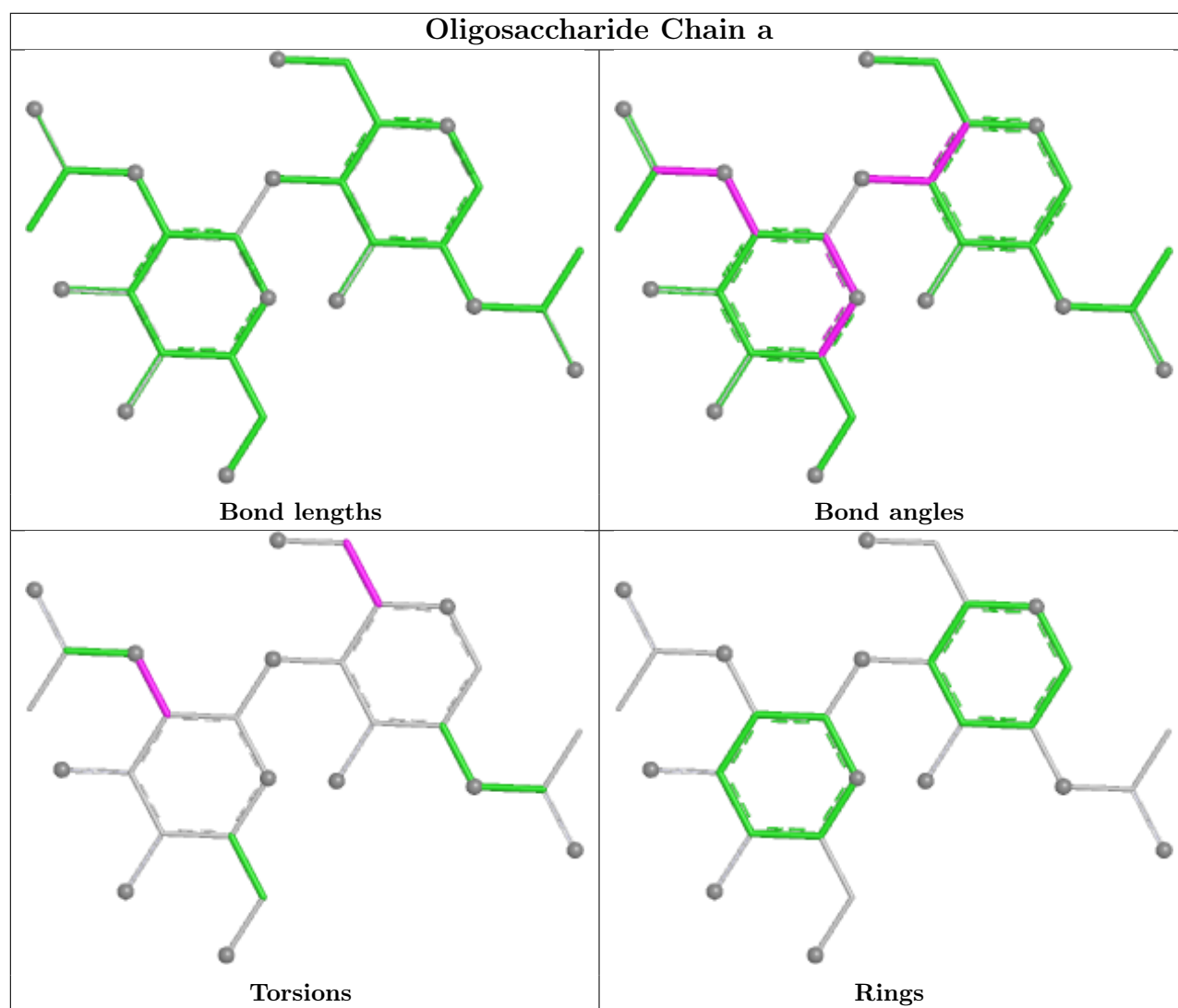


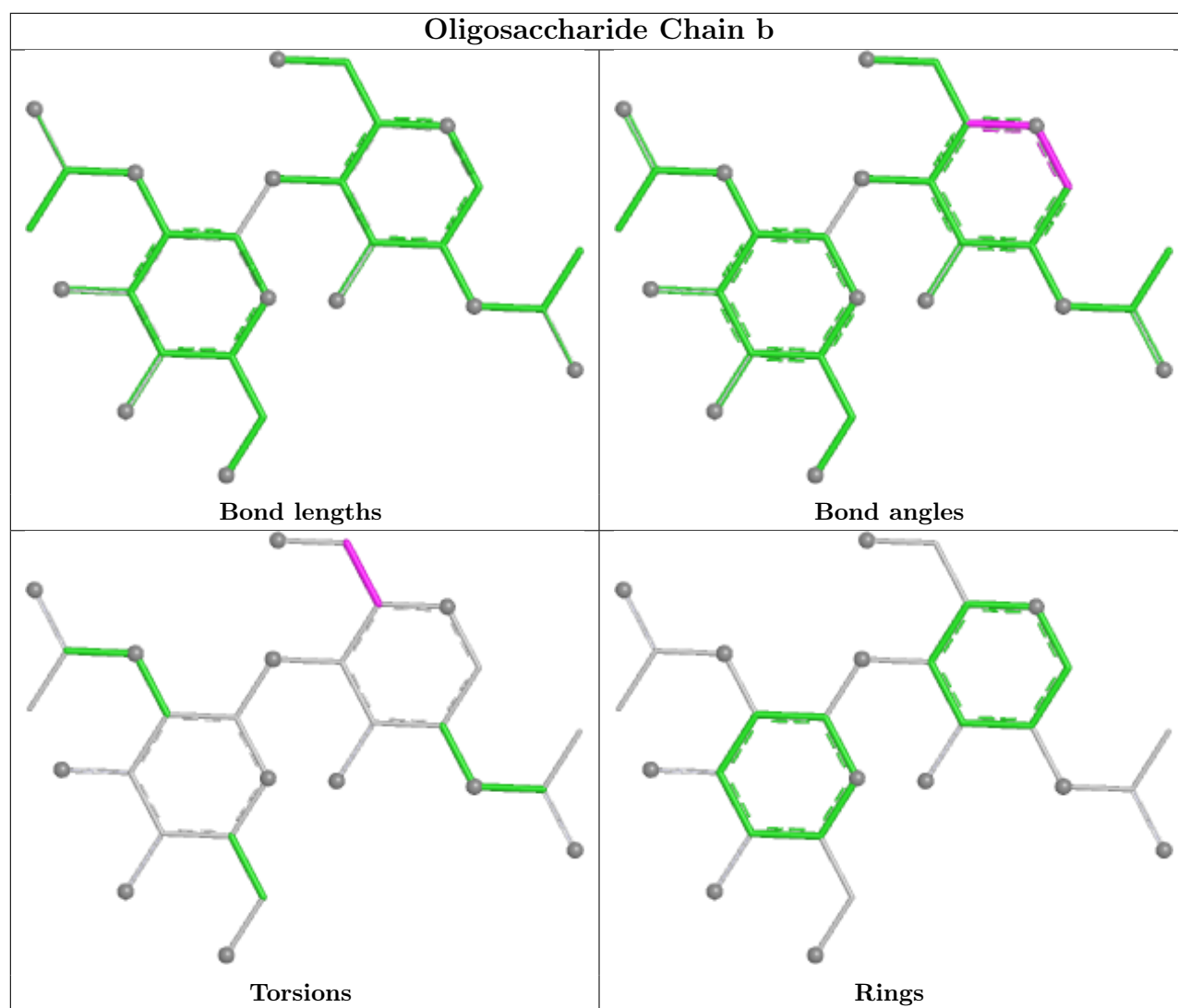


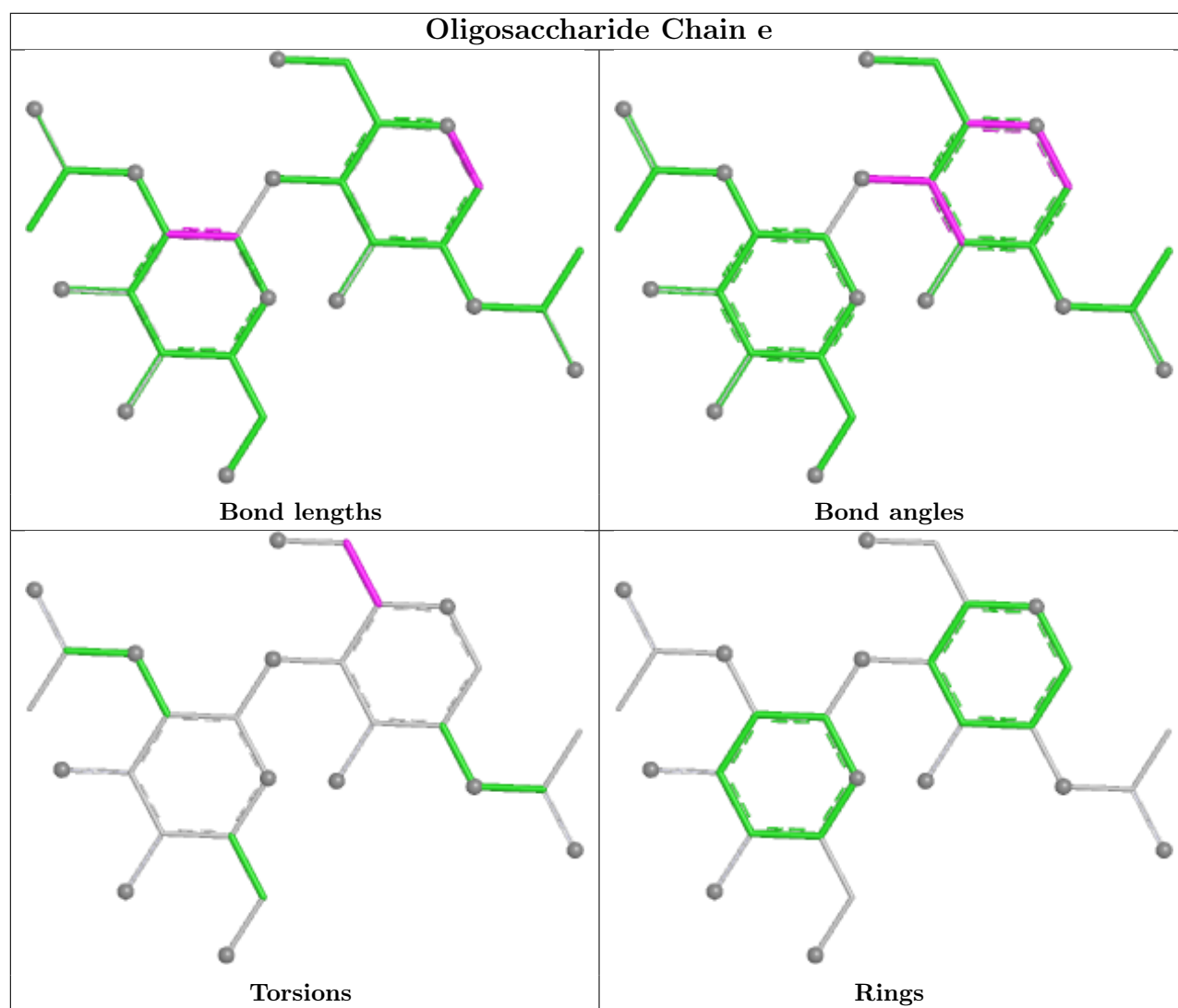


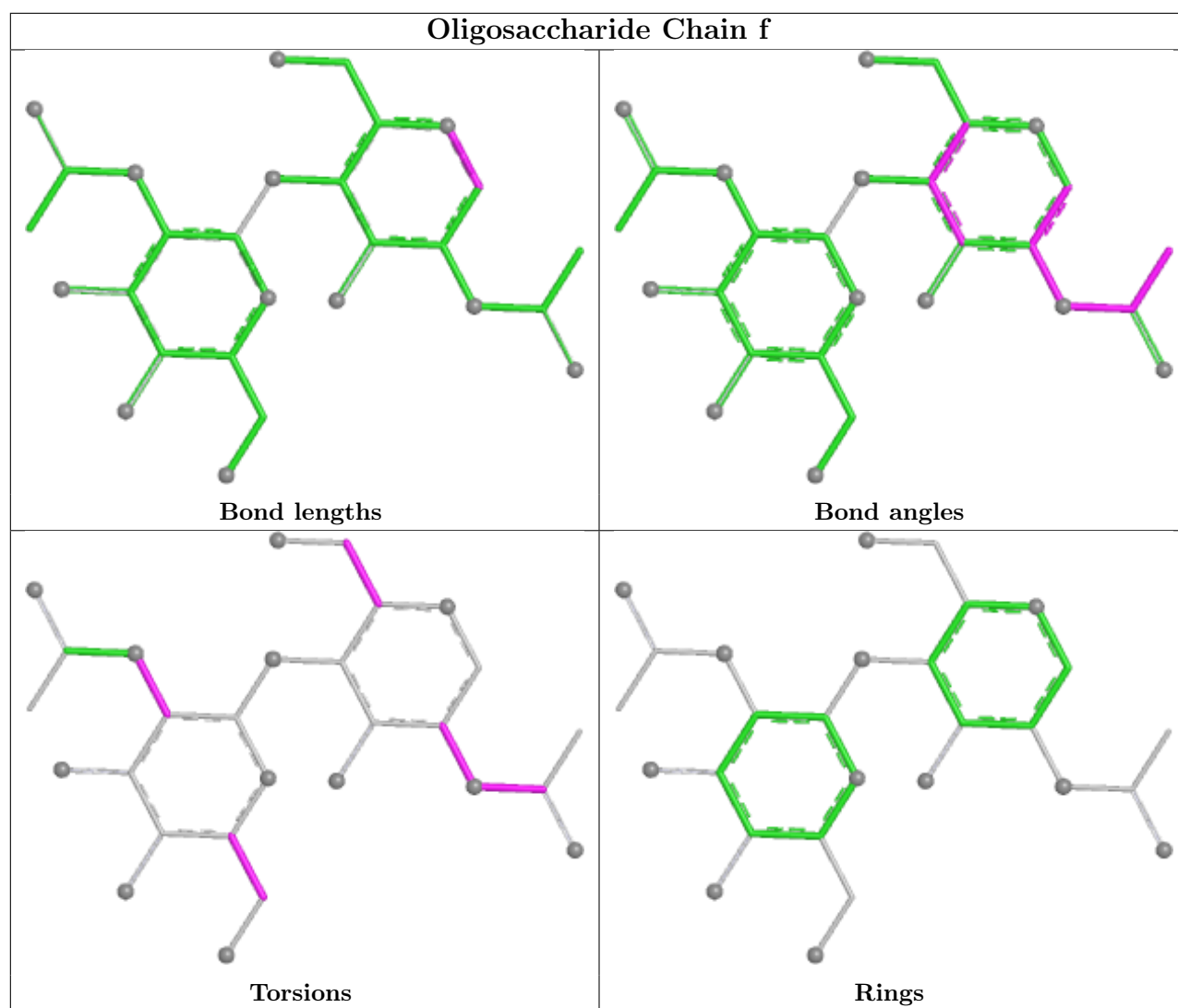


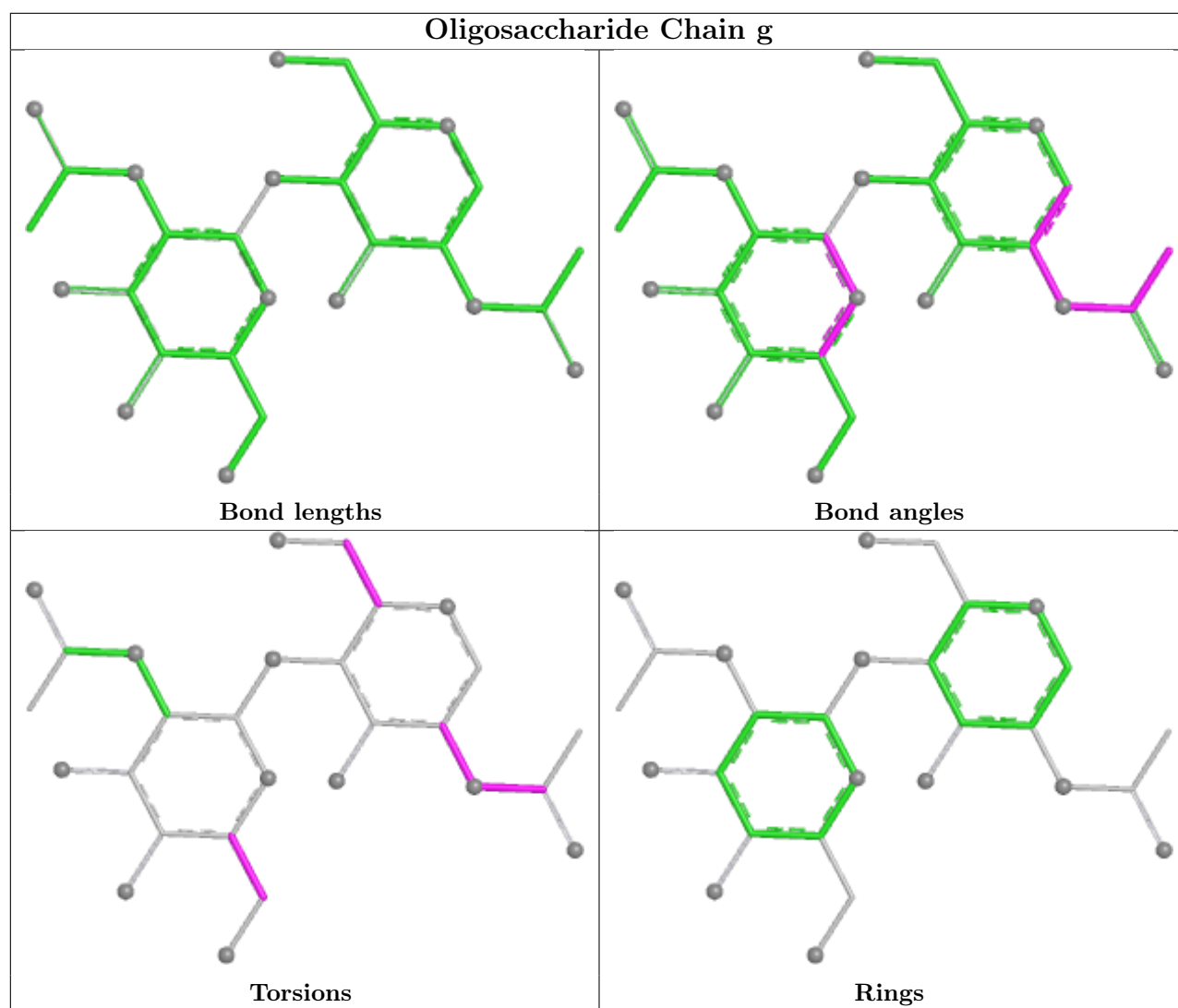


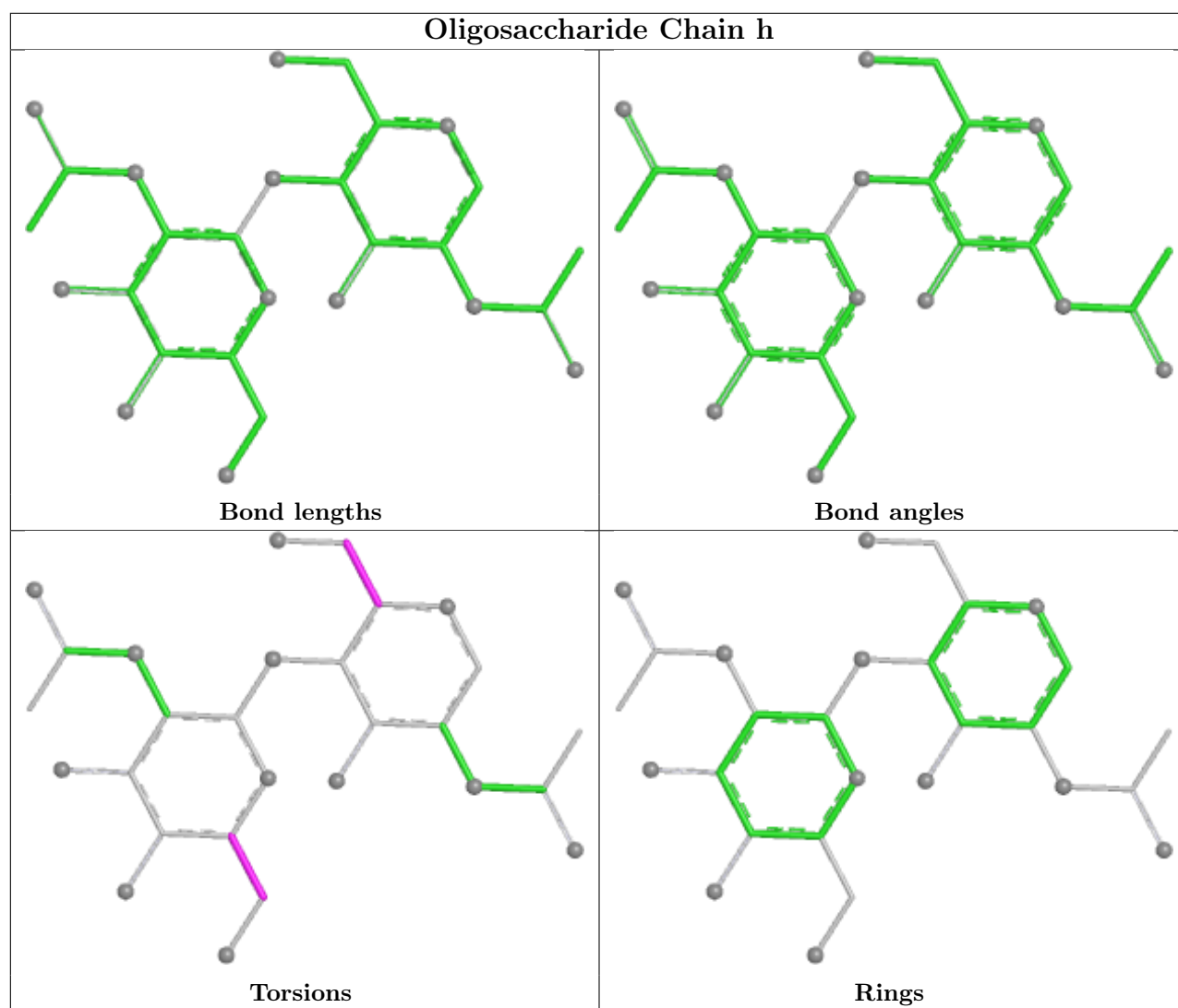


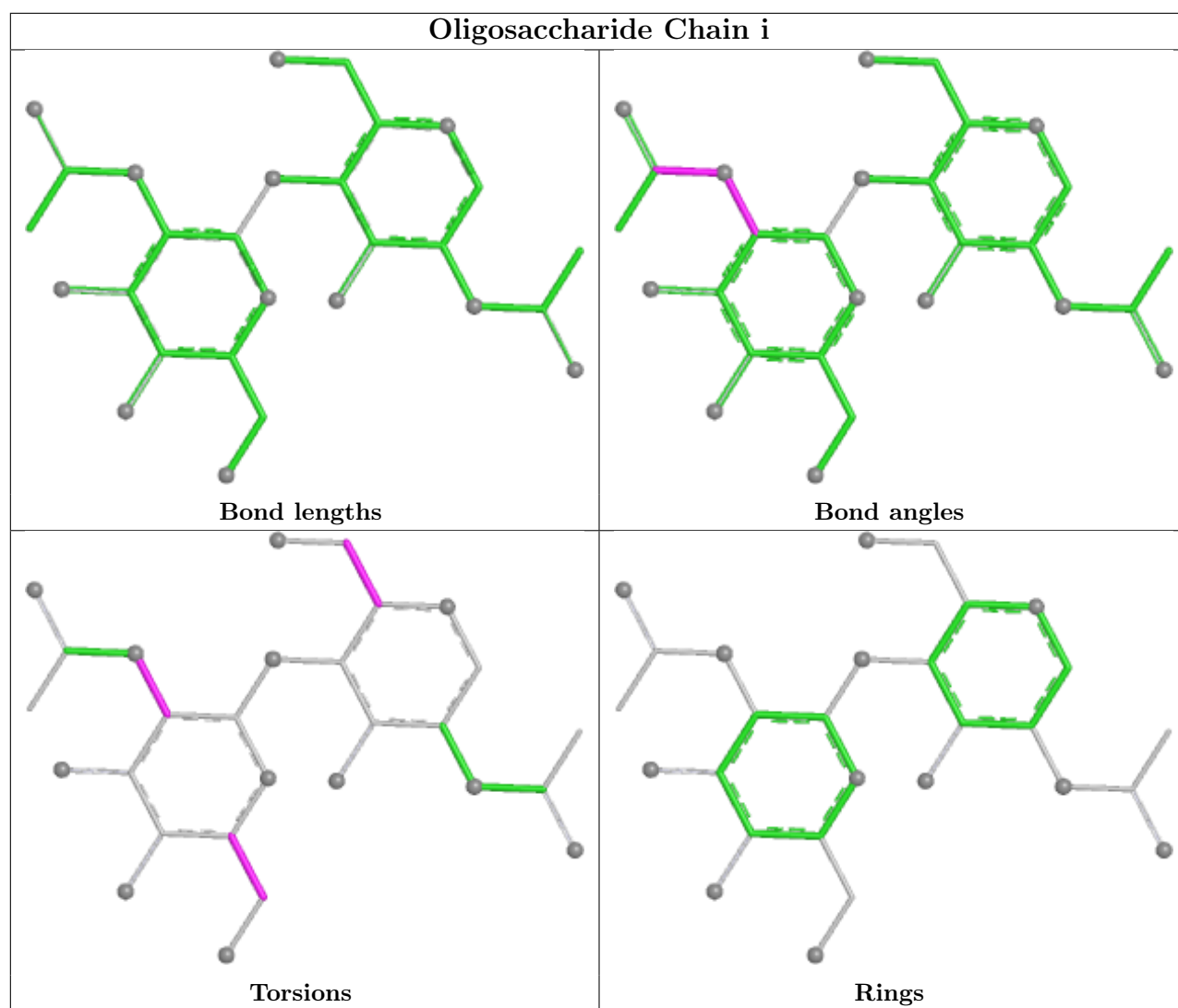


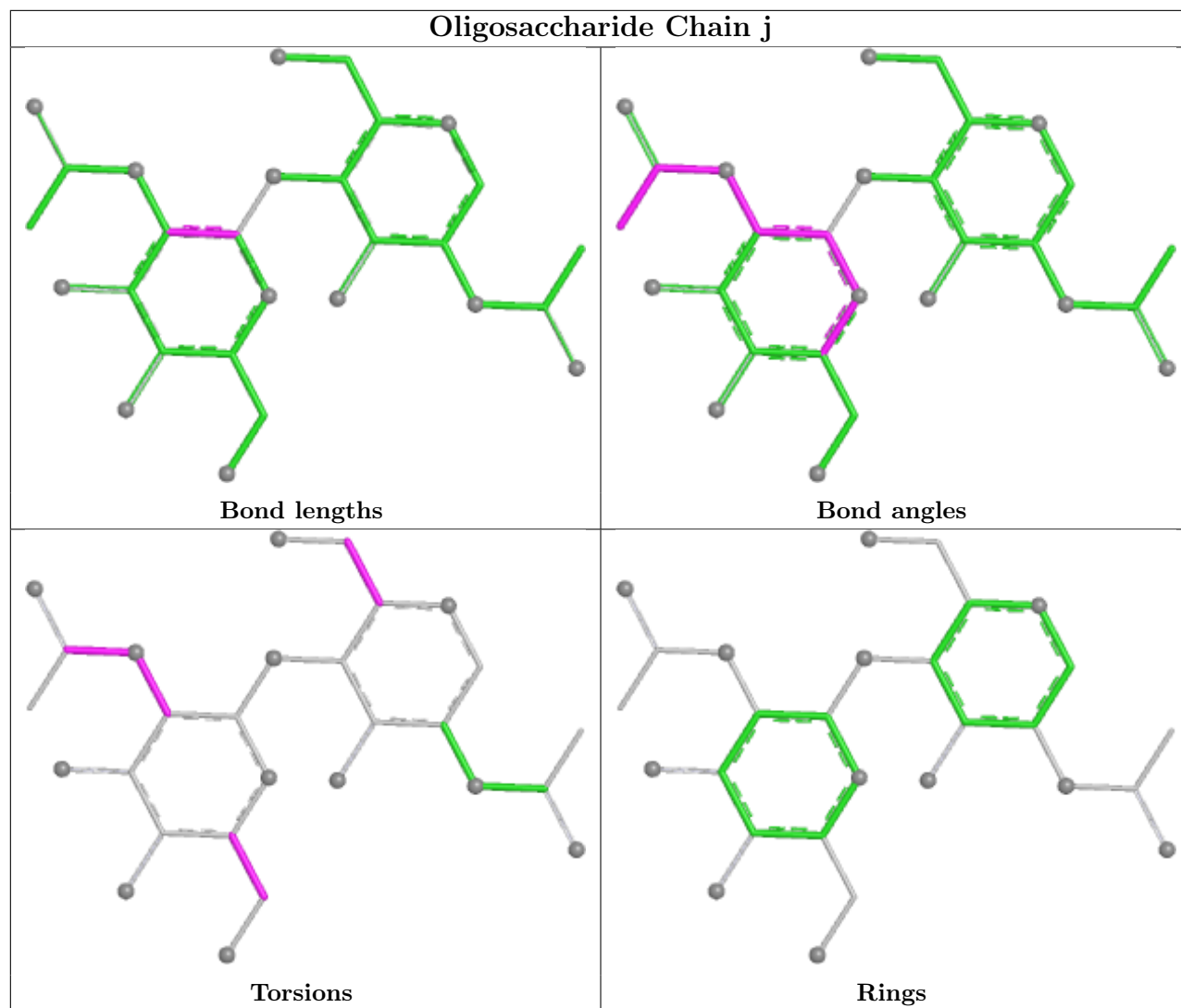


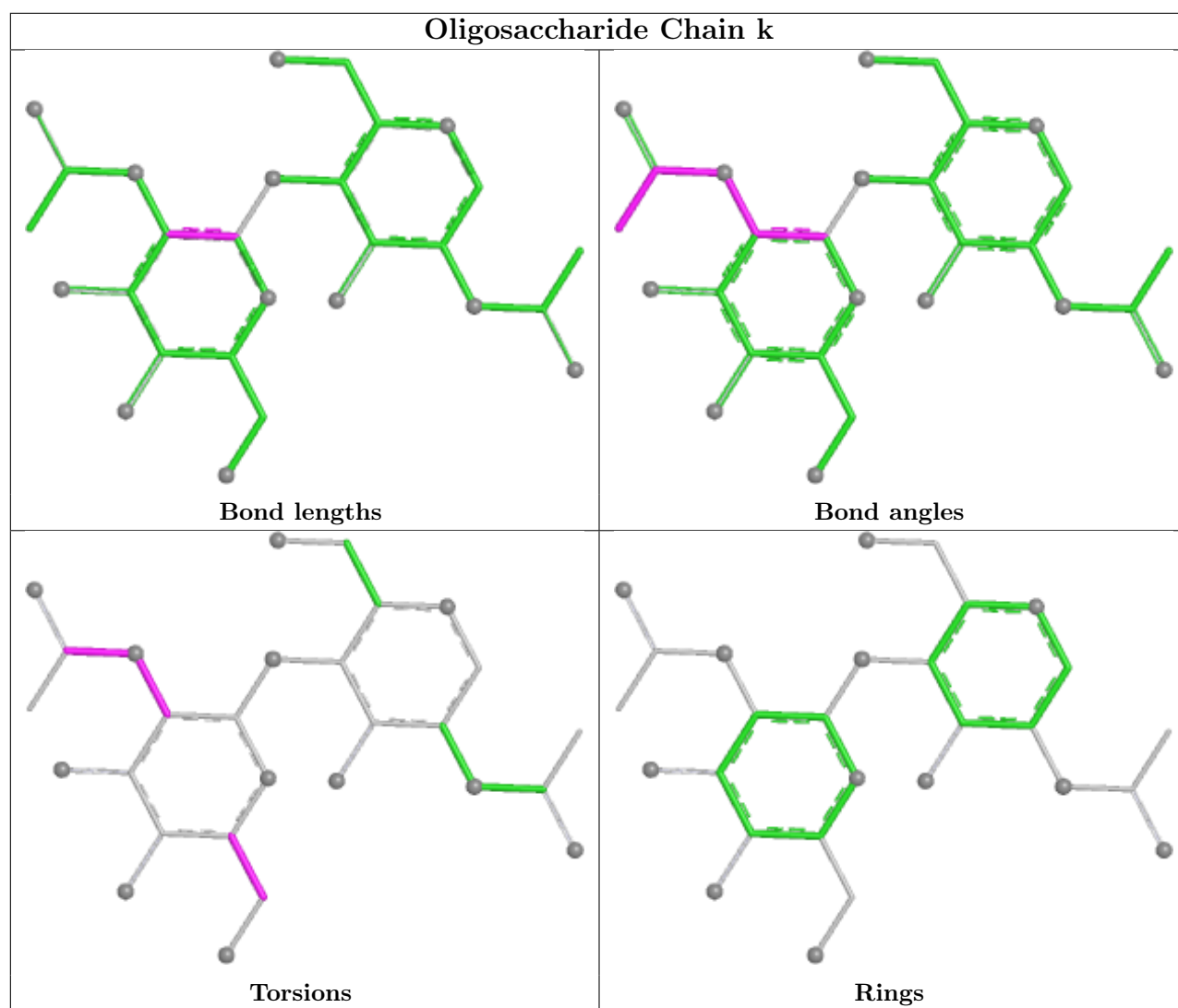


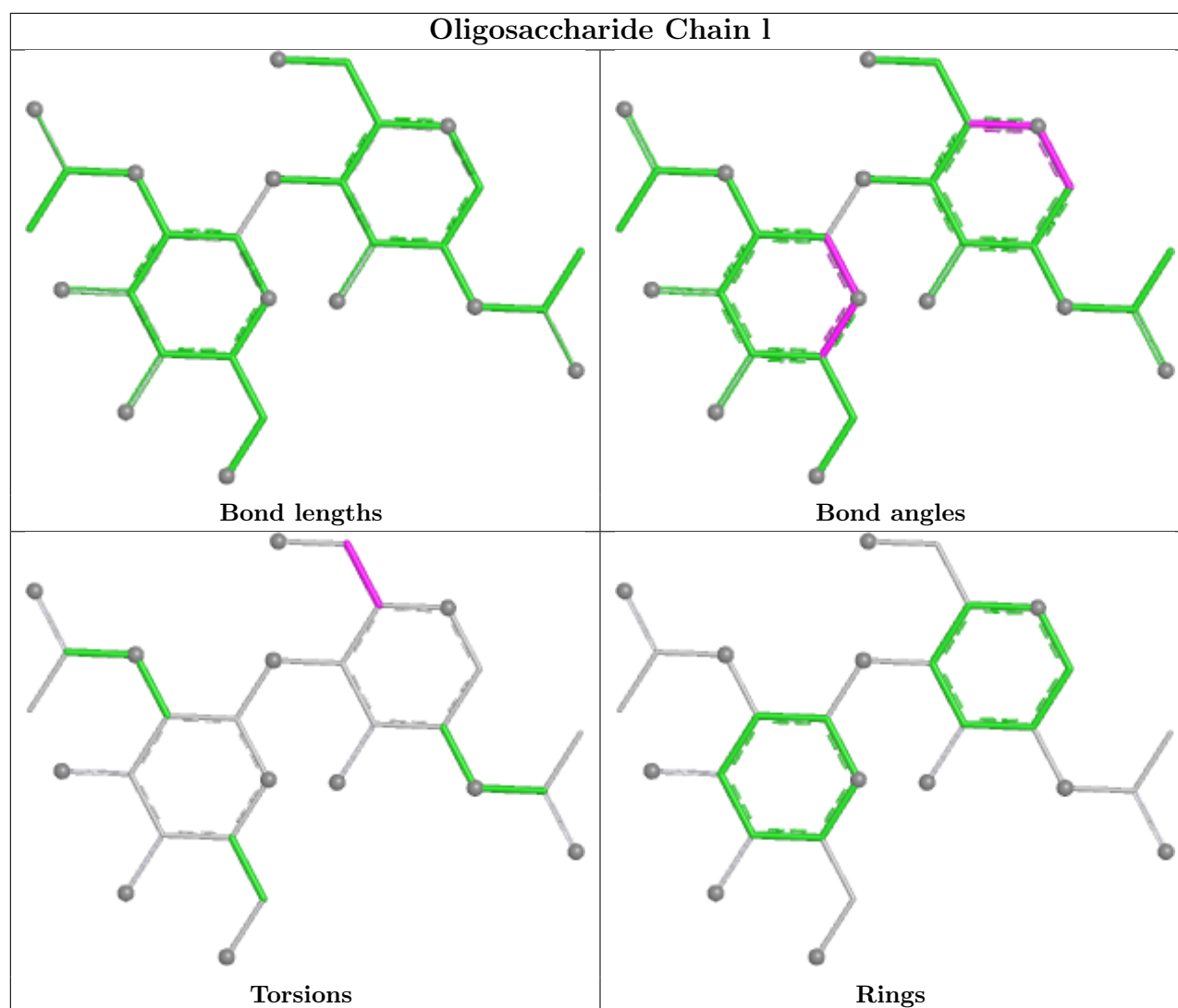












5.6 Ligand geometry [i](#)

25 ligands 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	$\# Z > 2$
6	NAG	A	1414	1	14,14,15	0.29	0	17,19,21	0.50	0
6	NAG	A	1415	1	14,14,15	0.39	0	17,19,21	0.41	0
6	NAG	A	1417	1	14,14,15	0.71	1 (7%)	17,19,21	0.72	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	NAG	A	1419	1	14,14,15	0.20	0	17,19,21	0.52	0
6	NAG	B	1416	1	14,14,15	0.60	1 (7%)	17,19,21	1.14	2 (11%)
6	NAG	A	1418	1	14,14,15	0.90	1 (7%)	17,19,21	1.08	1 (5%)
6	NAG	B	1417	1	14,14,15	0.30	0	17,19,21	0.62	1 (5%)
6	NAG	A	1402	1	14,14,15	0.21	0	17,19,21	0.56	0
6	NAG	A	1401	1	14,14,15	0.42	0	17,19,21	1.15	2 (11%)
6	NAG	B	1406	1	14,14,15	0.36	0	17,19,21	0.54	0
6	NAG	C	1401	1	14,14,15	0.41	0	17,19,21	1.16	2 (11%)
6	NAG	B	1418	1	14,14,15	0.19	0	17,19,21	0.47	0
6	NAG	C	1417	1	14,14,15	0.58	0	17,19,21	1.11	2 (11%)
6	NAG	B	1414	1	14,14,15	0.52	0	17,19,21	0.56	0
6	NAG	C	1402	1	14,14,15	0.21	0	17,19,21	0.56	0
6	NAG	C	1414	1	14,14,15	0.52	0	17,19,21	0.52	0
6	NAG	C	1415	1	14,14,15	0.33	0	17,19,21	0.57	0
6	NAG	C	1416	1	14,14,15	0.28	0	17,19,21	0.67	0
6	NAG	C	1406	1	14,14,15	0.36	0	17,19,21	0.55	0
6	NAG	B	1415	1	14,14,15	0.46	0	17,19,21	1.10	2 (11%)
6	NAG	A	1416	1	14,14,15	0.43	0	17,19,21	0.48	0
6	NAG	B	1402	1	14,14,15	0.22	0	17,19,21	0.57	0
6	NAG	C	1418	1	14,14,15	0.51	0	17,19,21	0.61	1 (5%)
6	NAG	B	1401	1	14,14,15	0.43	0	17,19,21	1.15	2 (11%)
6	NAG	A	1406	1	14,14,15	0.36	0	17,19,21	0.54	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
6	NAG	A	1414	1	-	1/6/23/26	0/1/1/1
6	NAG	A	1415	1	-	2/6/23/26	0/1/1/1
6	NAG	A	1417	1	-	2/6/23/26	0/1/1/1
6	NAG	A	1419	1	-	2/6/23/26	0/1/1/1
6	NAG	B	1416	1	-	4/6/23/26	0/1/1/1
6	NAG	A	1418	1	-	2/6/23/26	0/1/1/1
6	NAG	B	1417	1	-	2/6/23/26	0/1/1/1
6	NAG	A	1402	1	-	1/6/23/26	0/1/1/1
6	NAG	A	1401	1	-	0/6/23/26	0/1/1/1
6	NAG	B	1406	1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	C	1401	1	-	0/6/23/26	0/1/1/1
6	NAG	B	1418	1	-	0/6/23/26	0/1/1/1
6	NAG	C	1417	1	-	4/6/23/26	0/1/1/1
6	NAG	B	1414	1	-	4/6/23/26	0/1/1/1
6	NAG	C	1402	1	-	1/6/23/26	0/1/1/1
6	NAG	C	1414	1	-	1/6/23/26	0/1/1/1
6	NAG	C	1415	1	-	0/6/23/26	0/1/1/1
6	NAG	C	1416	1	-	4/6/23/26	0/1/1/1
6	NAG	C	1406	1	-	2/6/23/26	0/1/1/1
6	NAG	B	1415	1	-	4/6/23/26	0/1/1/1
6	NAG	A	1416	1	-	2/6/23/26	0/1/1/1
6	NAG	B	1402	1	-	1/6/23/26	0/1/1/1
6	NAG	C	1418	1	-	2/6/23/26	0/1/1/1
6	NAG	B	1401	1	-	0/6/23/26	0/1/1/1
6	NAG	A	1406	1	-	2/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1418	NAG	C1-C2	2.65	1.56	1.52
6	A	1417	NAG	O5-C1	2.01	1.47	1.43
6	B	1416	NAG	C1-C2	2.00	1.55	1.52

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	1418	NAG	C1-O5-C5	4.01	117.56	112.19
6	B	1416	NAG	C2-N2-C7	3.21	127.20	122.90
6	B	1415	NAG	C2-N2-C7	3.18	127.17	122.90
6	C	1417	NAG	C2-N2-C7	3.17	127.15	122.90
6	A	1417	NAG	C1-O5-C5	2.47	115.50	112.19
6	B	1416	NAG	C1-O5-C5	2.46	115.49	112.19
6	C	1417	NAG	C1-O5-C5	2.42	115.42	112.19
6	C	1401	NAG	C8-C7-N2	2.39	120.08	116.12
6	A	1401	NAG	C8-C7-N2	2.36	120.03	116.12
6	B	1401	NAG	C8-C7-N2	2.34	120.00	116.12
6	A	1401	NAG	C2-N2-C7	-2.15	120.02	122.90
6	B	1401	NAG	C2-N2-C7	-2.14	120.03	122.90
6	C	1401	NAG	C2-N2-C7	-2.13	120.05	122.90
6	B	1417	NAG	C1-O5-C5	2.08	114.97	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	1418	NAG	C1-O5-C5	2.06	114.94	112.19
6	B	1415	NAG	C1-O5-C5	2.02	114.89	112.19

There are no chirality outliers.

All (45) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	1417	NAG	O5-C5-C6-O6
6	C	1417	NAG	C4-C5-C6-O6
6	A	1417	NAG	C4-C5-C6-O6
6	B	1416	NAG	O5-C5-C6-O6
6	C	1418	NAG	O5-C5-C6-O6
6	B	1417	NAG	C4-C5-C6-O6
6	C	1416	NAG	O5-C5-C6-O6
6	B	1416	NAG	C4-C5-C6-O6
6	A	1415	NAG	O5-C5-C6-O6
6	A	1418	NAG	O5-C5-C6-O6
6	C	1417	NAG	O5-C5-C6-O6
6	A	1417	NAG	O5-C5-C6-O6
6	B	1414	NAG	O5-C5-C6-O6
6	A	1415	NAG	C4-C5-C6-O6
6	A	1416	NAG	O5-C5-C6-O6
6	B	1414	NAG	C8-C7-N2-C2
6	B	1414	NAG	O7-C7-N2-C2
6	C	1416	NAG	C8-C7-N2-C2
6	C	1416	NAG	O7-C7-N2-C2
6	A	1406	NAG	O5-C5-C6-O6
6	B	1406	NAG	O5-C5-C6-O6
6	C	1406	NAG	O5-C5-C6-O6
6	C	1418	NAG	C4-C5-C6-O6
6	C	1416	NAG	C4-C5-C6-O6
6	A	1419	NAG	C4-C5-C6-O6
6	A	1418	NAG	C4-C5-C6-O6
6	A	1402	NAG	O5-C5-C6-O6
6	B	1402	NAG	O5-C5-C6-O6
6	C	1402	NAG	O5-C5-C6-O6
6	B	1414	NAG	C4-C5-C6-O6
6	B	1415	NAG	C4-C5-C6-O6
6	A	1419	NAG	O5-C5-C6-O6
6	A	1416	NAG	C4-C5-C6-O6
6	C	1414	NAG	O5-C5-C6-O6
6	C	1406	NAG	C4-C5-C6-O6

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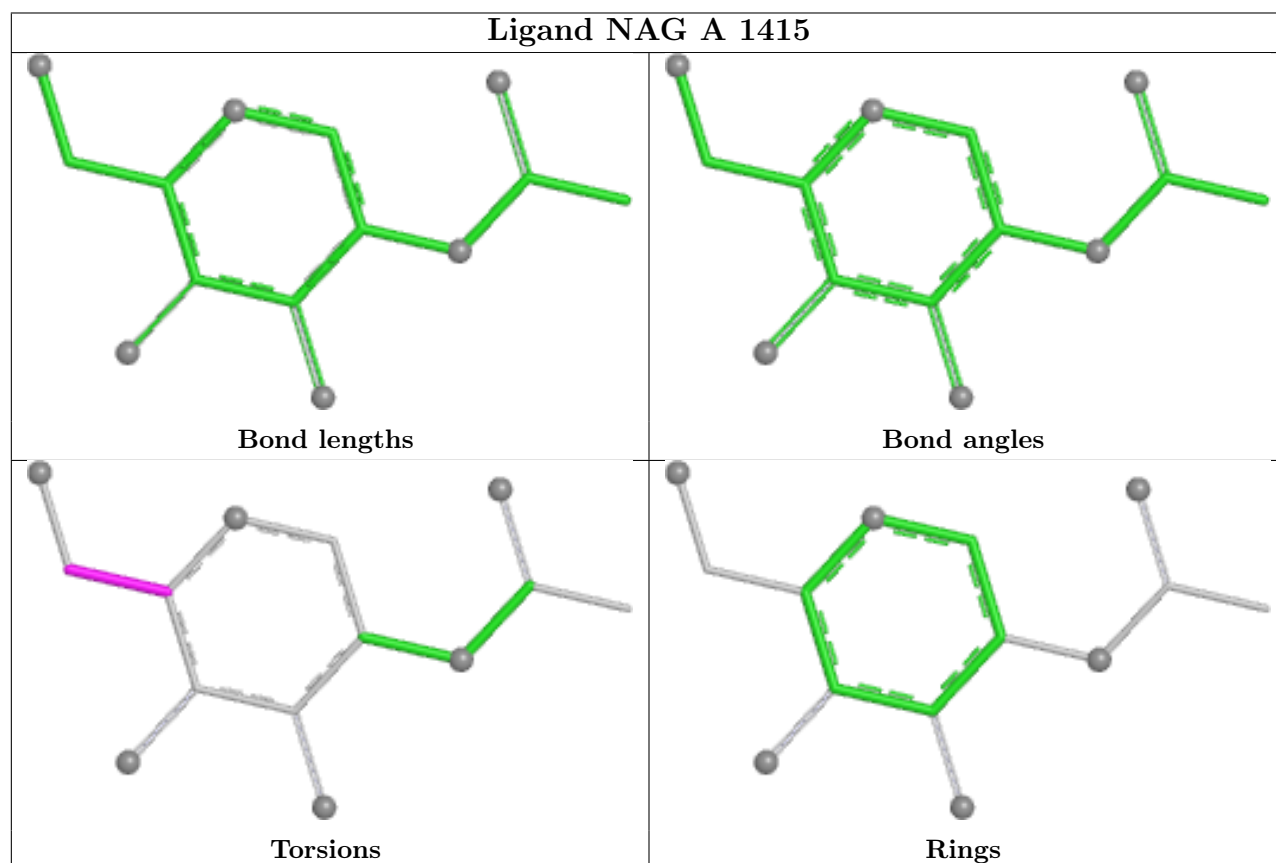
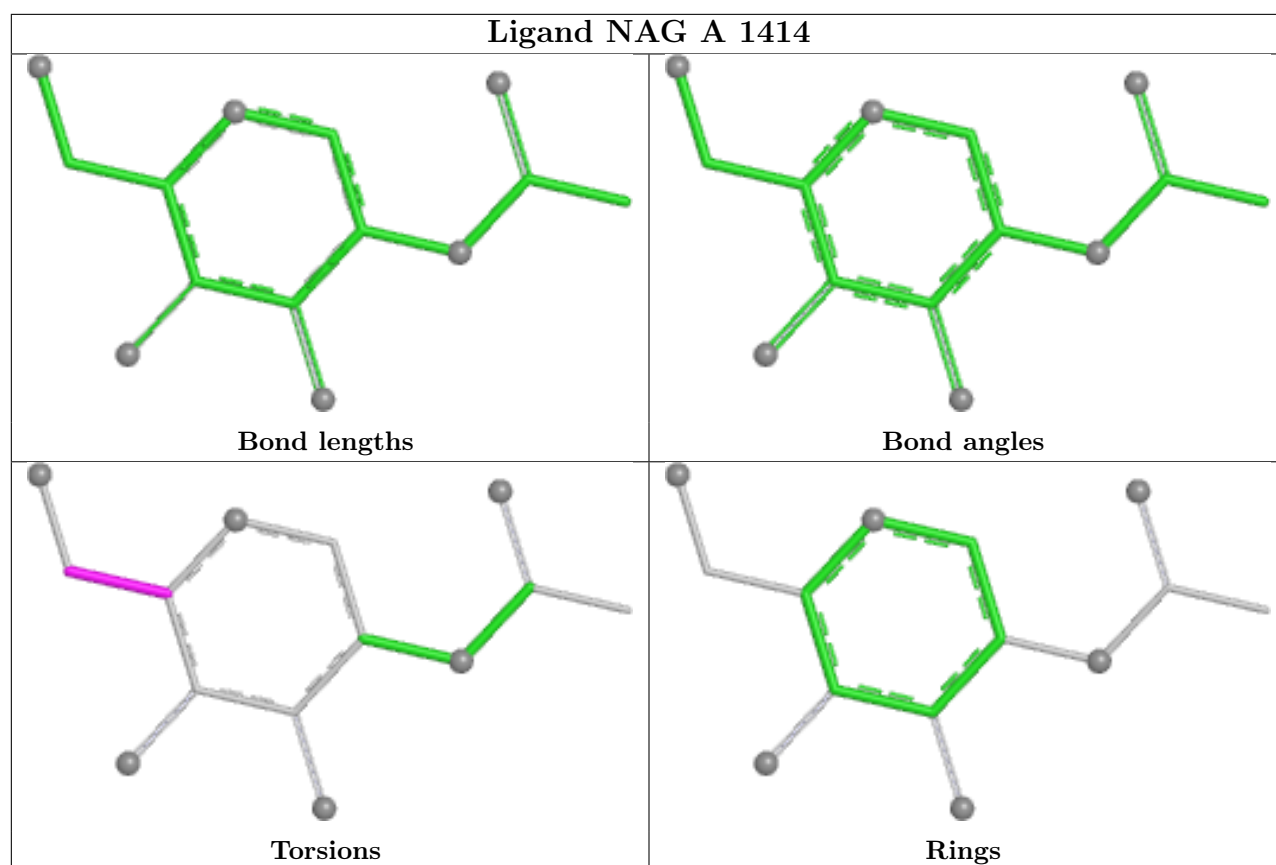
Mol	Chain	Res	Type	Atoms
6	A	1406	NAG	C4-C5-C6-O6
6	B	1406	NAG	C4-C5-C6-O6
6	B	1415	NAG	O5-C5-C6-O6
6	A	1414	NAG	C4-C5-C6-O6
6	B	1416	NAG	C3-C2-N2-C7
6	B	1415	NAG	C1-C2-N2-C7
6	B	1416	NAG	C1-C2-N2-C7
6	C	1417	NAG	C1-C2-N2-C7
6	B	1415	NAG	C3-C2-N2-C7
6	C	1417	NAG	C3-C2-N2-C7

There are no ring outliers.

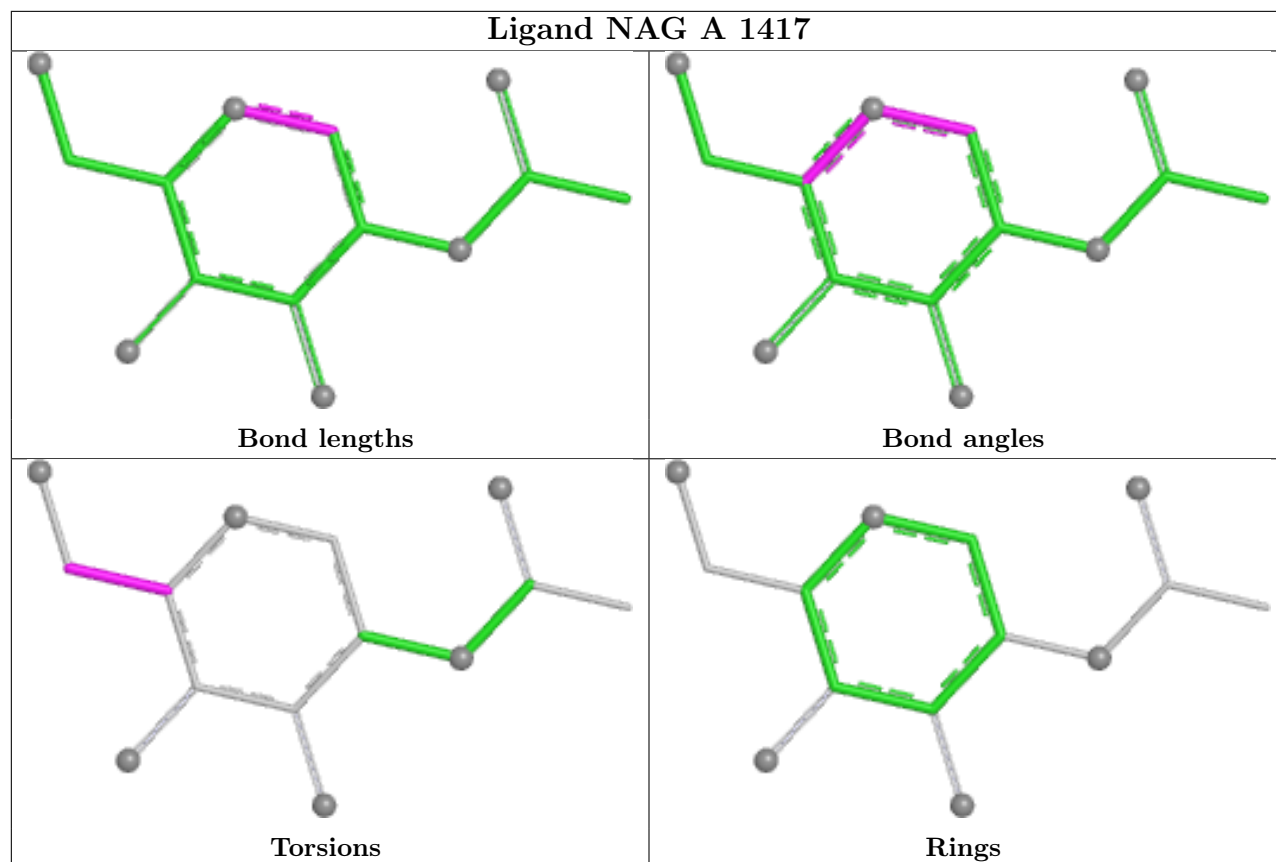
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	1417	NAG	1	0

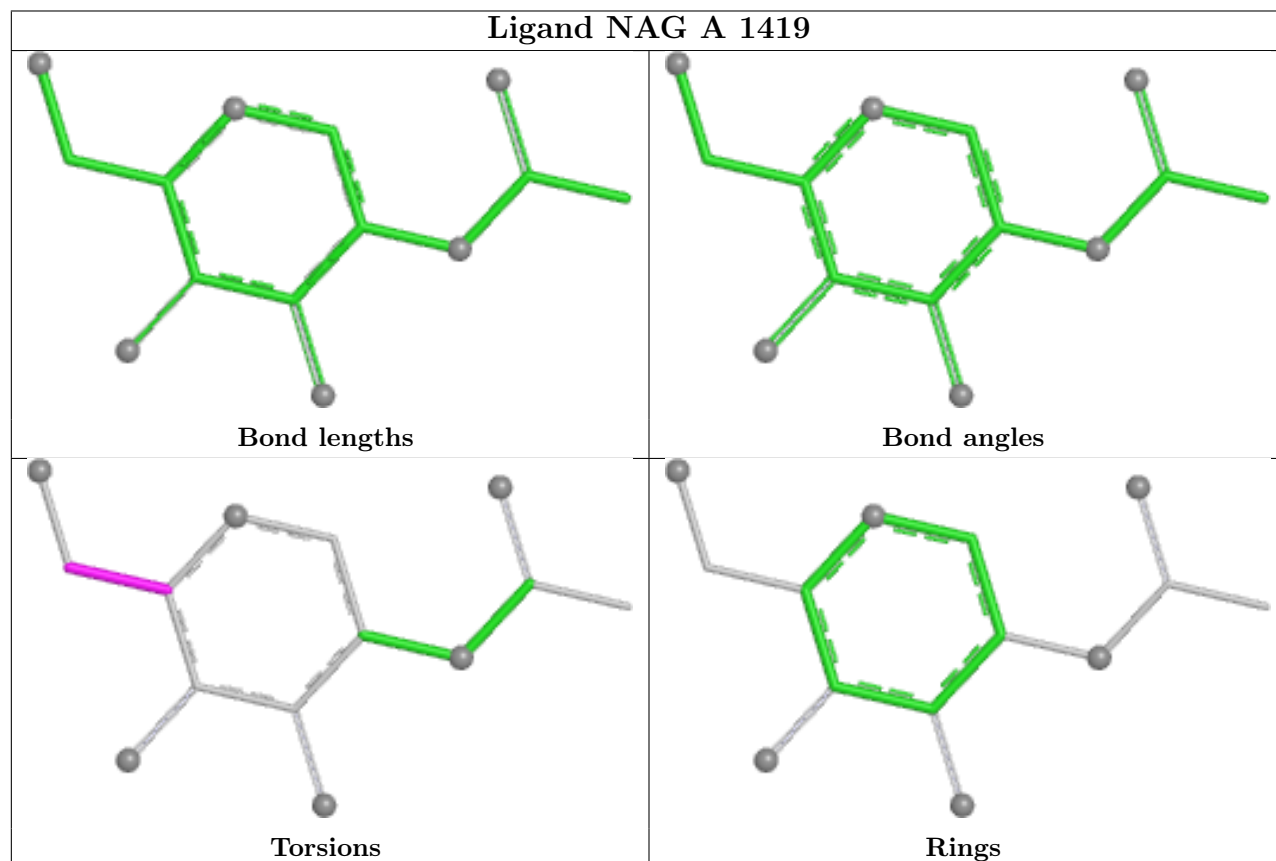
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



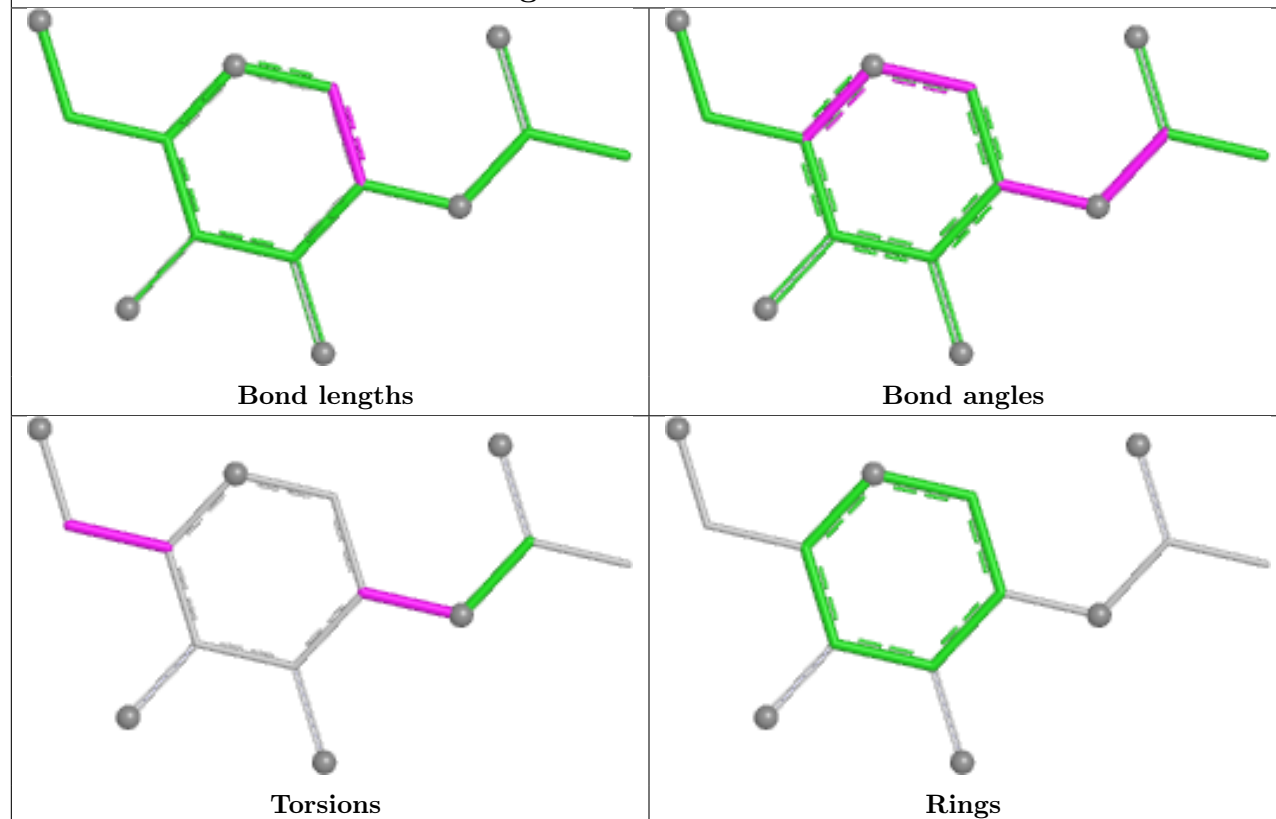
Ligand NAG A 1417



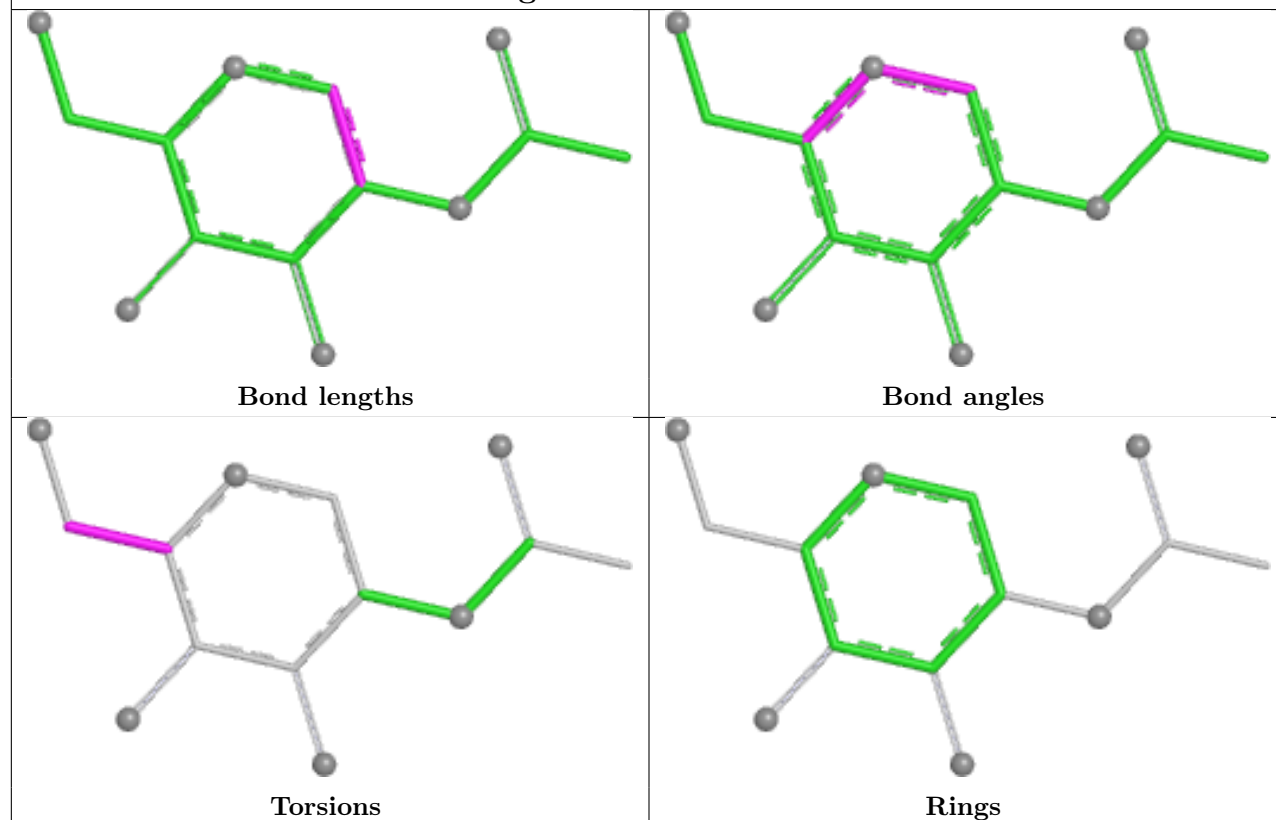
Ligand NAG A 1419

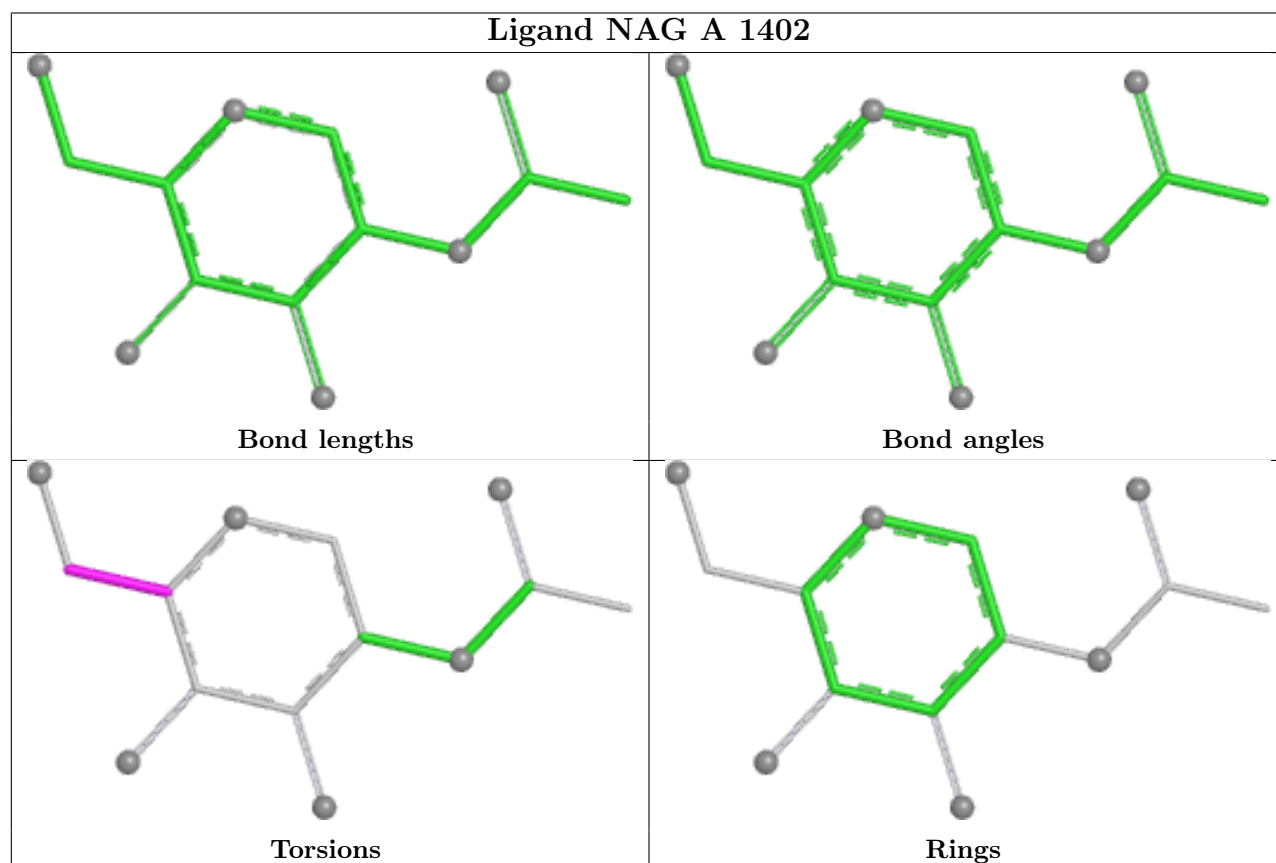
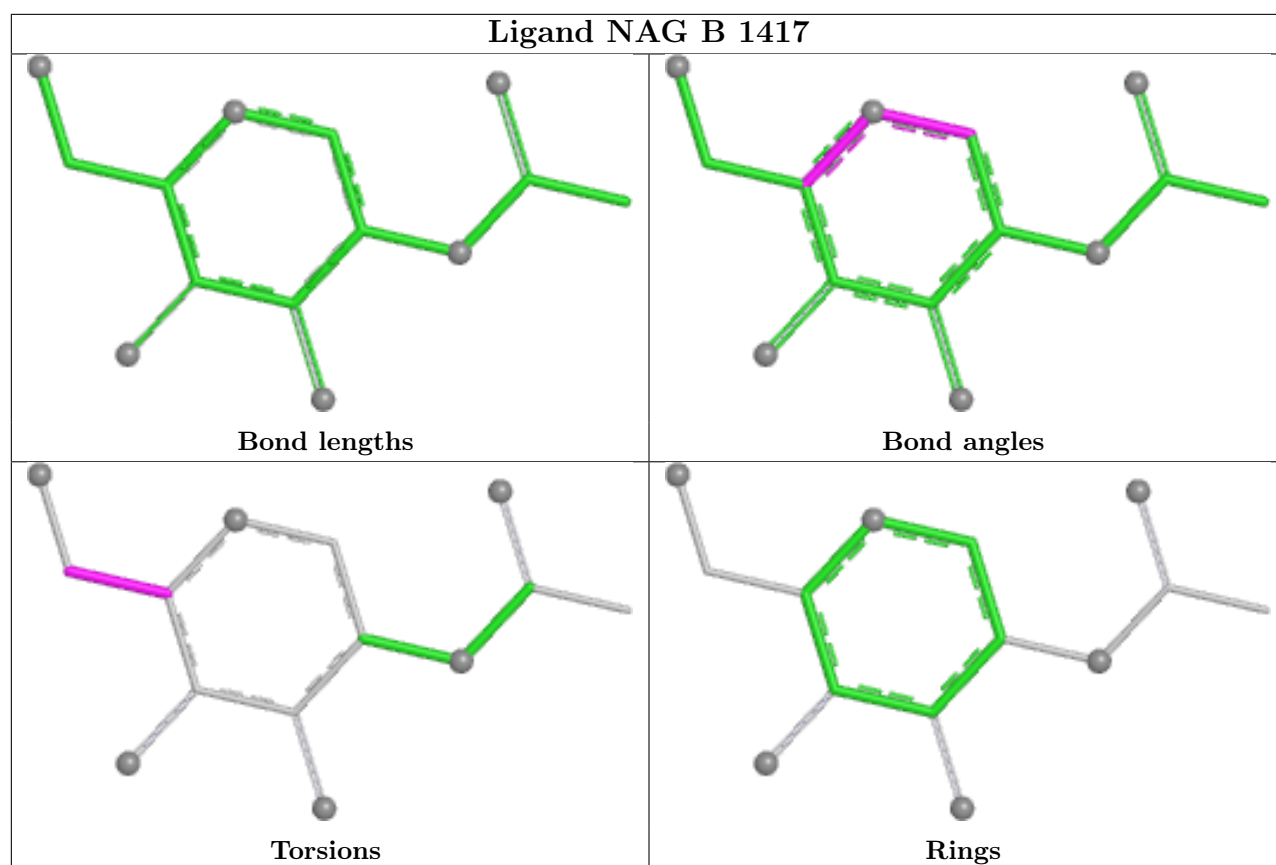


Ligand NAG B 1416

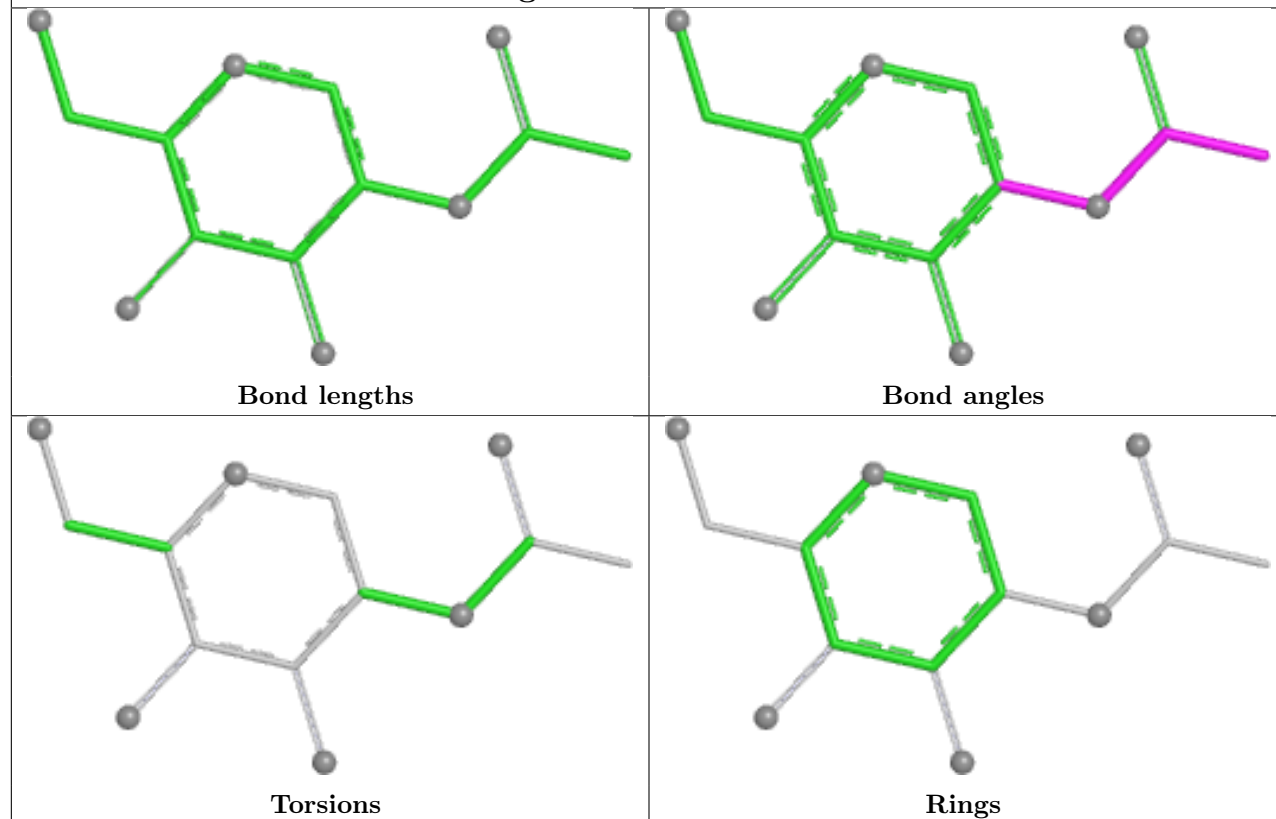


Ligand NAG A 1418

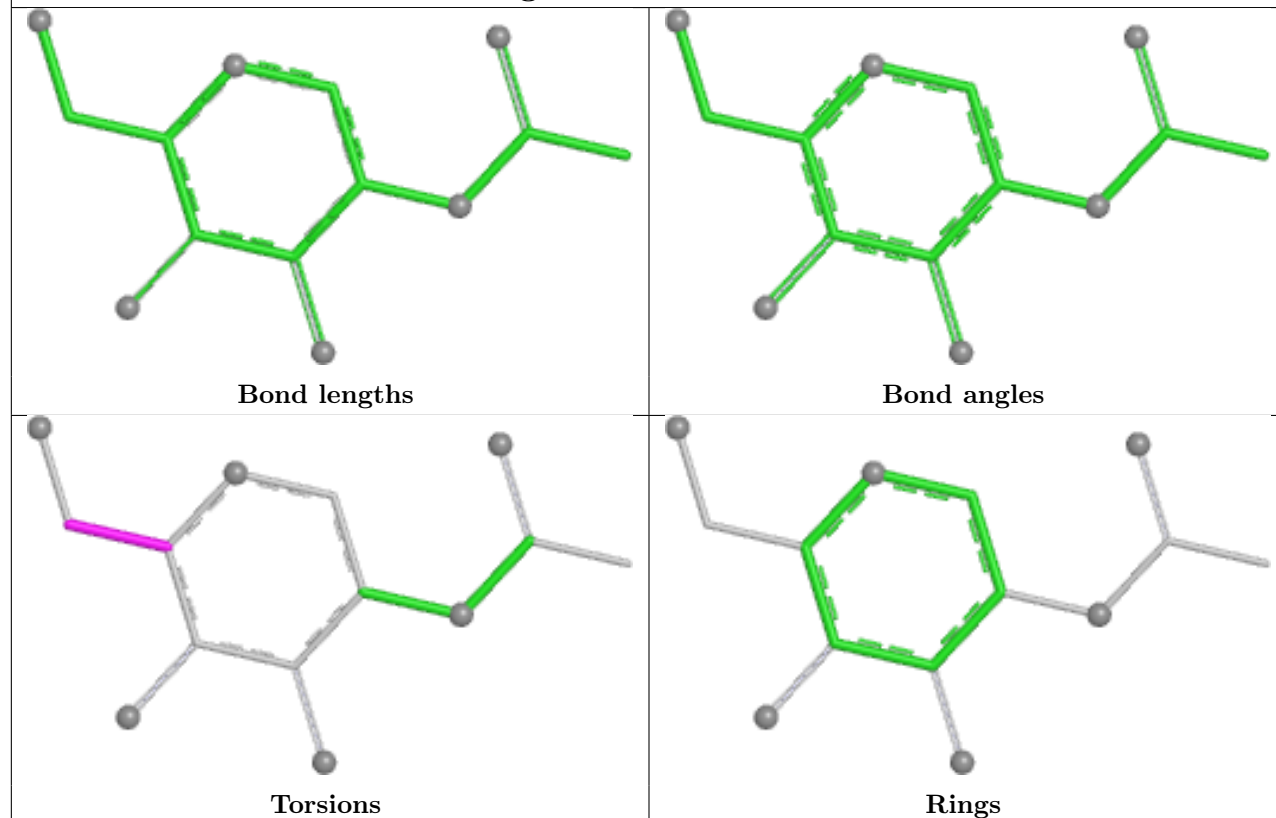




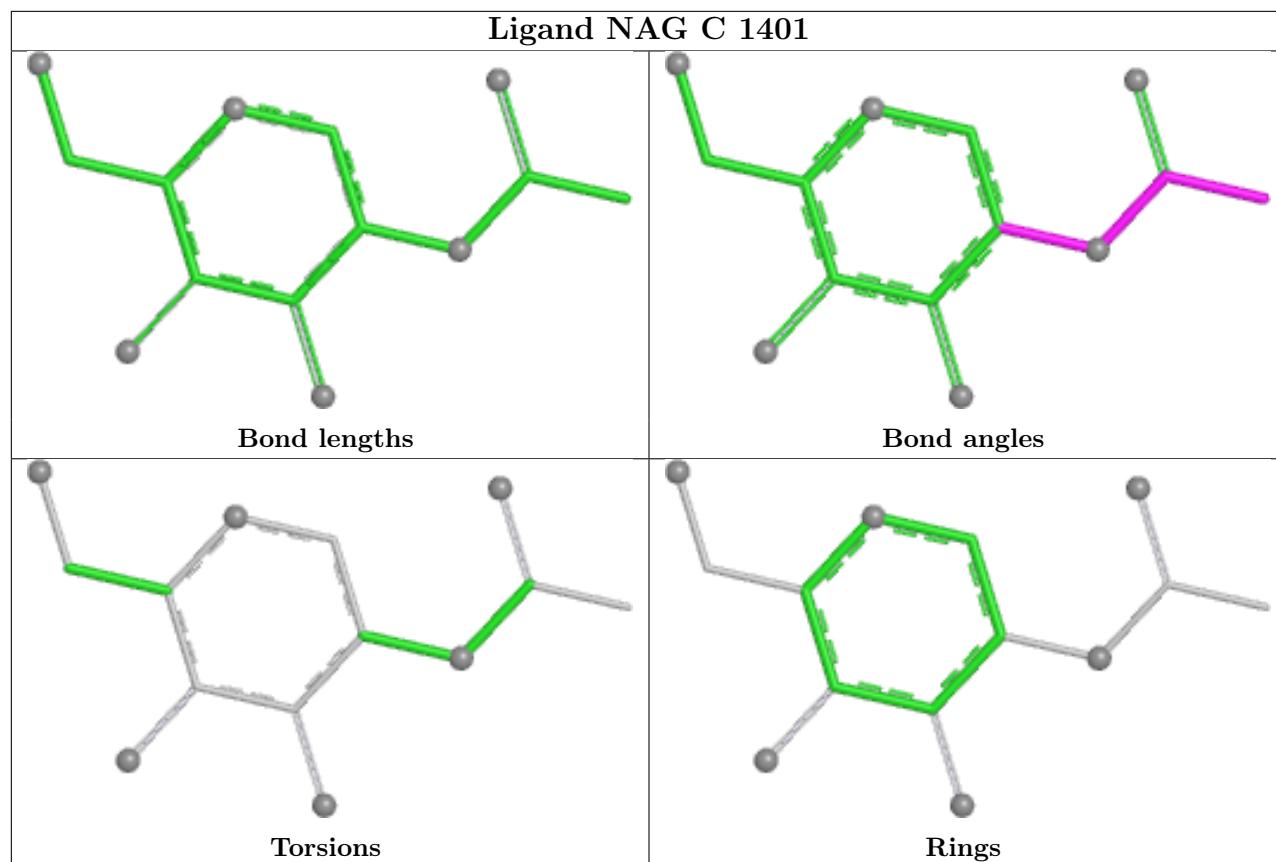
Ligand NAG A 1401



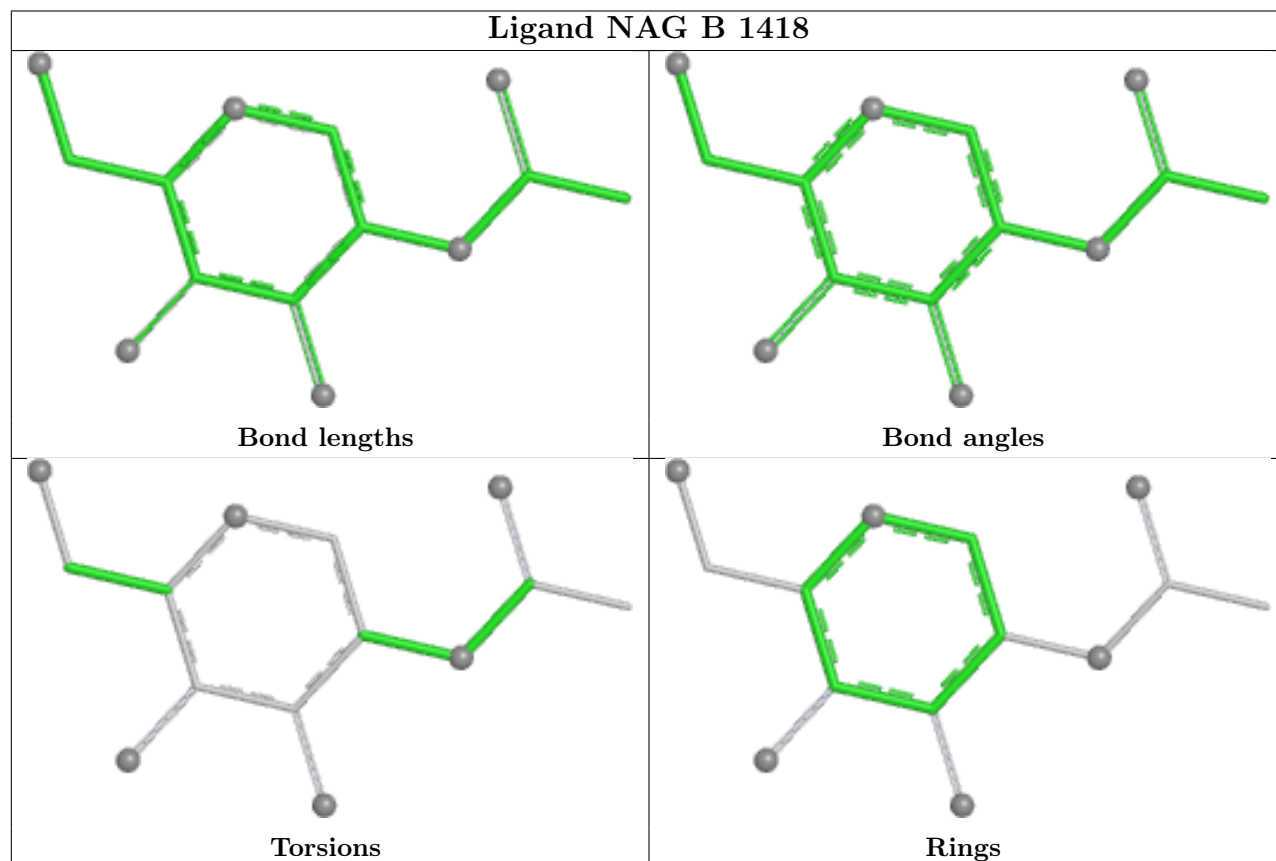
Ligand NAG B 1406



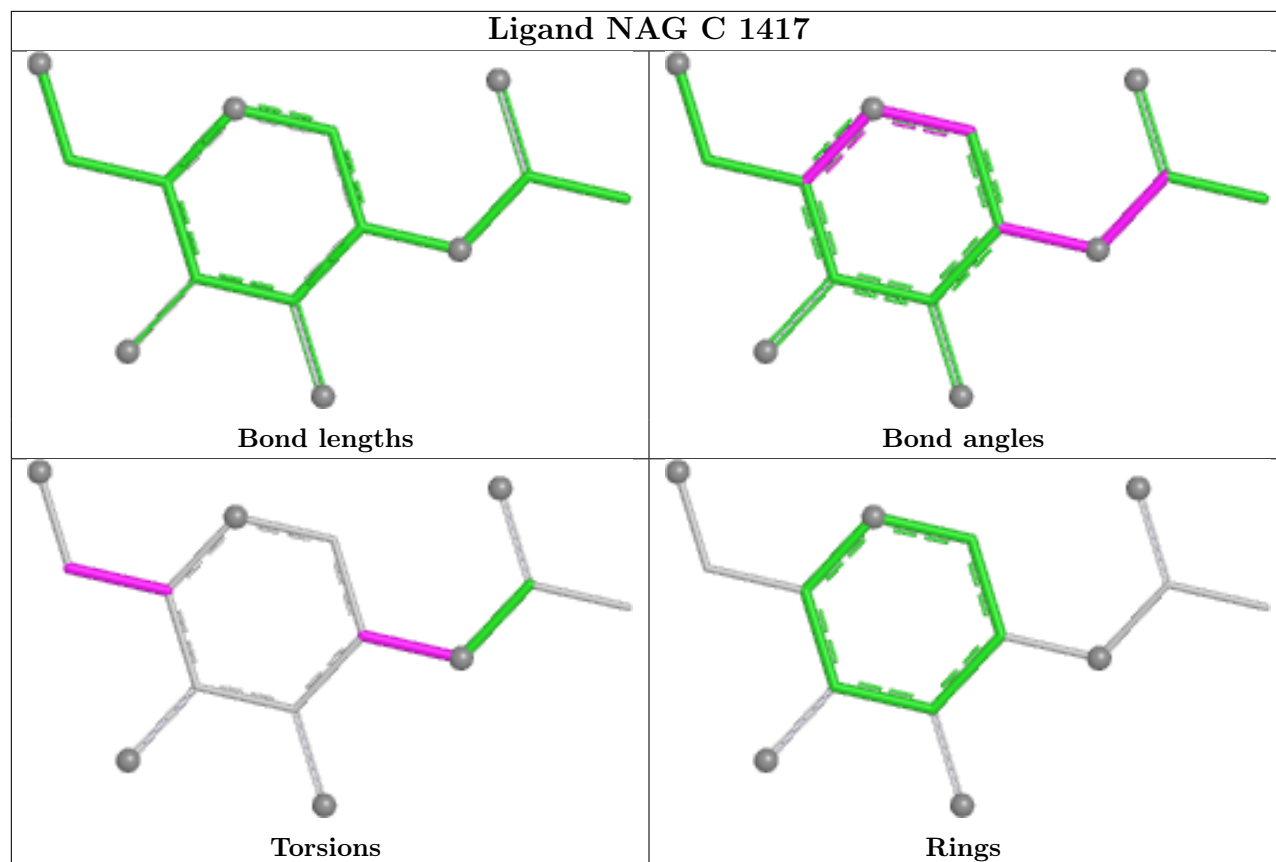
Ligand NAG C 1401



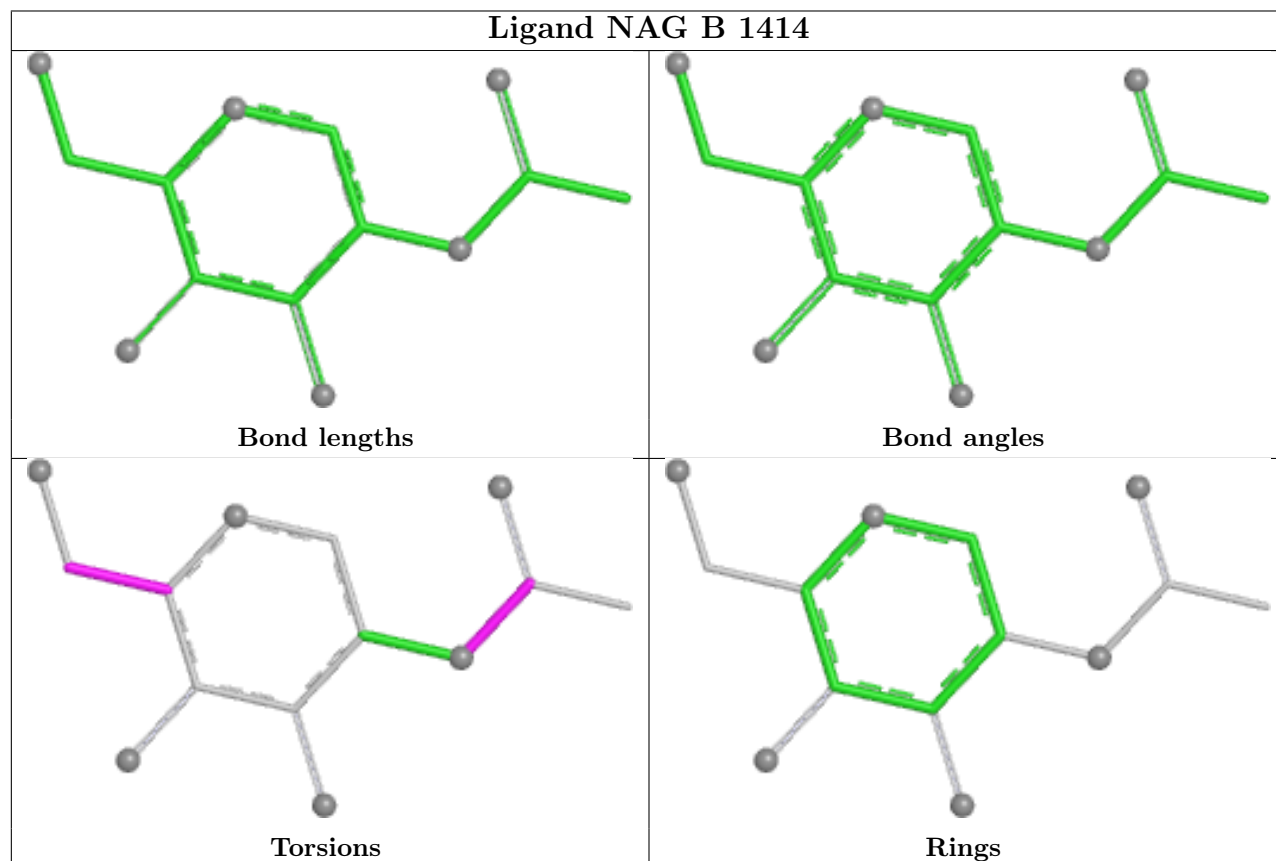
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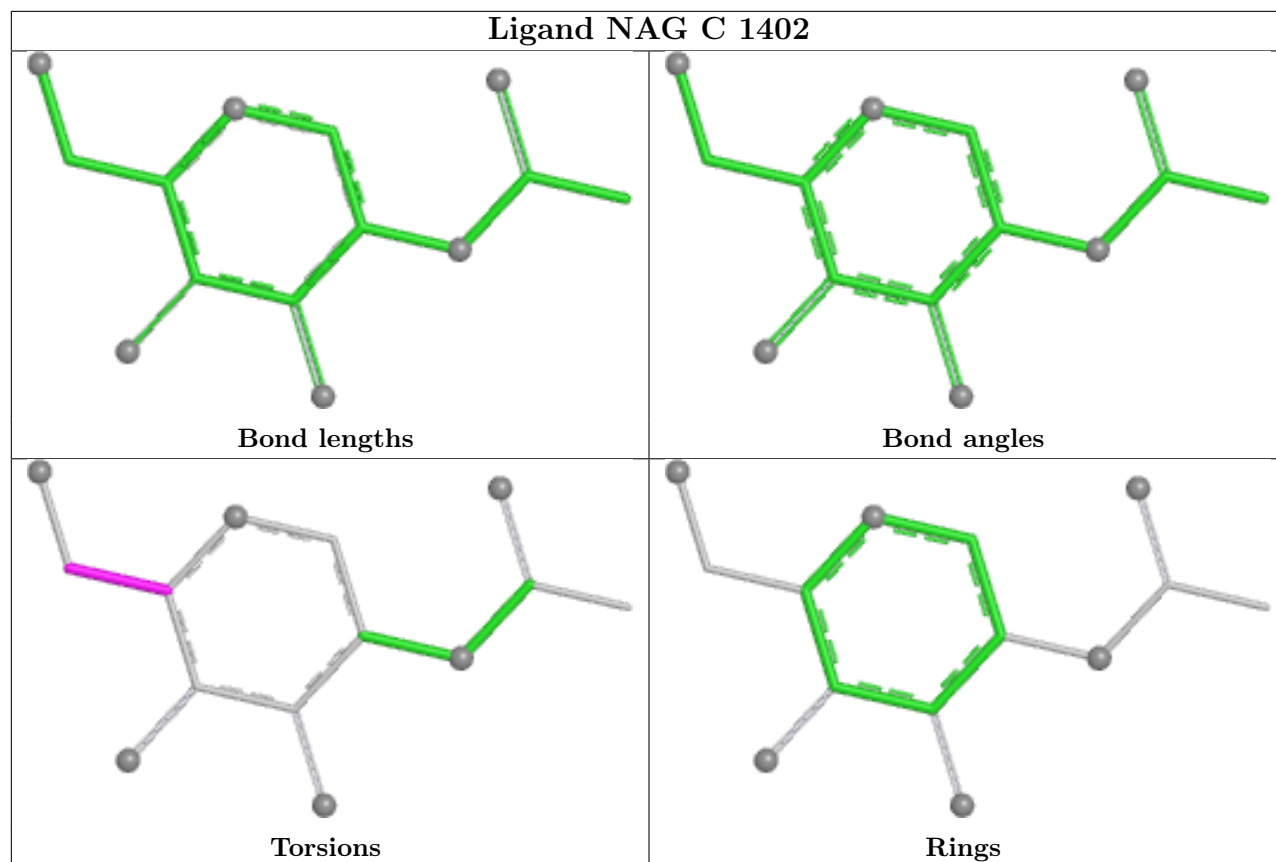
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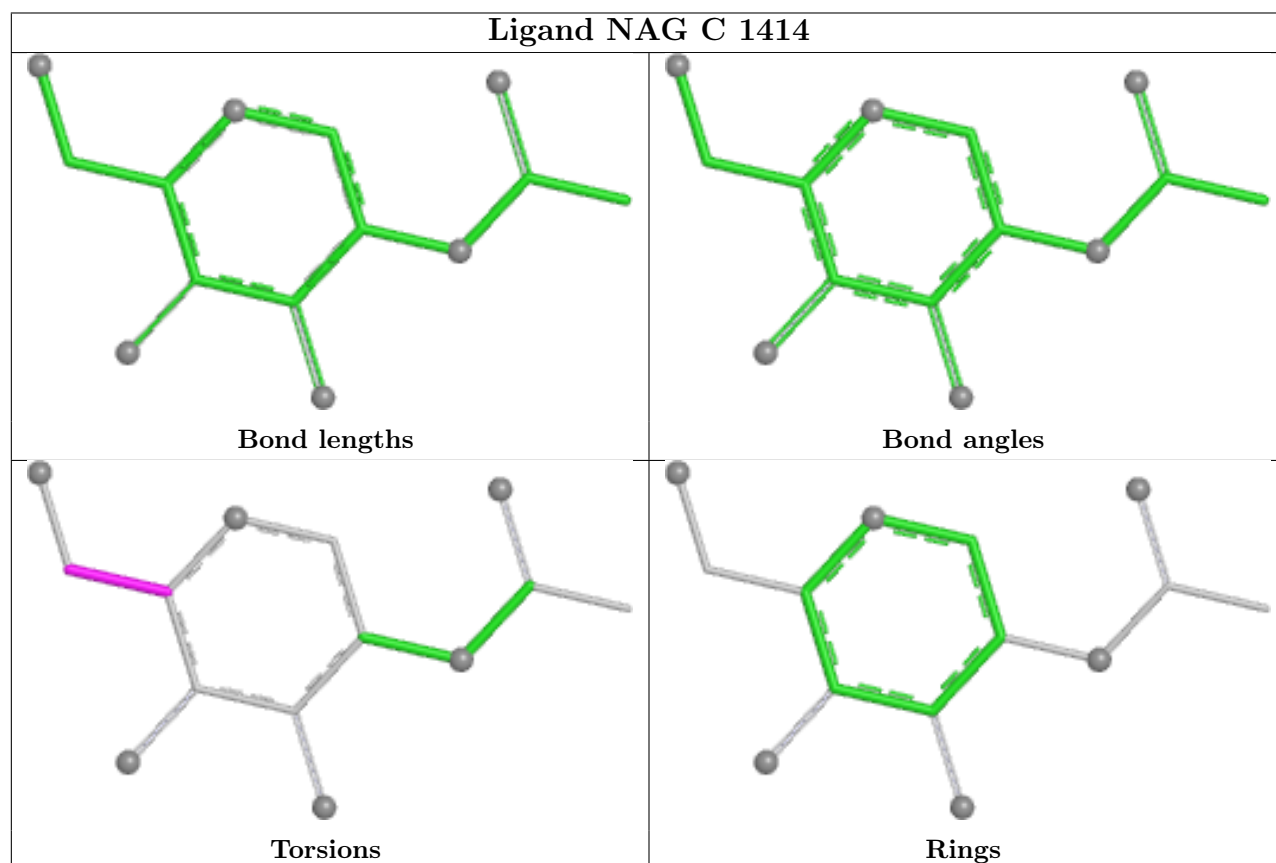
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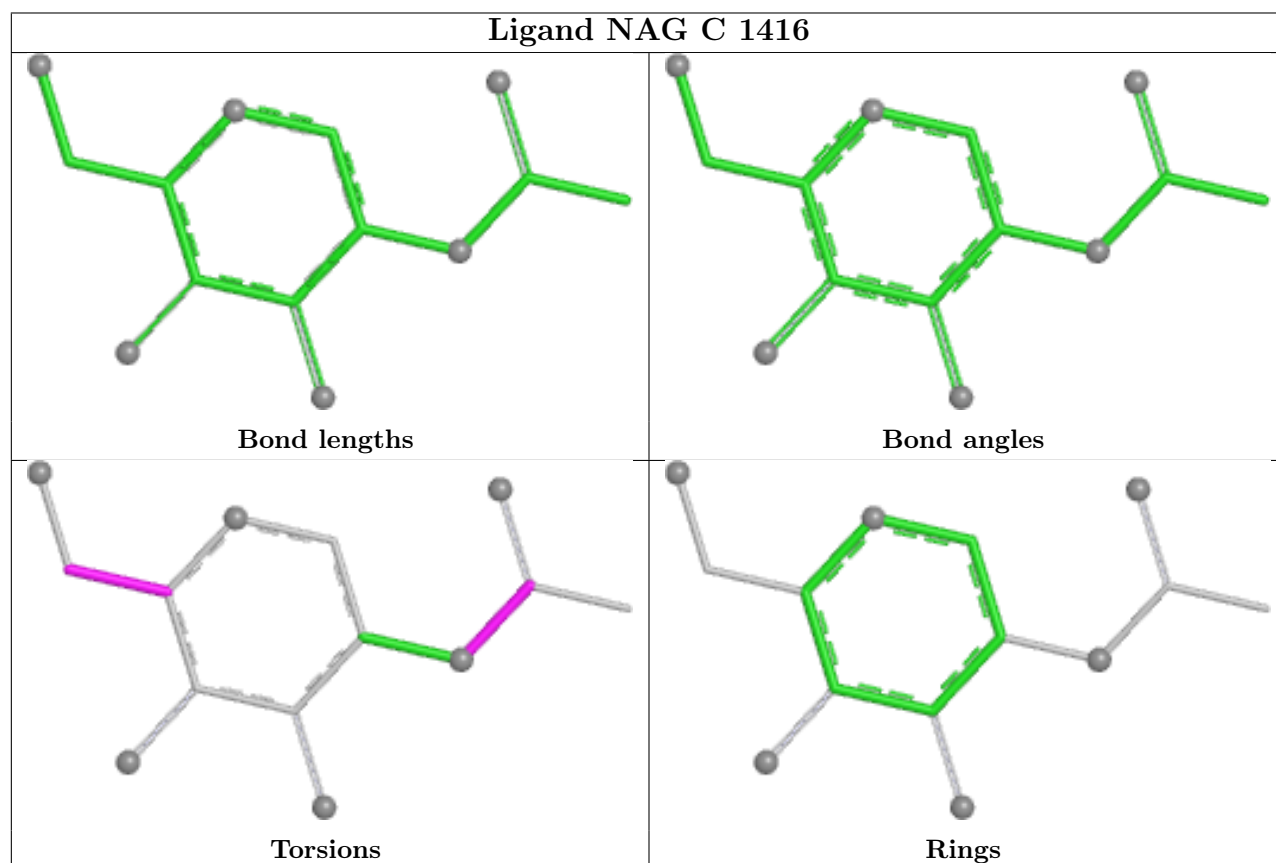
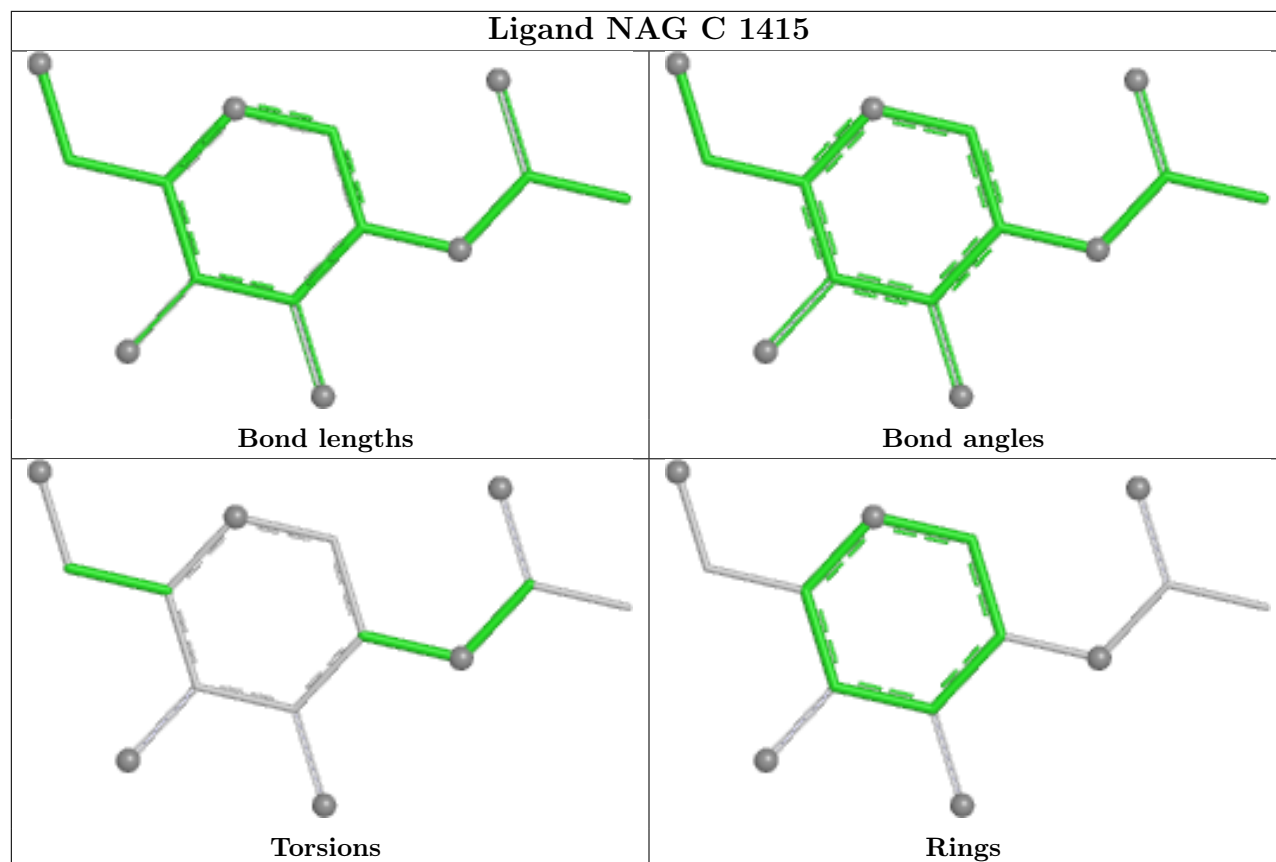


Ligand NAG C 1402

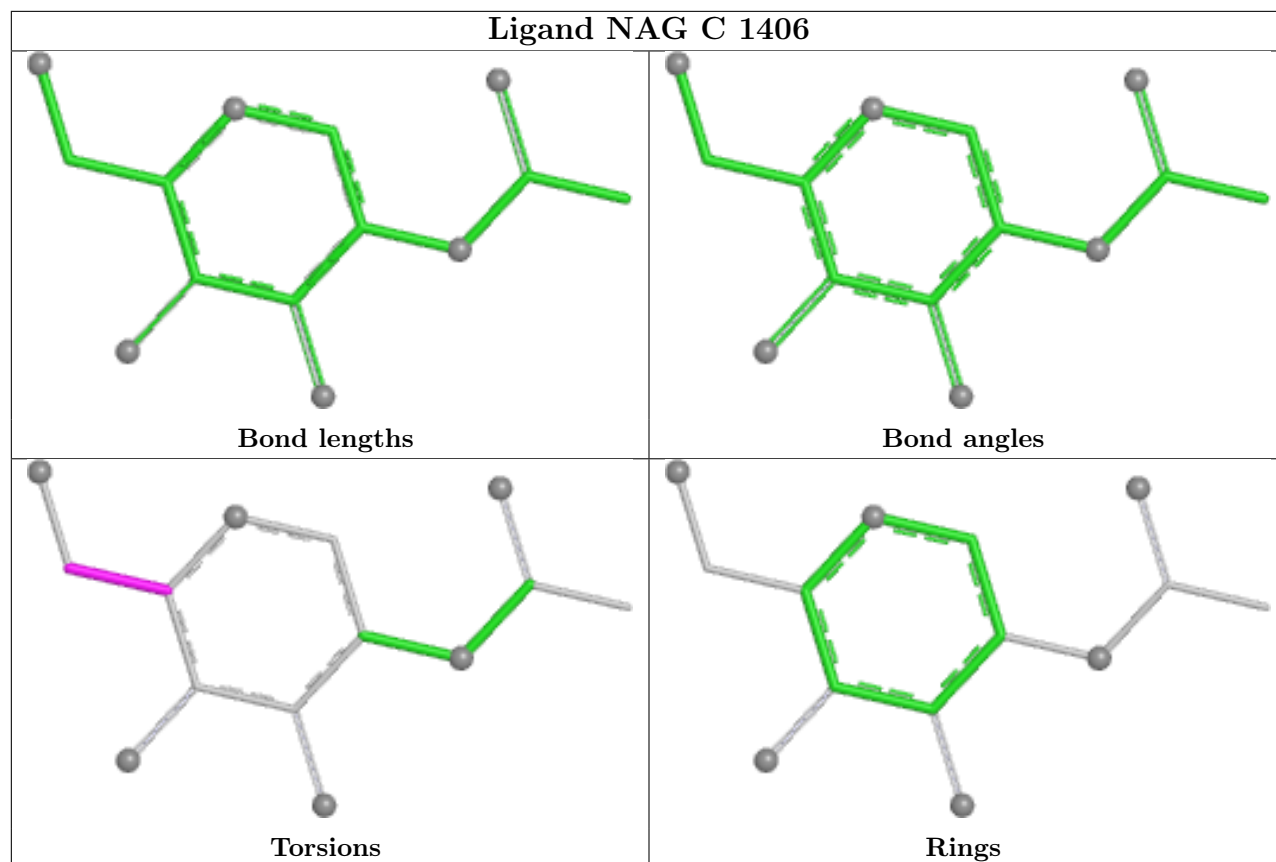


Ligand NAG C 1414

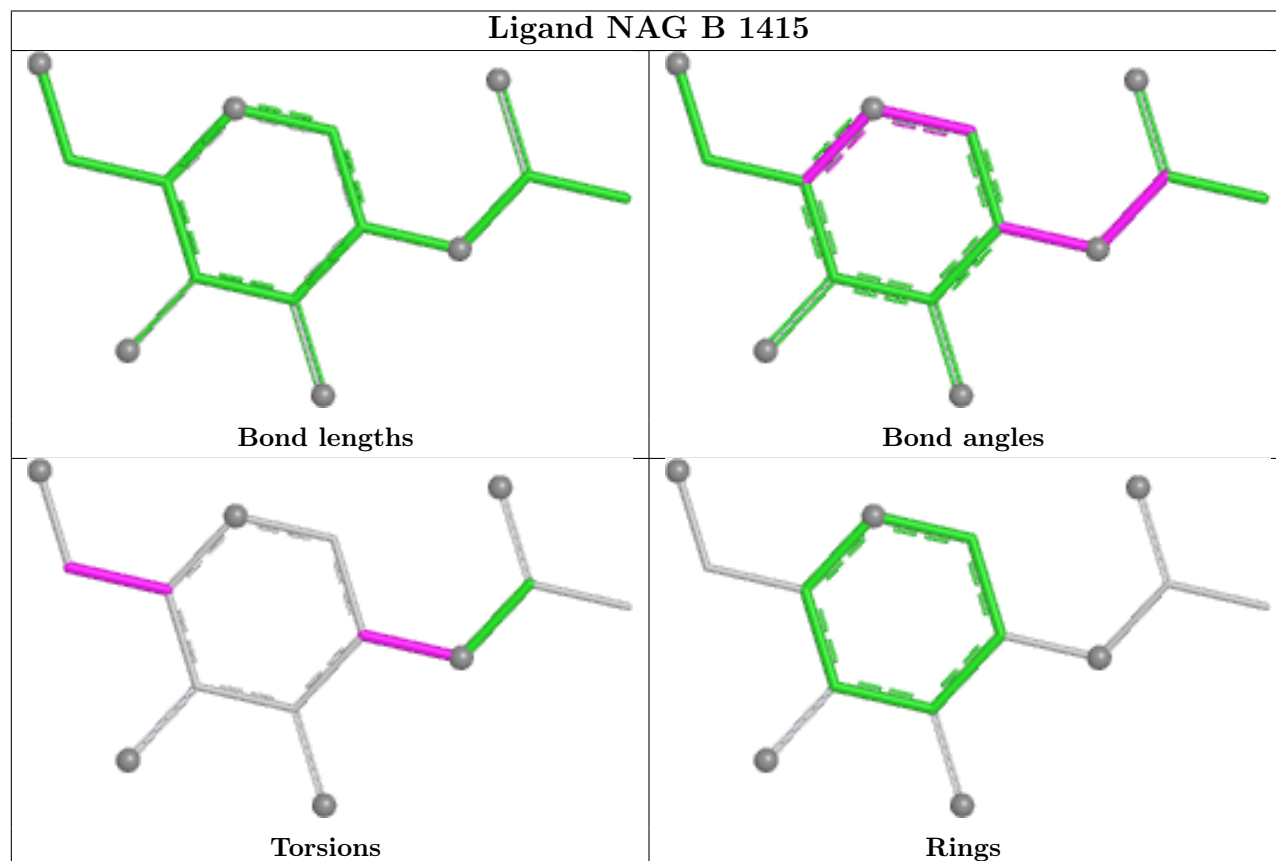




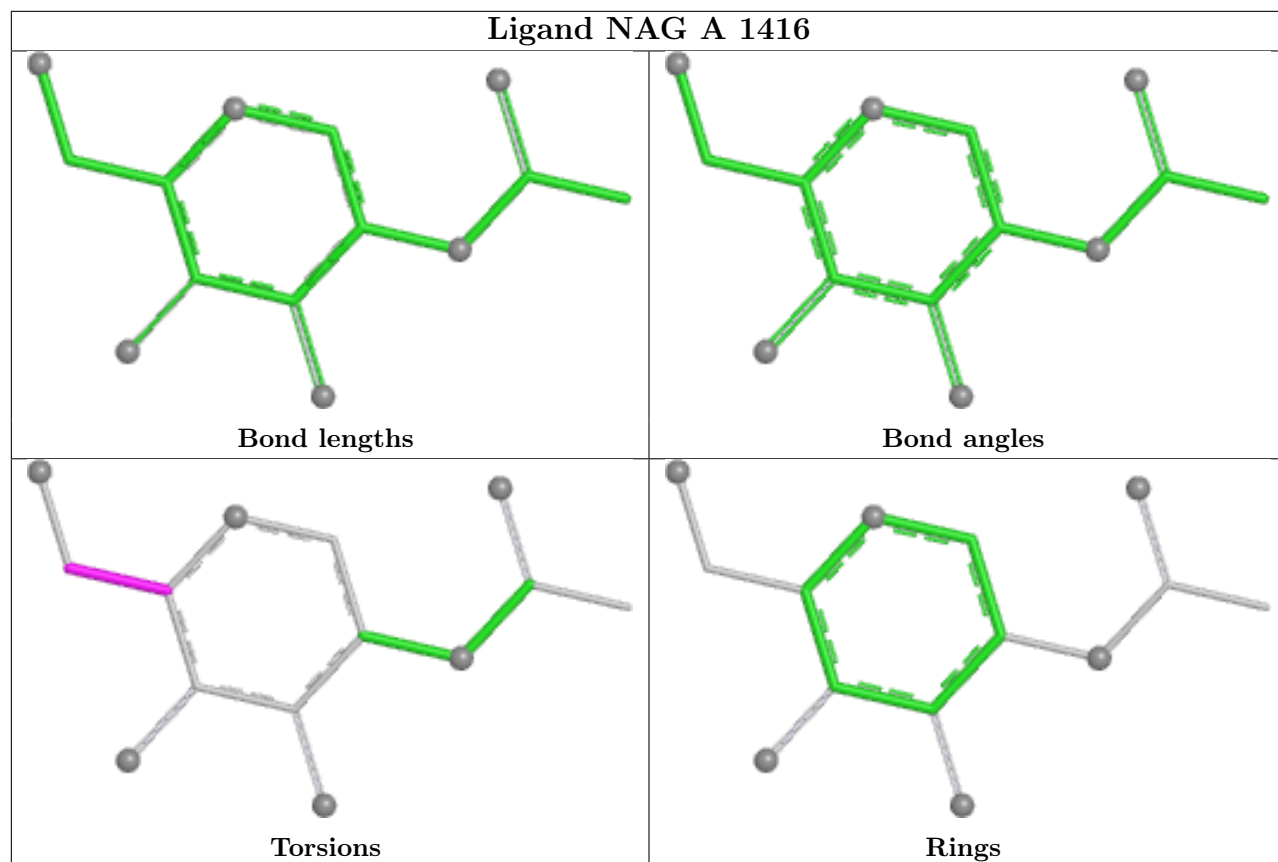
Ligand NAG C 1406



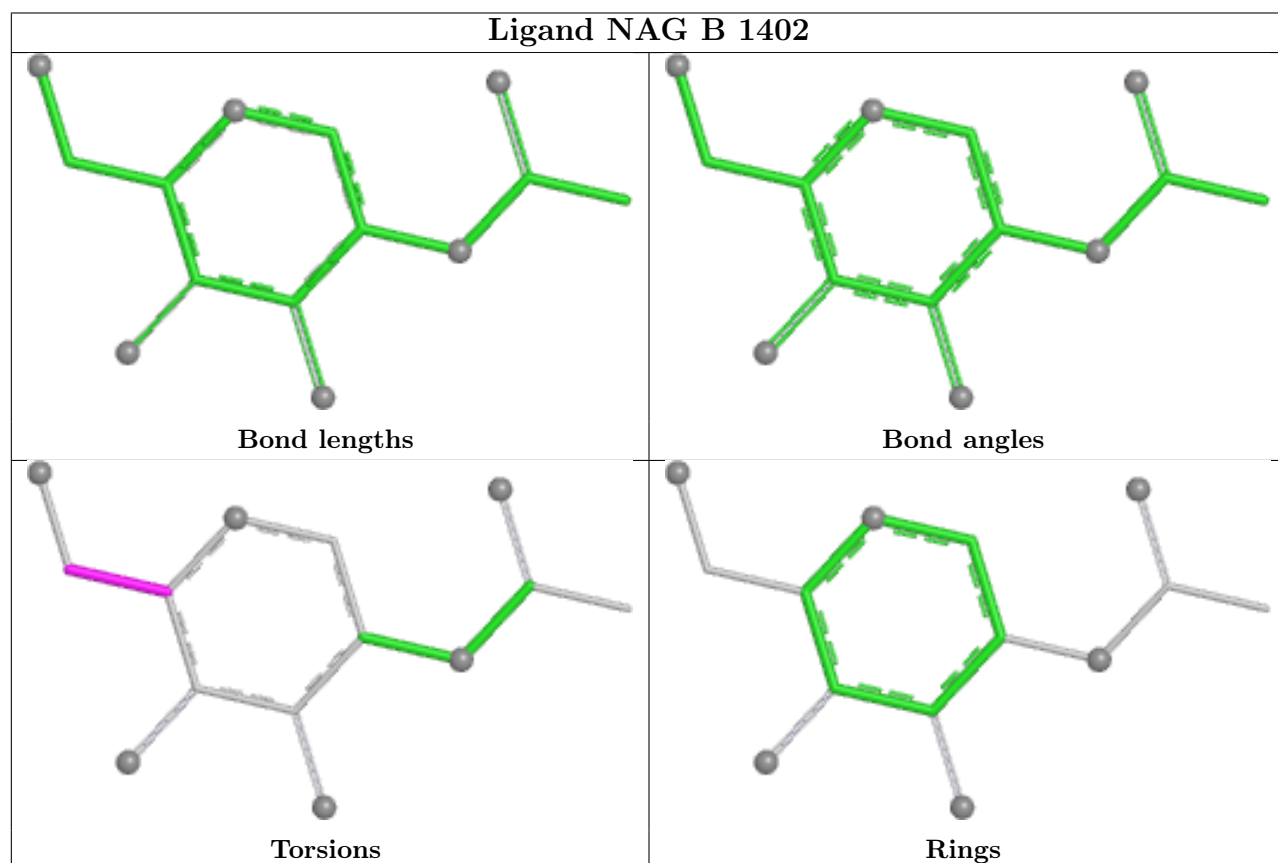
Ligand NAG B 1415



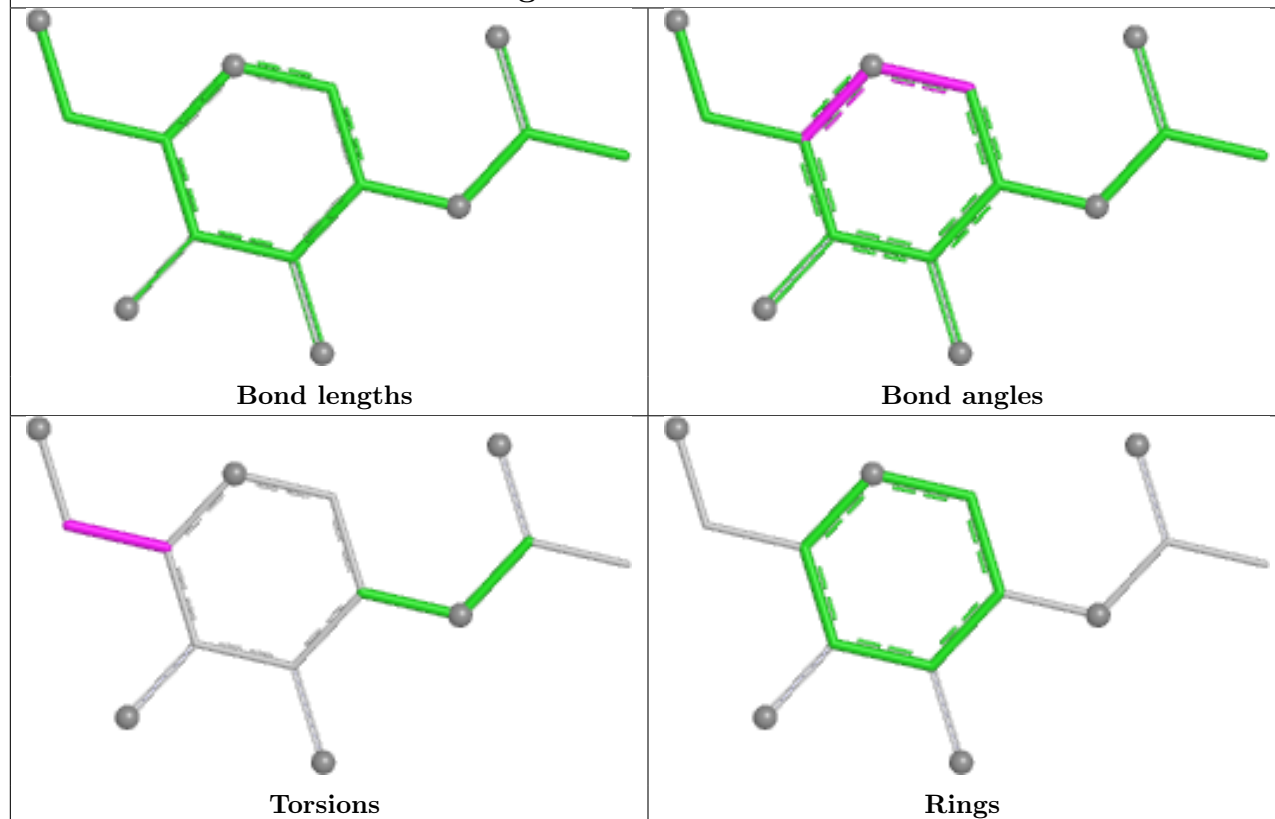
Ligand NAG A 1416



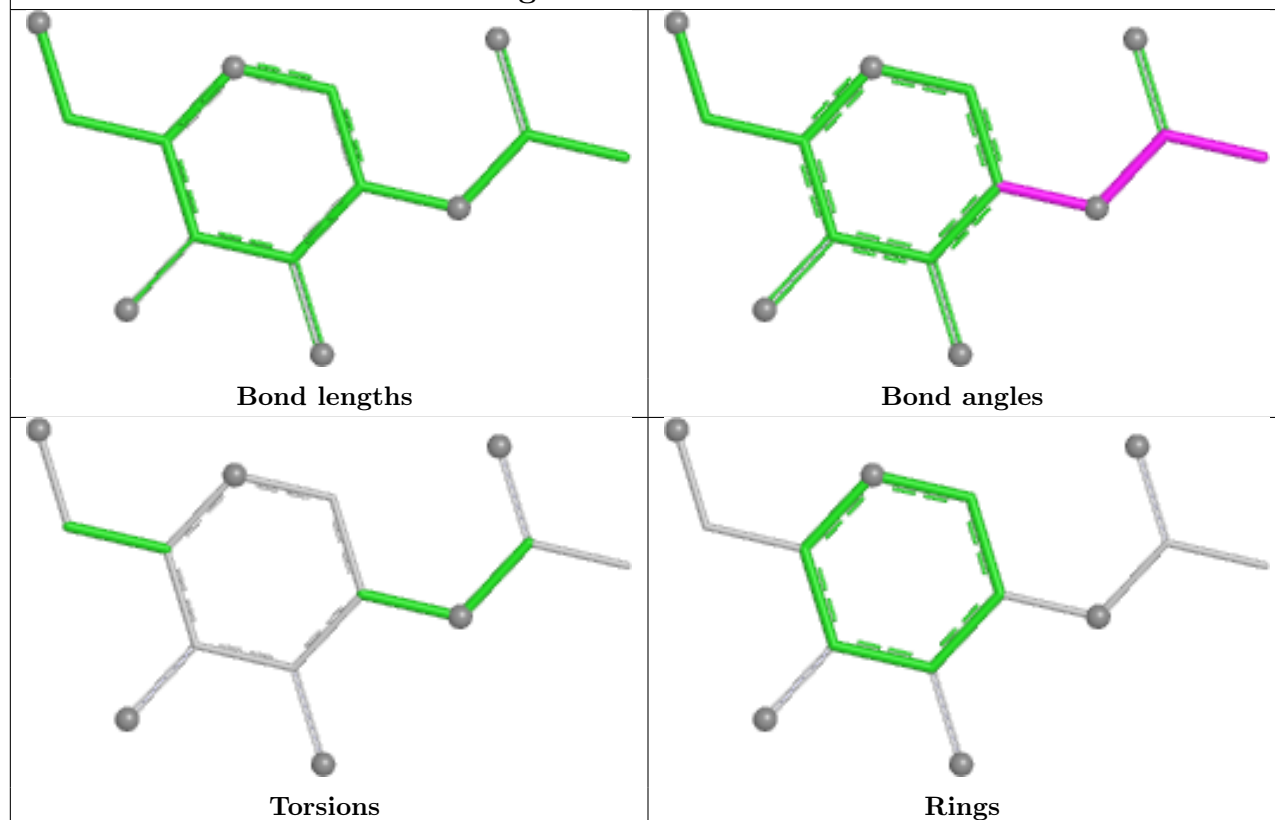
Ligand NAG B 1402

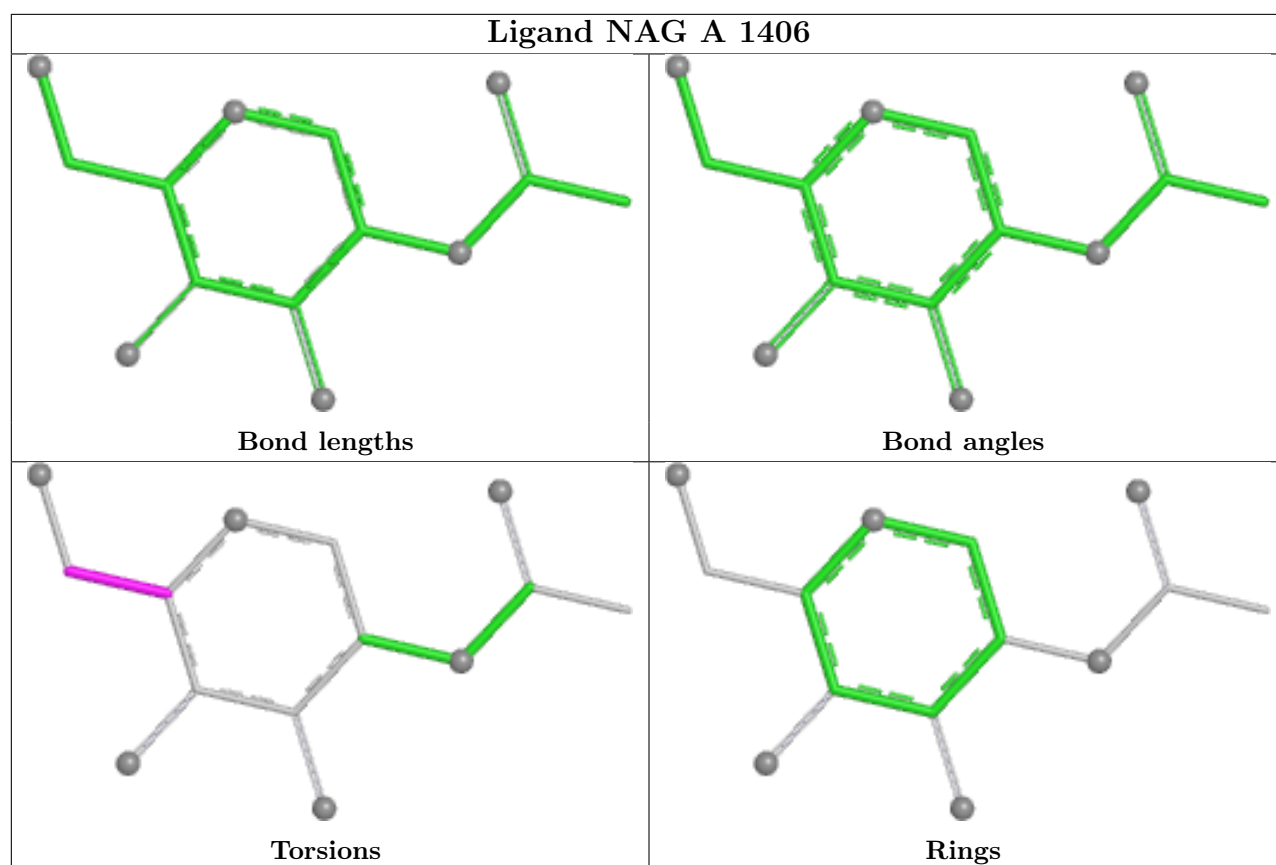


Ligand NAG C 1418



Ligand NAG B 1401





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.

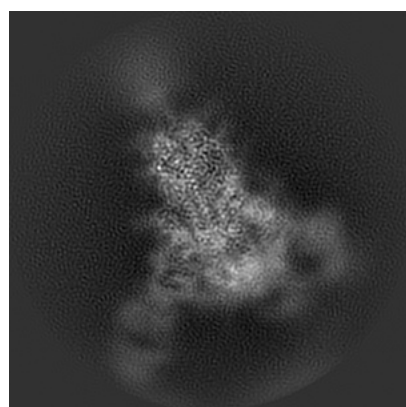
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-30276. These allow visual inspection of the internal detail of the map and identification of artifacts.

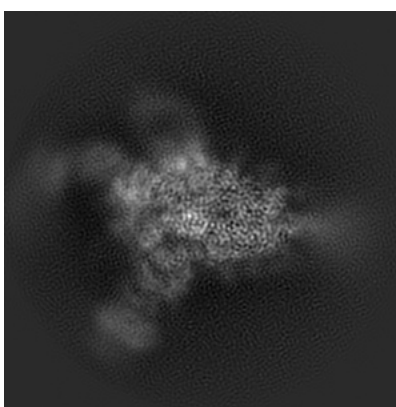
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

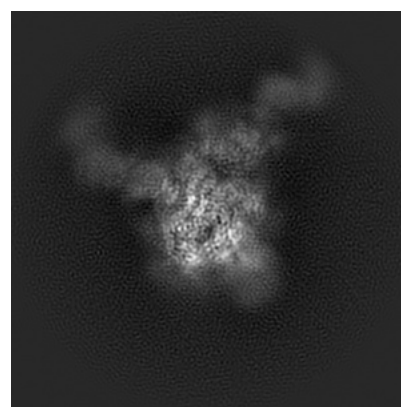
6.1.1 Primary map



X



Y

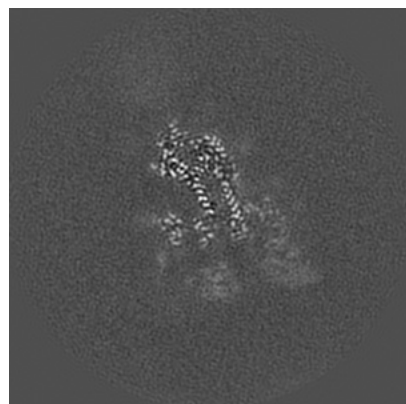


Z

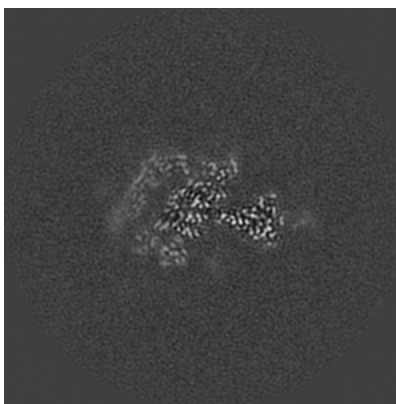
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

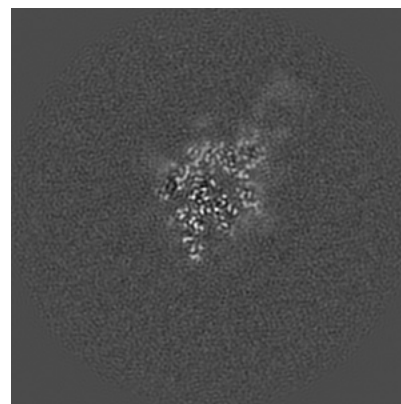
6.2.1 Primary map



X Index: 144



Y Index: 144

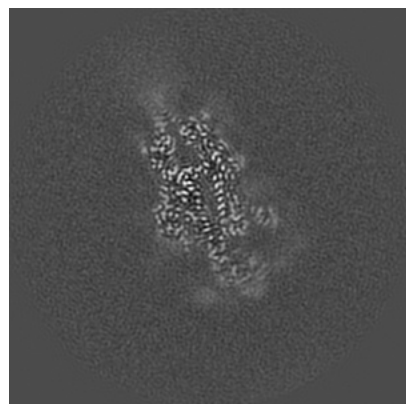


Z Index: 144

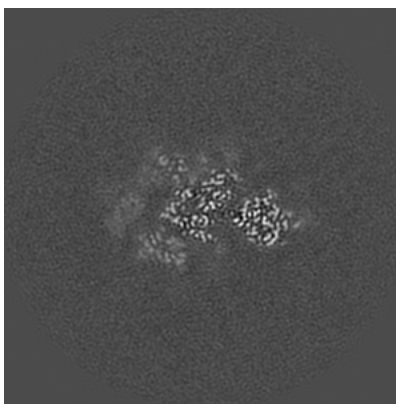
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

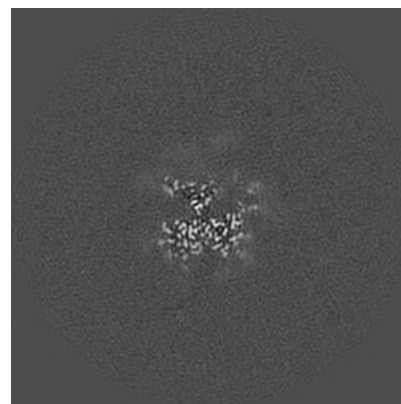
6.3.1 Primary map



X Index: 131



Y Index: 141

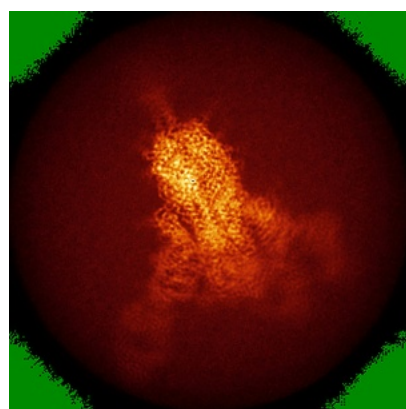


Z Index: 165

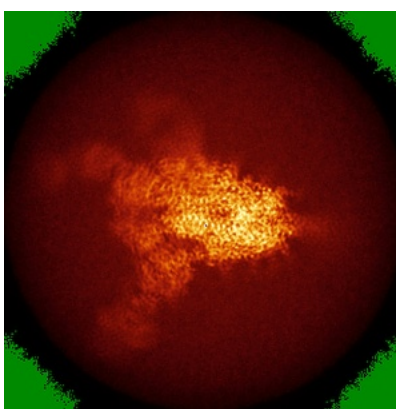
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

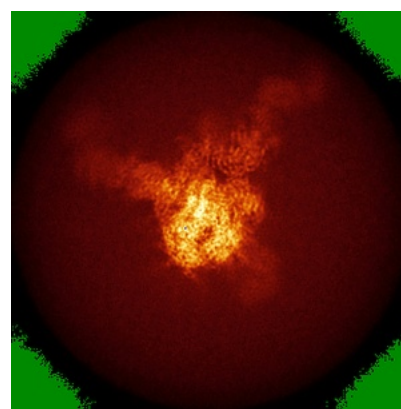
6.4.1 Primary map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views

This section was not generated.

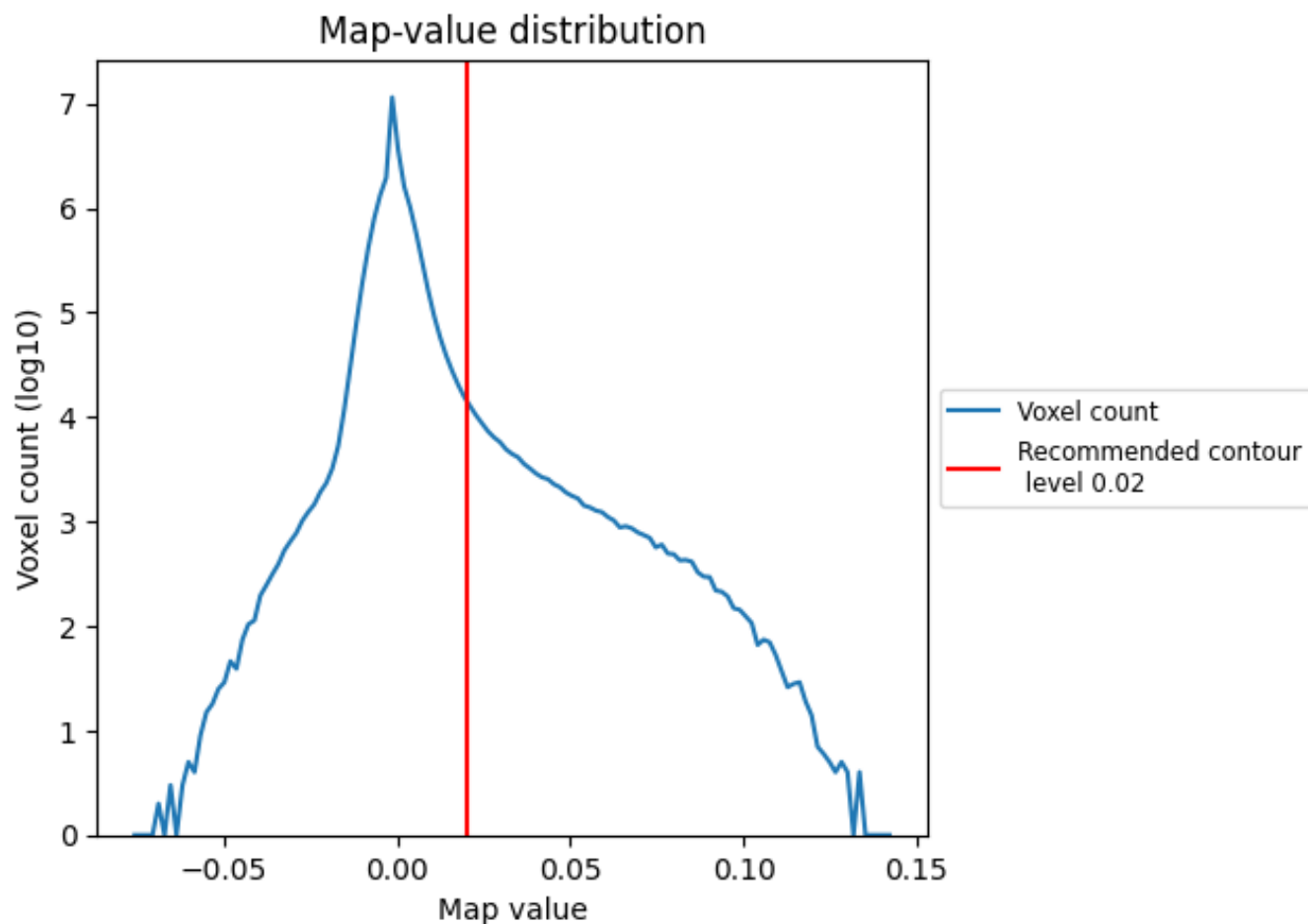
6.6 Mask visualisation

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

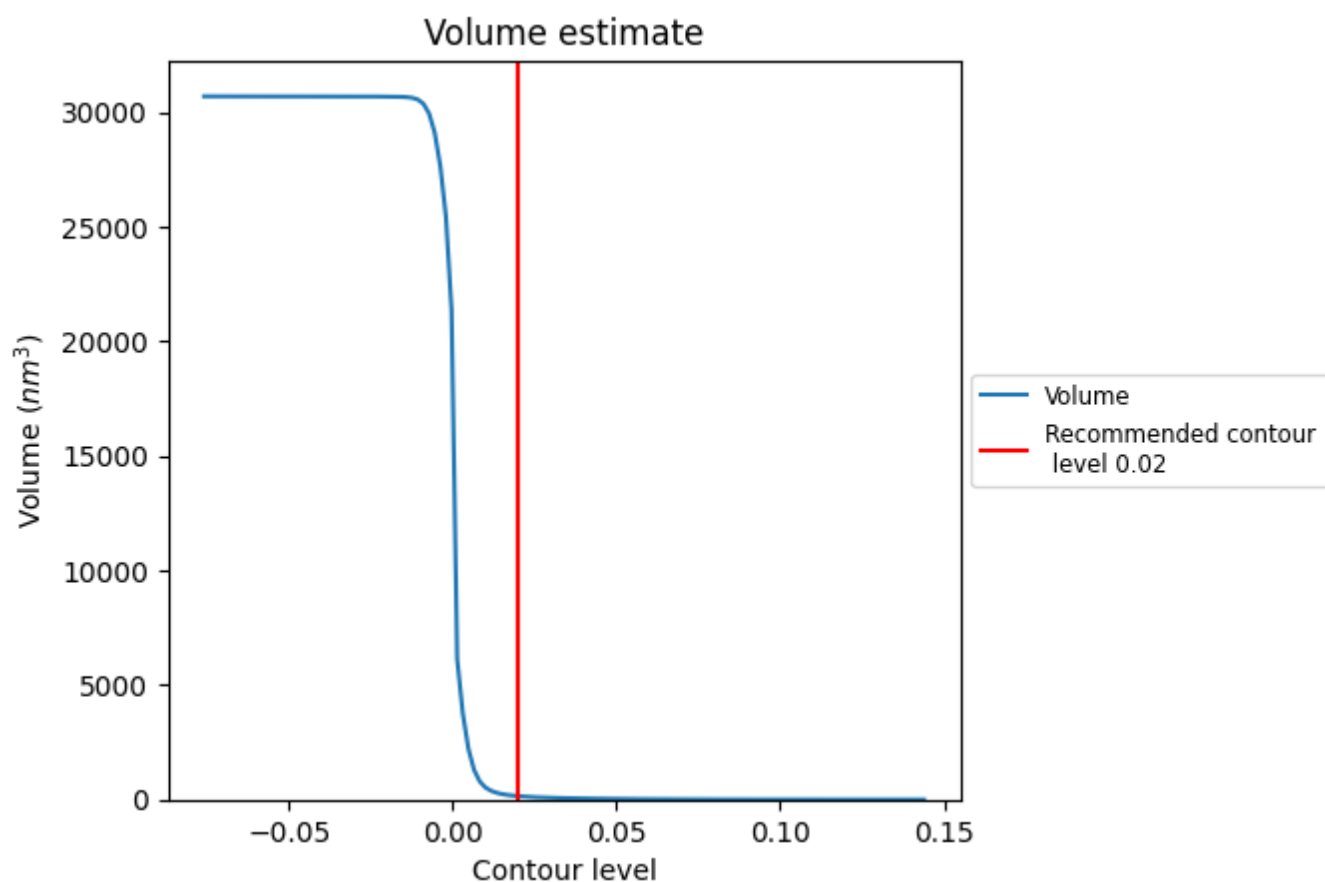
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

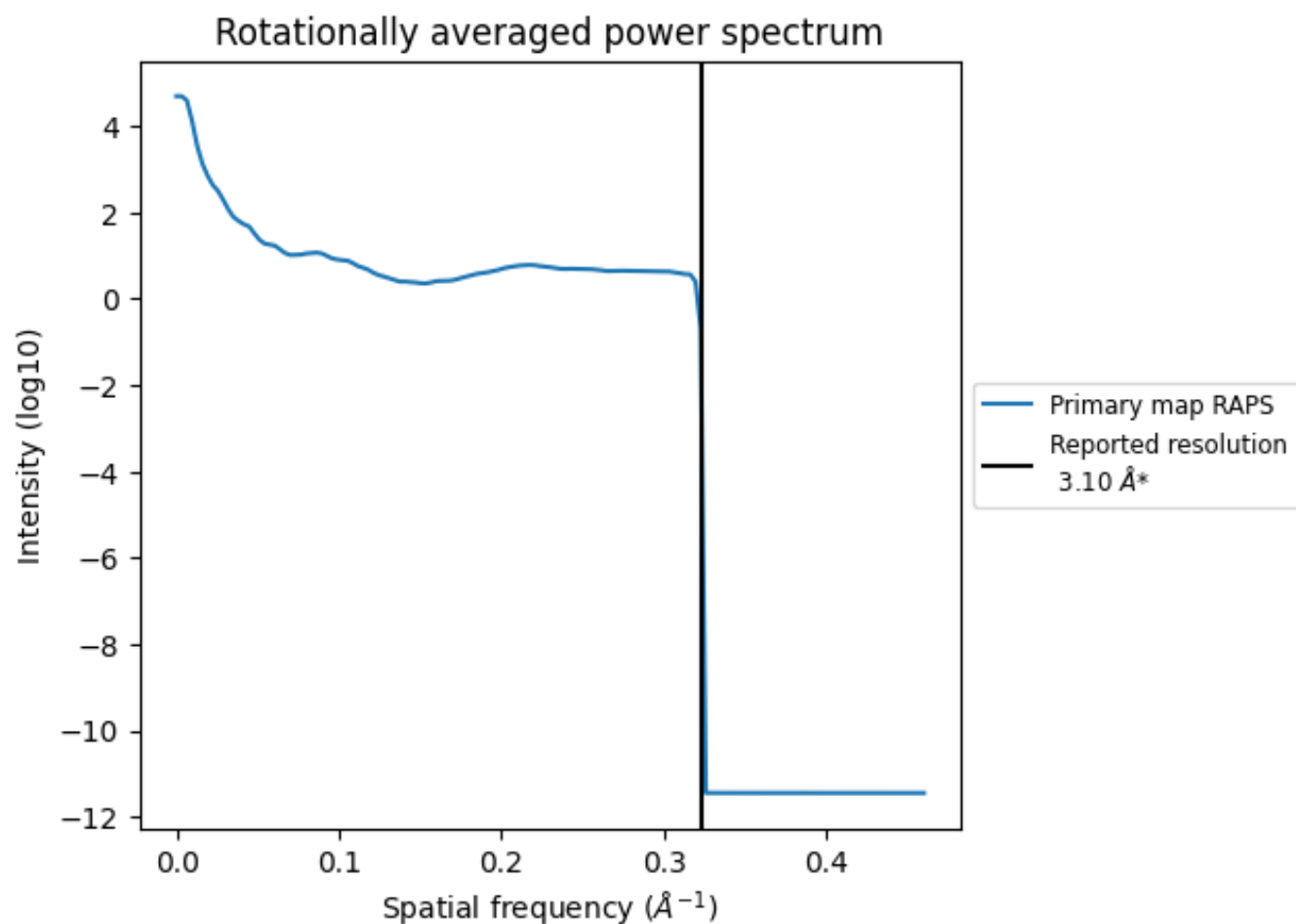
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 150 nm³; this corresponds to an approximate mass of 135 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.323 $\text{\AA}^{-1}$

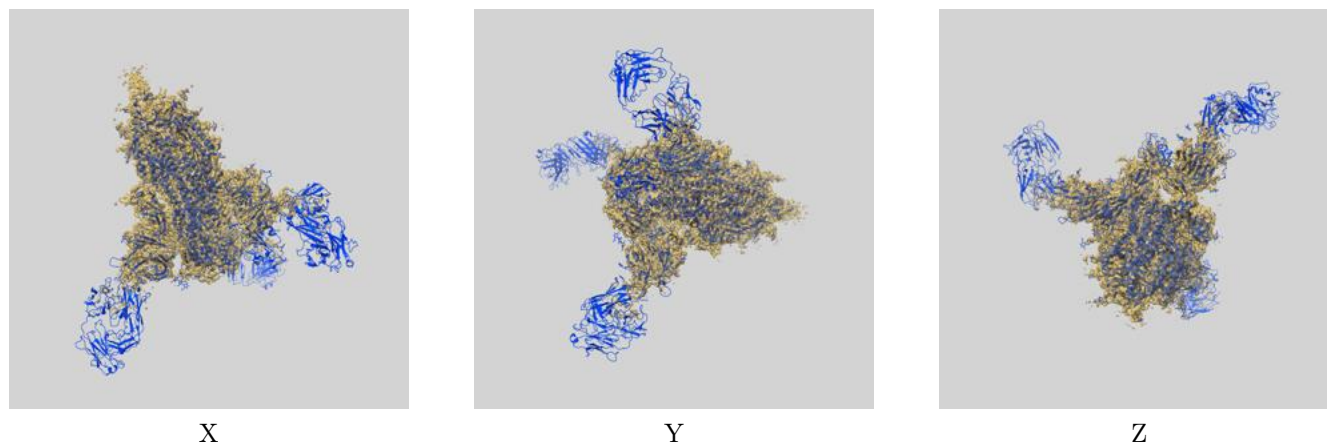
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

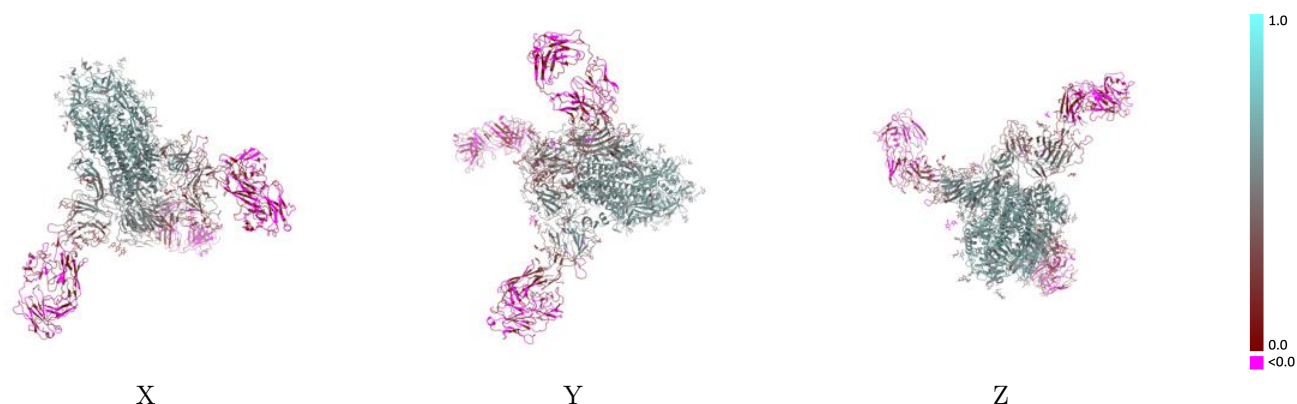
This section contains information regarding the fit between EMDB map EMD-30276 and PDB model 7C2L. Per-residue inclusion information can be found in section [3](#) on page [11](#).

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



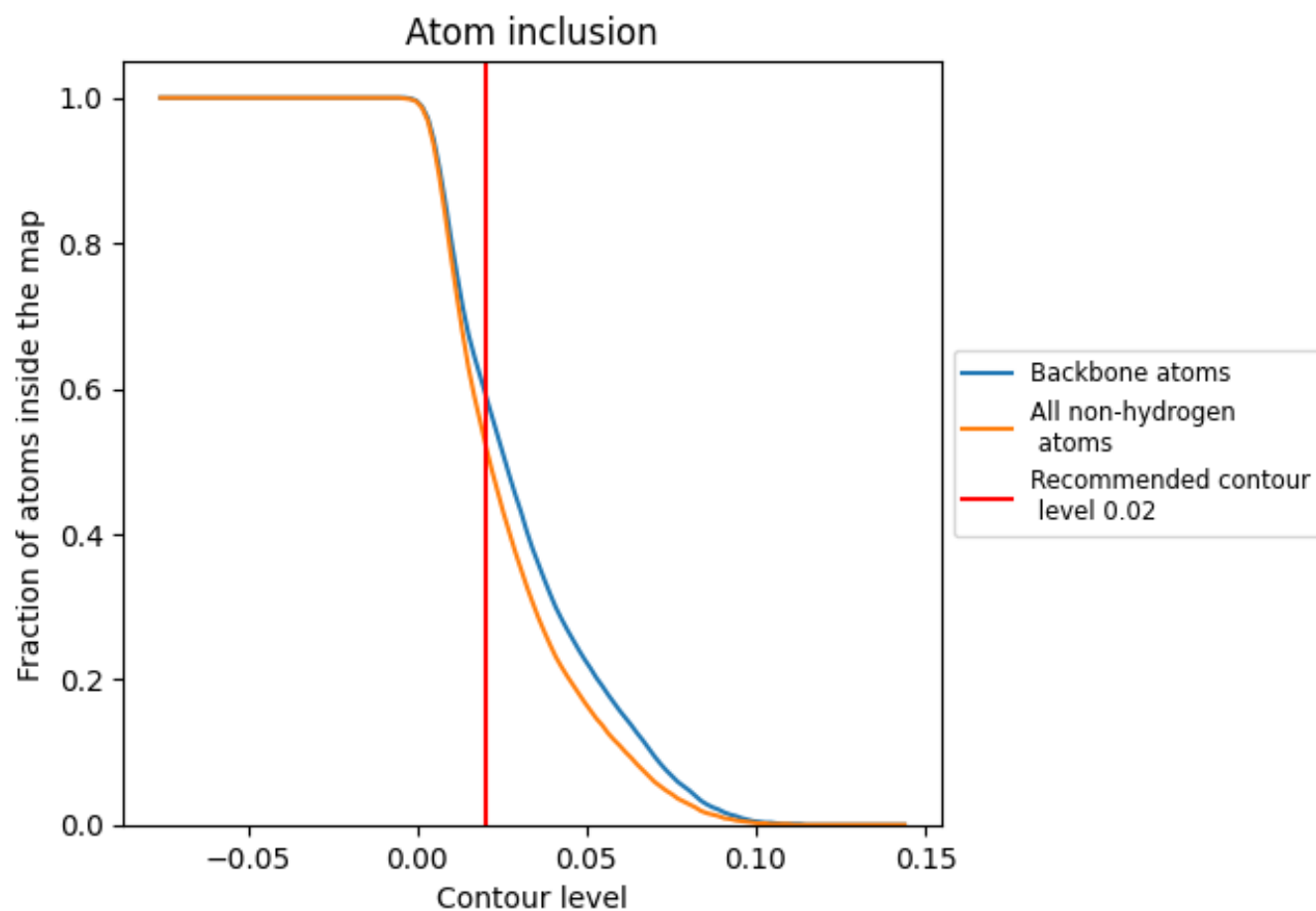
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.02).

9.4 Atom inclusion [i](#)



At the recommended contour level, 59% of all backbone atoms, 52% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5250	 0.3620
A	 0.7010	 0.4840
B	 0.7510	 0.4970
C	 0.7690	 0.5040
D	 0.1670	 0.1760
E	 0.0480	 0.0460
F	 0.3570	 0.3390
G	 0.0710	 -0.0930
H	 0.0220	 0.0660
I	 0.0130	 0.0430
J	 0.0180	 0.0630
K	 0.8210	 0.5000
L	 0.0040	 0.0310
M	 0.0030	 0.0140
N	 0.0020	 0.0200
O	 0.6430	 0.4190
P	 0.5360	 0.4520
Q	 0.6790	 0.4500
R	 0.7140	 0.4960
S	 0.2380	 0.3150
T	 0.0000	 0.0360
U	 0.0000	 0.1590
V	 0.1070	 0.2230
W	 0.3210	 0.3320
X	 0.7500	 0.4970
Y	 0.6430	 0.4980
Z	 0.3930	 0.4150
a	 0.7860	 0.4630
b	 0.6070	 0.4720
c	 0.0950	 0.1920
d	 0.0000	 0.1420
e	 0.1430	 0.3100
f	 0.1790	 0.1020
g	 0.3930	 0.4640
h	 0.7860	 0.5370



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Chain	Atom inclusion	Q-score
i	 0.6430	 0.3860
j	 0.4290	 0.3970
k	 0.8210	 0.4770
l	 0.5710	 0.4660