



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 05:38 AM UTC

PDB ID : 6H04 / pdb_00006h04
EMDB ID : EMD-0107
Title : Closed conformation of the Membrane Attack Complex
Authors : Menny, A.; Serna, M.; Boyd, C.M.; Gardner, S.; Joseph, A.P.; Topf, M.; Bubeck, D.
Deposited on : 2018-07-06
Resolution : 5.60 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:

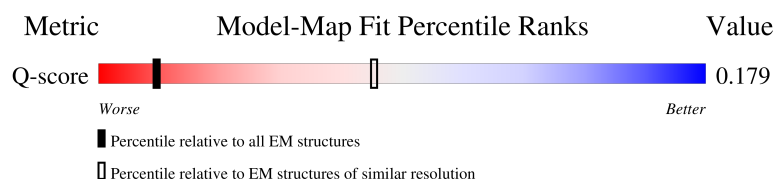
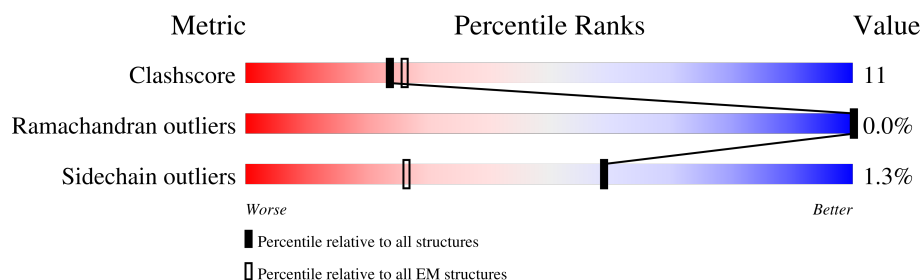
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
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 5.60 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.



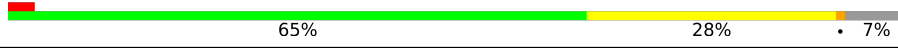
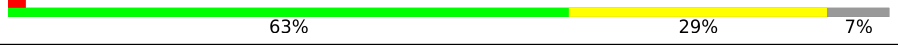
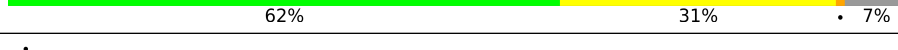
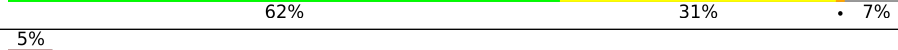
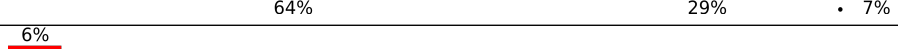
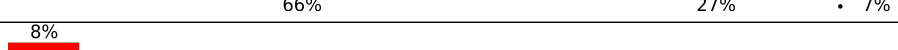
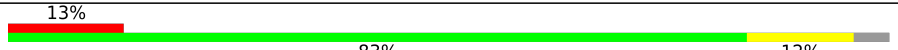
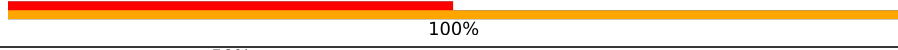
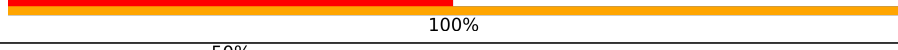
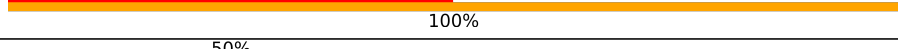
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	513 (5.10 - 6.10)

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	G	538	 11% 61% 31% • 7%
1	H	538	 69% 23% • 7%
1	I	538	 67% 25% • 7%
1	J	538	 68% 25% • 7%

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Mol	Chain	Length	Quality of chain
1	K	538	
1	L	538	
1	M	538	
1	N	538	
1	O	538	
1	P	538	
1	Q	538	
1	R	538	
1	S	538	
1	T	538	
1	U	538	
1	V	538	
1	W	538	
1	X	538	
2	A	1580	
3	C	537	
4	D	821	
5	E	182	
6	F	554	
7	B	913	
8	Y	2	
8	Z	2	
8	a	2	
8	b	2	
8	c	2	

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Mol	Chain	Length	Quality of chain
8	d	2	50% 50% 50%
8	e	2	50% 100%
8	f	2	50% 50%
8	g	2	50% 50%
8	h	2	50% 50%
8	i	2	50% 50%
8	j	2	50% 50%
8	k	2	50% 50%
8	l	2	50% 100%
8	m	2	50% 100%
8	n	2	50% 50%
8	o	2	50% 50%
8	p	2	50% 100%
8	q	2	50% 50%

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 97178 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 Complement component C9.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	L	501	Total	C	N	O	S	0	0
			3785	2363	670	721	31		
1	M	501	Total	C	N	O	S	0	0
			3785	2363	670	721	31		
1	N	501	Total	C	N	O	S	0	0
			3785	2363	670	721	31		
1	O	501	Total	C	N	O	S	0	0
			3785	2363	670	721	31		
1	Q	501	Total	C	N	O	S	0	0
			3785	2363	670	721	31		
1	R	501	Total	C	N	O	S	0	0
			3785	2363	670	721	31		
1	S	501	Total	C	N	O	S	0	0
			3785	2363	670	721	31		
1	T	501	Total	C	N	O	S	0	0
			3785	2363	670	721	31		
1	U	501	Total	C	N	O	S	0	0
			3785	2363	670	721	31		
1	V	501	Total	C	N	O	S	0	0
			3785	2363	670	721	31		
1	W	501	Total	C	N	O	S	0	0
			3785	2363	670	721	31		
1	X	501	Total	C	N	O	S	0	0
			3785	2363	670	721	31		
1	P	501	Total	C	N	O	S	0	0
			3785	2363	670	721	31		
1	H	501	Total	C	N	O	S	0	0
			3785	2363	670	721	31		
1	I	501	Total	C	N	O	S	0	0
			3785	2363	670	721	31		
1	J	501	Total	C	N	O	S	0	0
			3785	2363	670	721	31		
1	K	501	Total	C	N	O	S	0	0
			3785	2363	670	721	31		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	G	501	Total	C	N	O	S	0	0
			3770	2352	668	720	30		

- Molecule 2 is a protein called Complement C5, Complement C5.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	1219	Total	C	N	O	S	0	0
			9497	6097	1572	1801	27		

- Molecule 3 is a protein called Complement component C8 beta chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	513	Total	C	N	O	S	0	0
			3752	2345	664	713	30		

- Molecule 4 is a protein called Complement component C7.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	660	Total	C	N	O	S	0	0
			4578	2844	825	867	42		

- Molecule 5 is a protein called Complement component C8 gamma chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	165	Total	C	N	O	S	0	0
			1286	823	223	236	4		

- Molecule 6 is a protein called Complement component C8 alpha chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	510	Total	C	N	O	S	0	0
			3758	2331	660	730	37		

- Molecule 7 is a protein called Complement component C6.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	B	688	Total	C	N	O	S	0	0
			5128	3174	918	990	46		

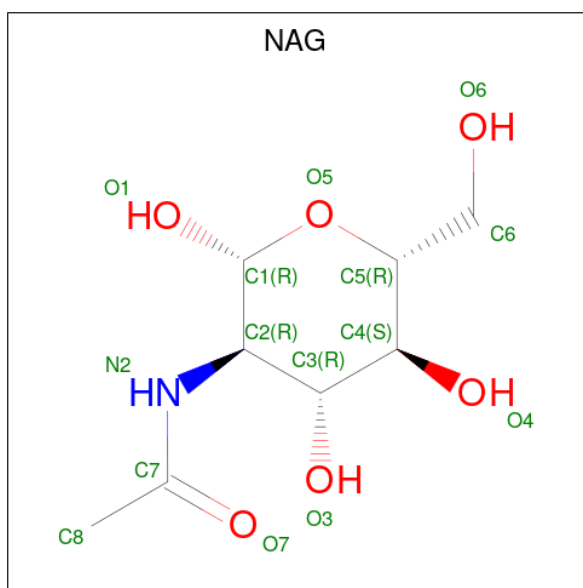
- Molecule 8 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
8	Y	2	Total	C	N	O	0	0
			28	16	2	10		
8	Z	2	Total	C	N	O	0	0
			28	16	2	10		
8	a	2	Total	C	N	O	0	0
			28	16	2	10		
8	b	2	Total	C	N	O	0	0
			28	16	2	10		
8	c	2	Total	C	N	O	0	0
			28	16	2	10		
8	d	2	Total	C	N	O	0	0
			28	16	2	10		
8	e	2	Total	C	N	O	0	0
			28	16	2	10		
8	f	2	Total	C	N	O	0	0
			28	16	2	10		
8	g	2	Total	C	N	O	0	0
			28	16	2	10		
8	h	2	Total	C	N	O	0	0
			28	16	2	10		
8	i	2	Total	C	N	O	0	0
			28	16	2	10		
8	j	2	Total	C	N	O	0	0
			28	16	2	10		
8	k	2	Total	C	N	O	0	0
			28	16	2	10		
8	l	2	Total	C	N	O	0	0
			28	16	2	10		
8	m	2	Total	C	N	O	0	0
			28	16	2	10		
8	n	2	Total	C	N	O	0	0
			28	16	2	10		
8	o	2	Total	C	N	O	0	0
			28	16	2	10		
8	p	2	Total	C	N	O	0	0
			28	16	2	10		
8	q	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 9 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula:

C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms				AltConf
9	L	1	Total	C	N	O	0
			14	8	1	5	
9	L	1	Total	C	N	O	0
			14	8	1	5	
9	M	1	Total	C	N	O	0
			14	8	1	5	
9	M	1	Total	C	N	O	0
			14	8	1	5	
9	N	1	Total	C	N	O	0
			14	8	1	5	
9	N	1	Total	C	N	O	0
			14	8	1	5	
9	O	1	Total	C	N	O	0
			14	8	1	5	
9	O	1	Total	C	N	O	0
			14	8	1	5	
9	Q	1	Total	C	N	O	0
			14	8	1	5	
9	Q	1	Total	C	N	O	0
			14	8	1	5	
9	R	1	Total	C	N	O	0
			14	8	1	5	
9	R	1	Total	C	N	O	0
			14	8	1	5	
9	S	1	Total	C	N	O	0
			14	8	1	5	

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Mol	Chain	Residues	Atoms				AltConf
9	S	1	Total 14	C 8	N 1	O 5	0
9	T	1	Total 14	C 8	N 1	O 5	0
9	T	1	Total 14	C 8	N 1	O 5	0
9	U	1	Total 14	C 8	N 1	O 5	0
9	U	1	Total 14	C 8	N 1	O 5	0
9	V	1	Total 14	C 8	N 1	O 5	0
9	V	1	Total 14	C 8	N 1	O 5	0
9	W	1	Total 14	C 8	N 1	O 5	0
9	W	1	Total 14	C 8	N 1	O 5	0
9	X	1	Total 14	C 8	N 1	O 5	0
9	X	1	Total 14	C 8	N 1	O 5	0
9	P	1	Total 14	C 8	N 1	O 5	0
9	P	1	Total 14	C 8	N 1	O 5	0
9	H	1	Total 14	C 8	N 1	O 5	0
9	H	1	Total 14	C 8	N 1	O 5	0
9	I	1	Total 14	C 8	N 1	O 5	0
9	I	1	Total 14	C 8	N 1	O 5	0
9	J	1	Total 14	C 8	N 1	O 5	0
9	J	1	Total 14	C 8	N 1	O 5	0
9	K	1	Total 14	C 8	N 1	O 5	0
9	K	1	Total 14	C 8	N 1	O 5	0

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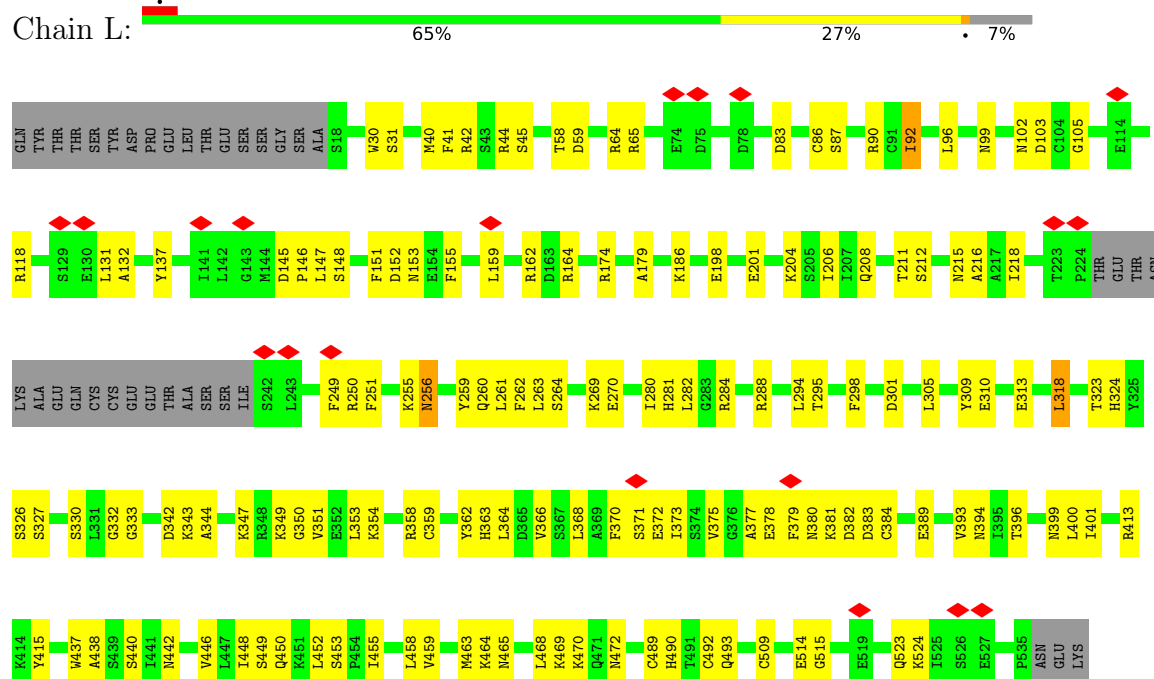
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Mol	Chain	Residues	Atoms				AltConf
9	G	1	Total	C	N	O	0
			14	8	1	5	
9	G	1	Total	C	N	O	0
			14	8	1	5	
9	D	1	Total	C	N	O	0
			14	8	1	5	
9	B	1	Total	C	N	O	0
			14	8	1	5	

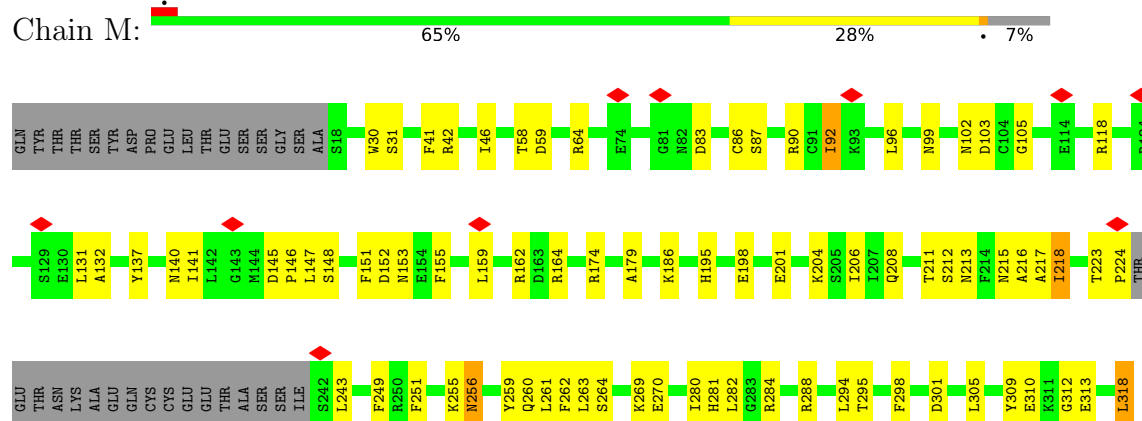
3 Residue-property plots

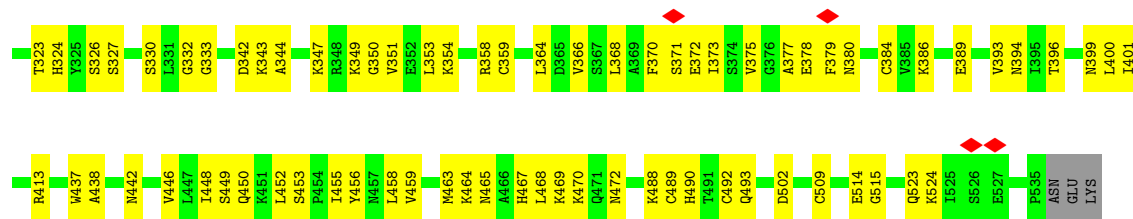
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Complement component C9

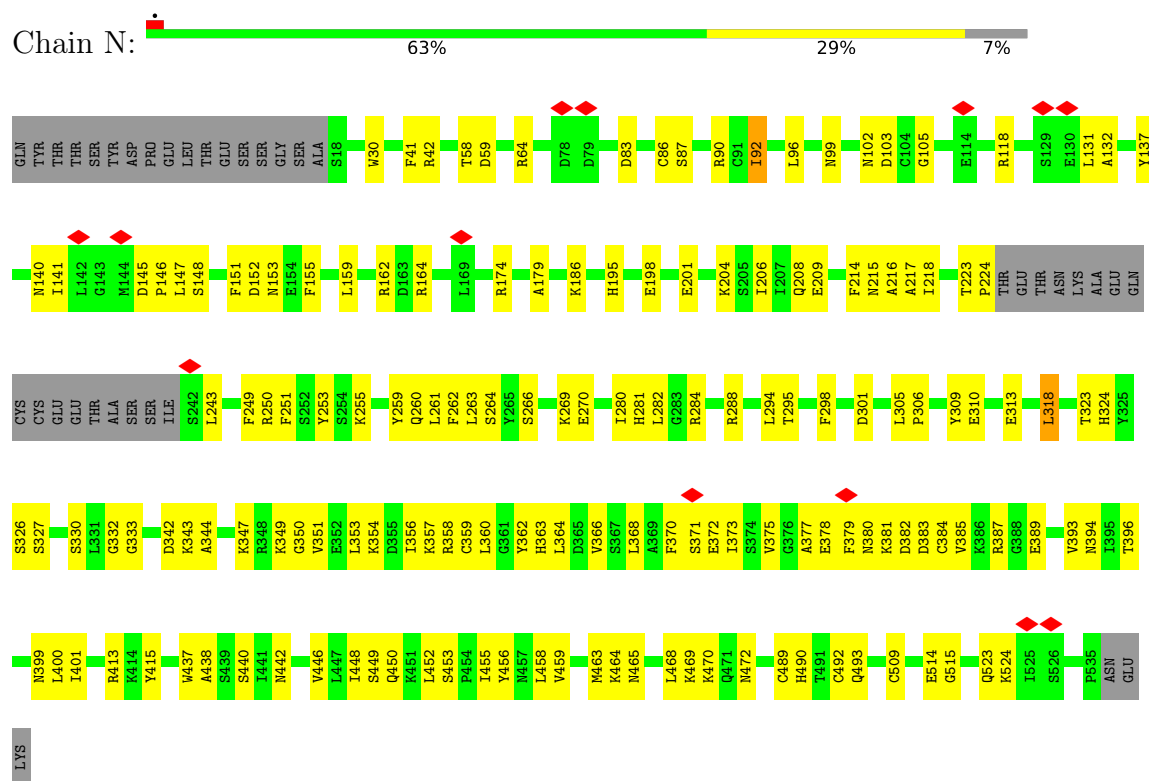


• Molecule 1: Complement component C9

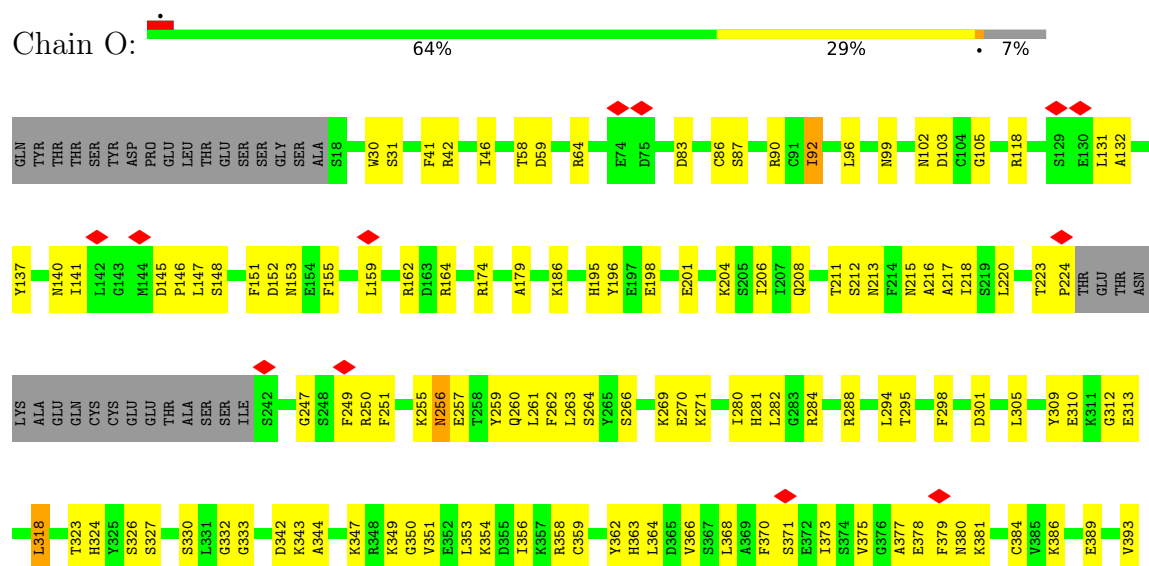




• Molecule 1: Complement component C9

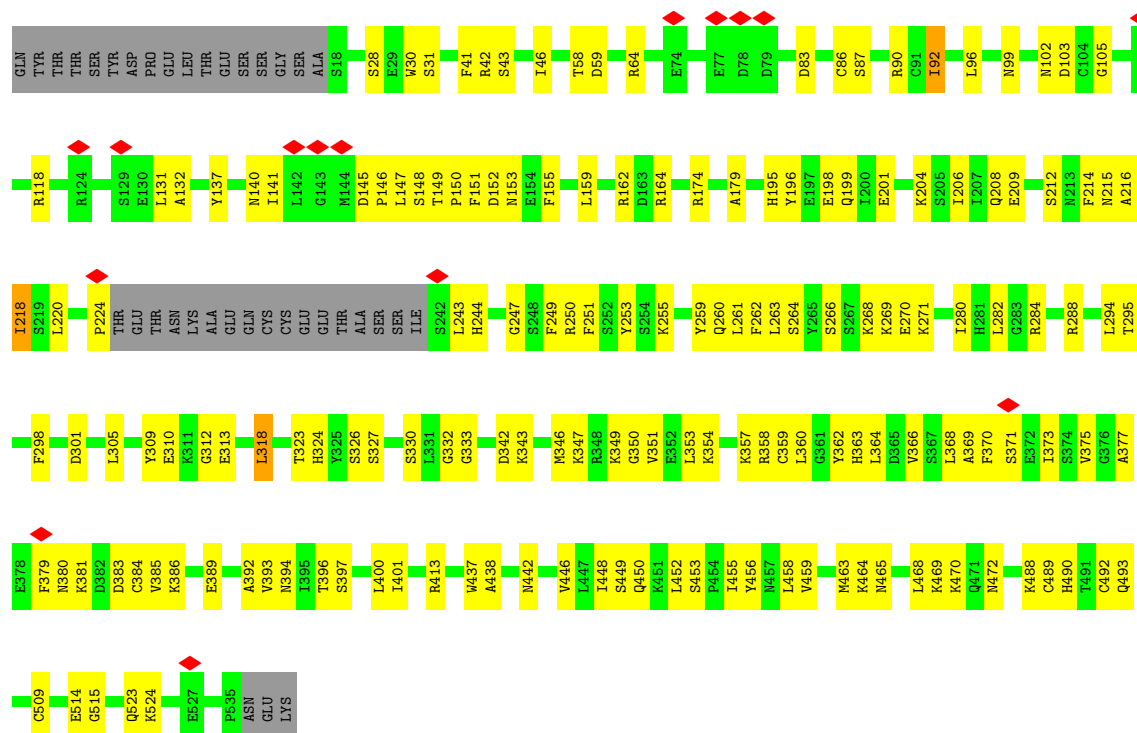


• Molecule 1: Complement component C9

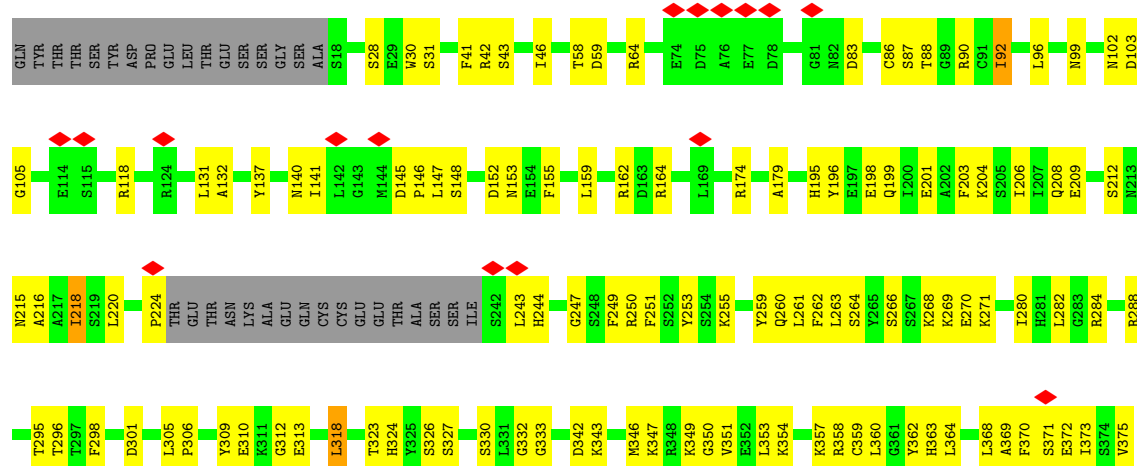


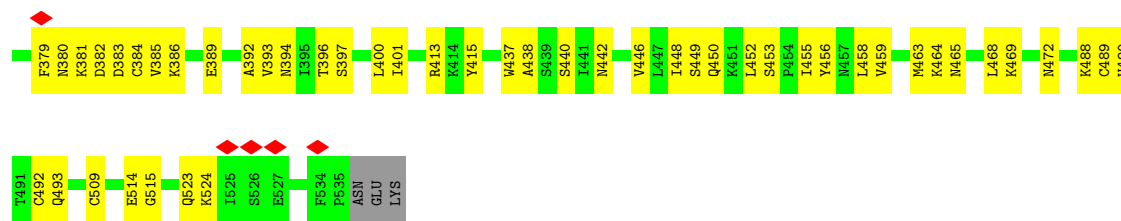


• Molecule 1: Complement component C9

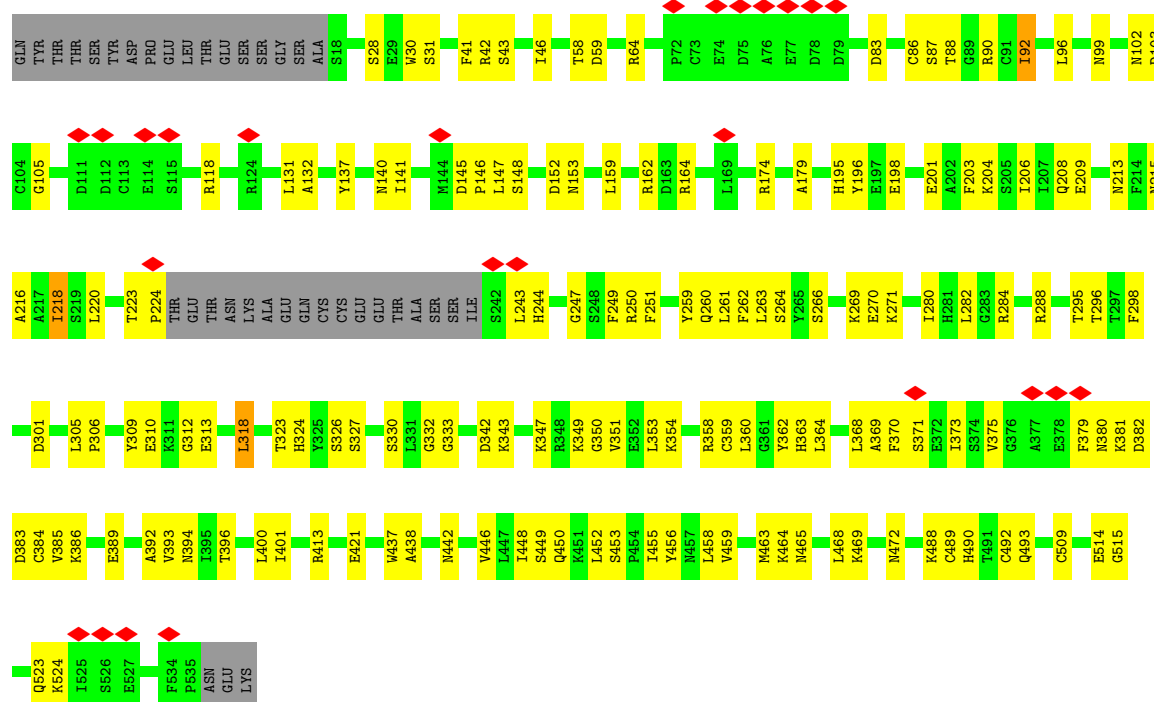


• Molecule 1: Complement component C9

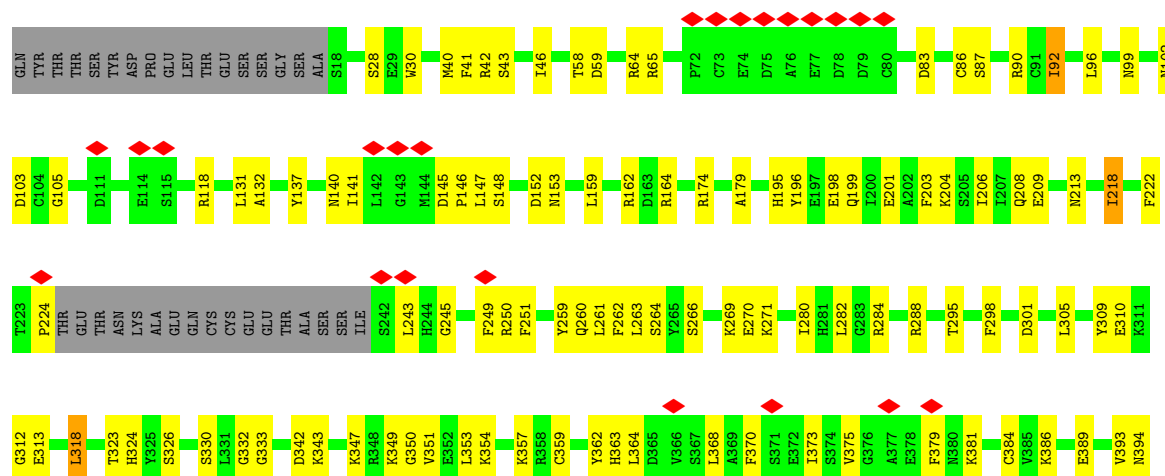




• Molecule 1: Complement component C9

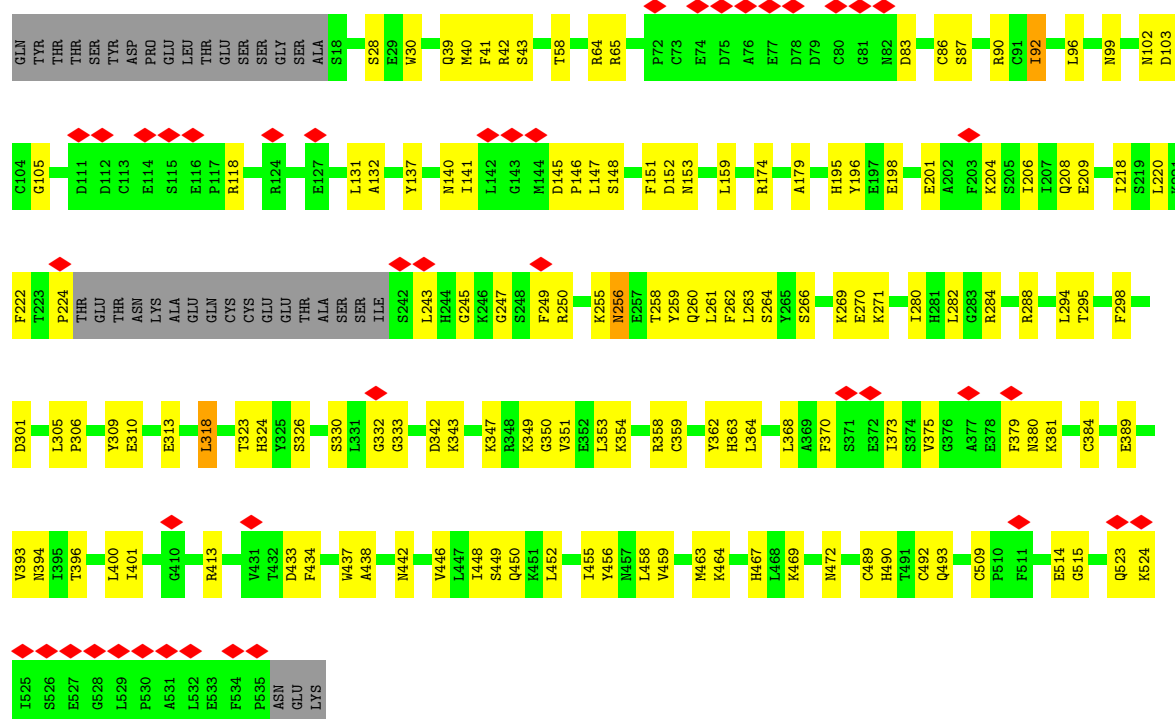


• Molecule 1: Complement component C9

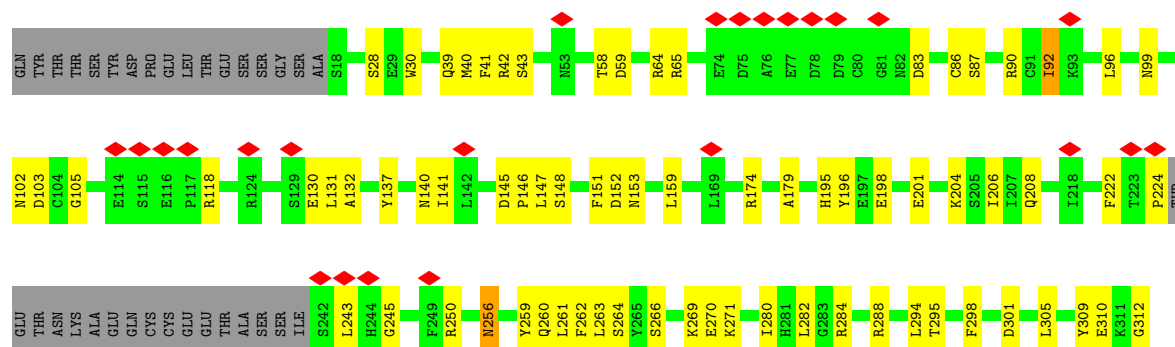


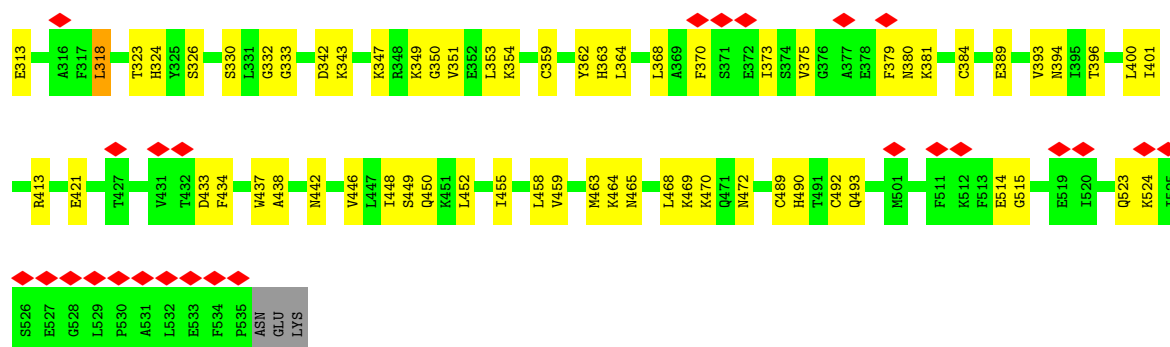


• Molecule 1: Complement component C9

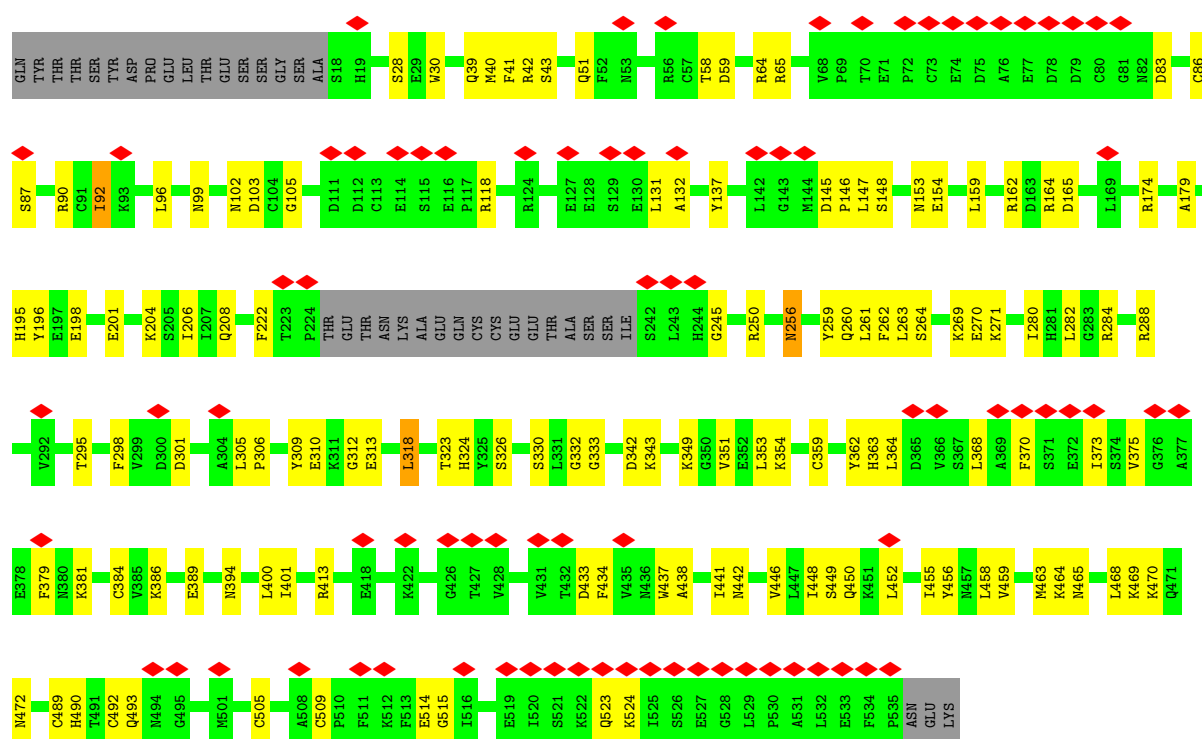


• Molecule 1: Complement component C9

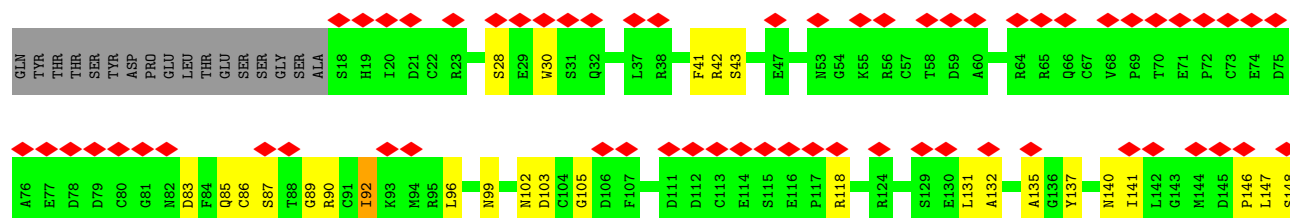


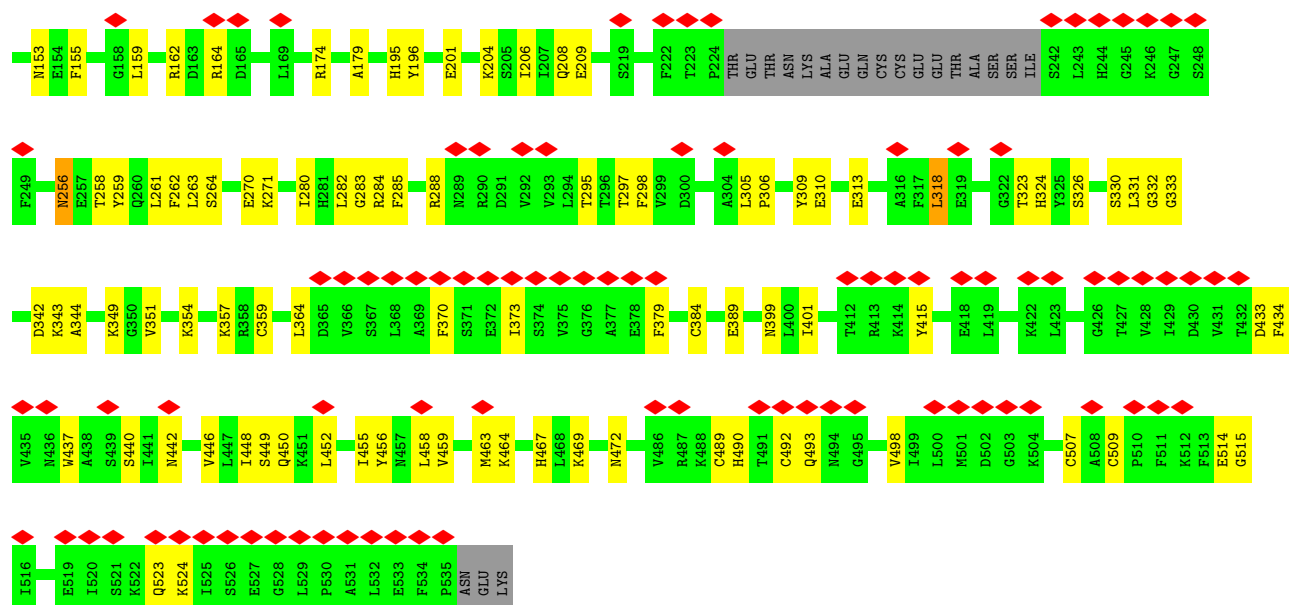


• Molecule 1: Complement component C9

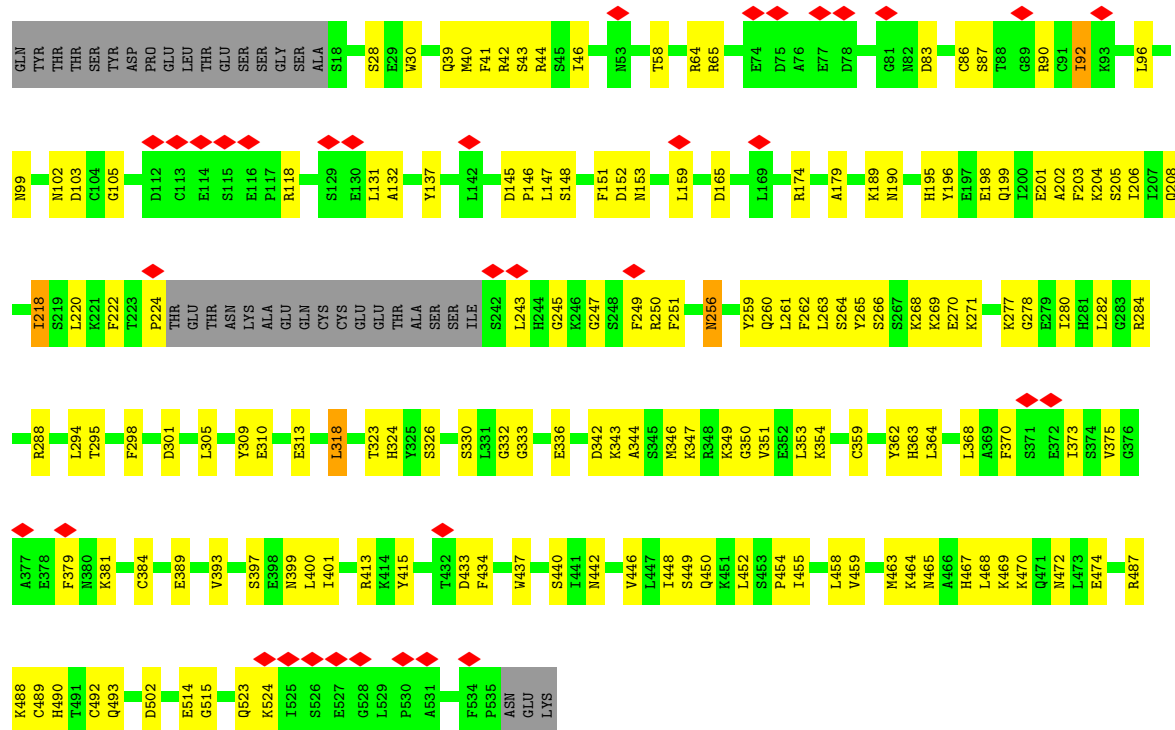


• Molecule 1: Complement component C9



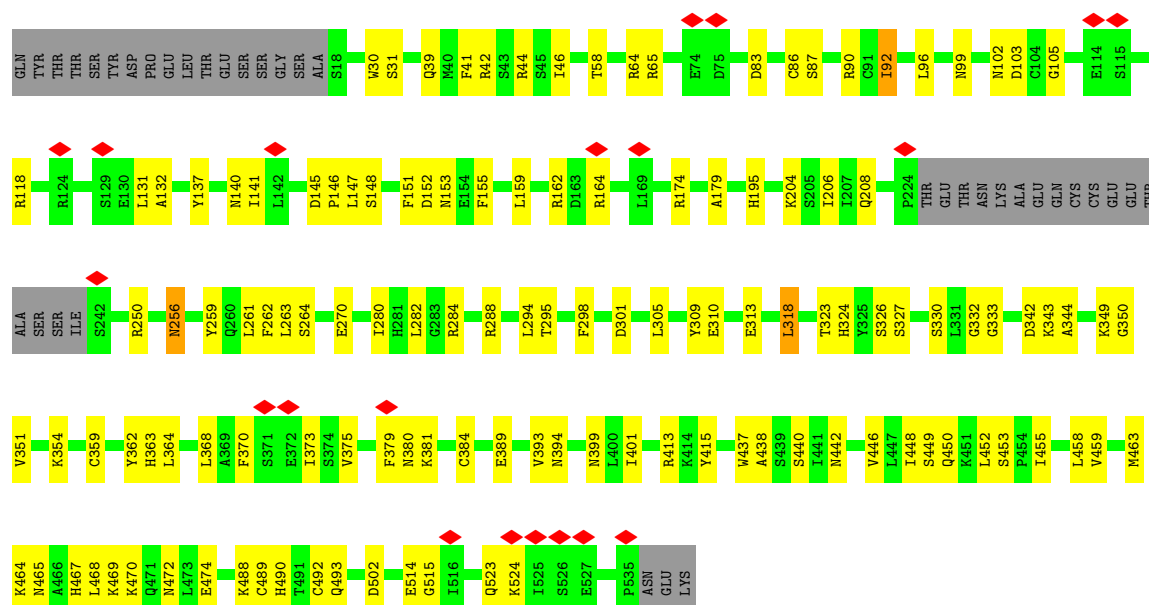


• Molecule 1: Complement component C9



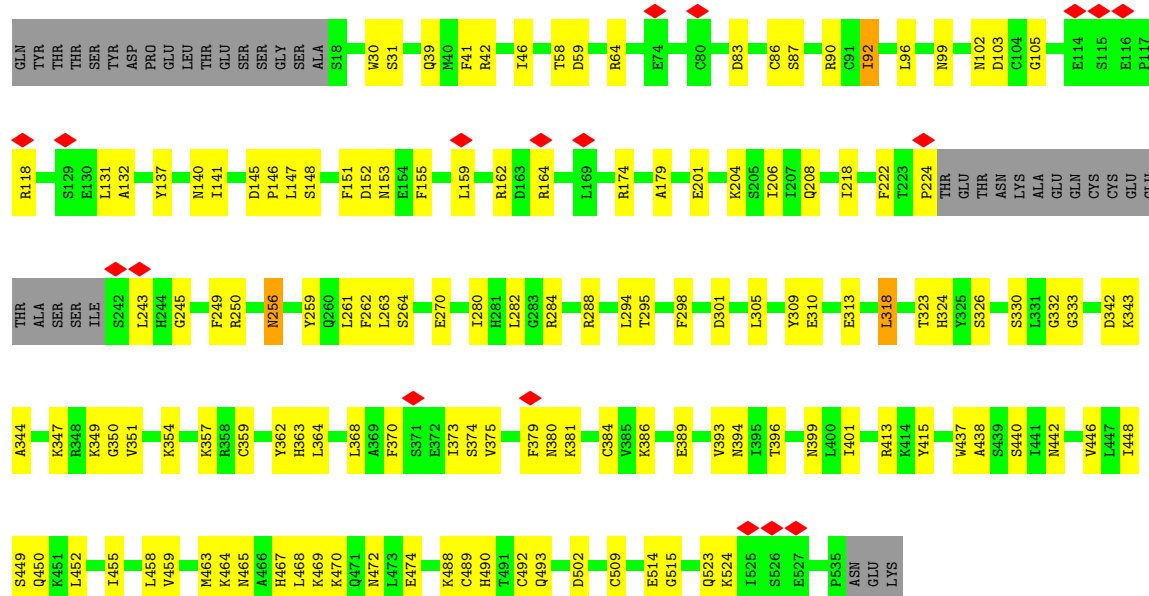
• Molecule 1: Complement component C9





• Molecule 1: Complement component C9

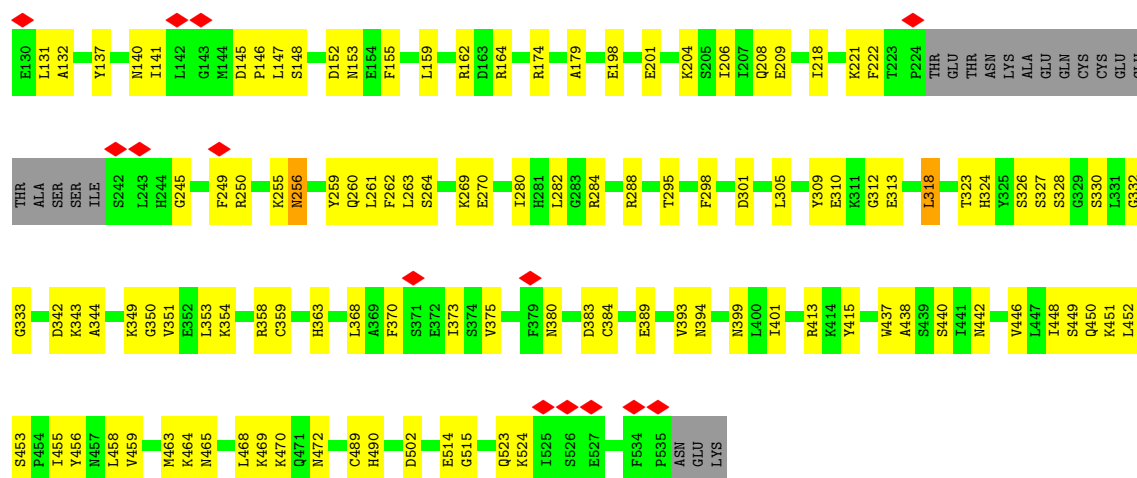
Chain I: 67% 25% 7%



• Molecule 1: Complement component C9

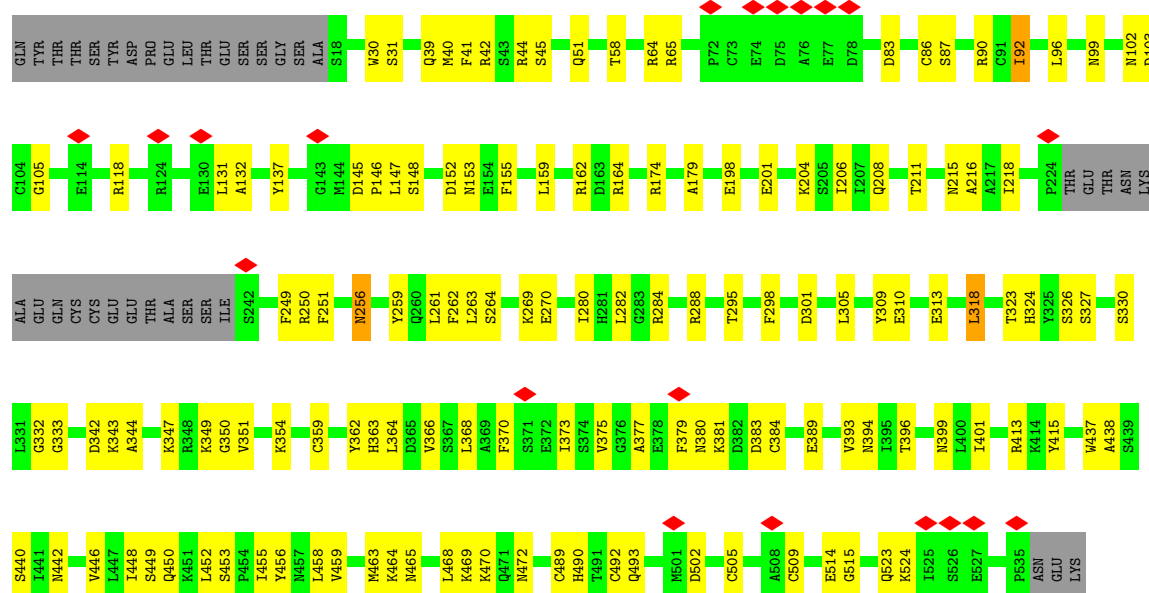
Chain J: 68% 25% 7%





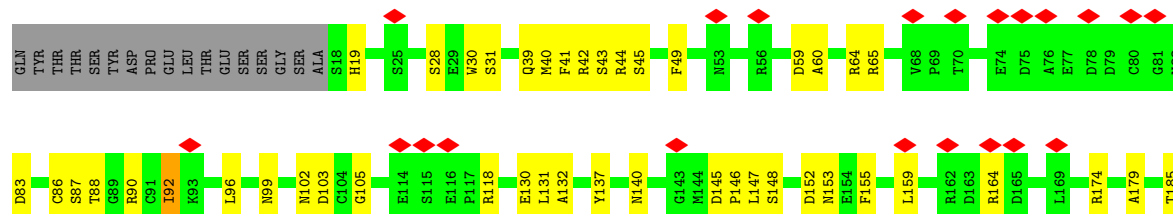
• Molecule 1: Complement component C9

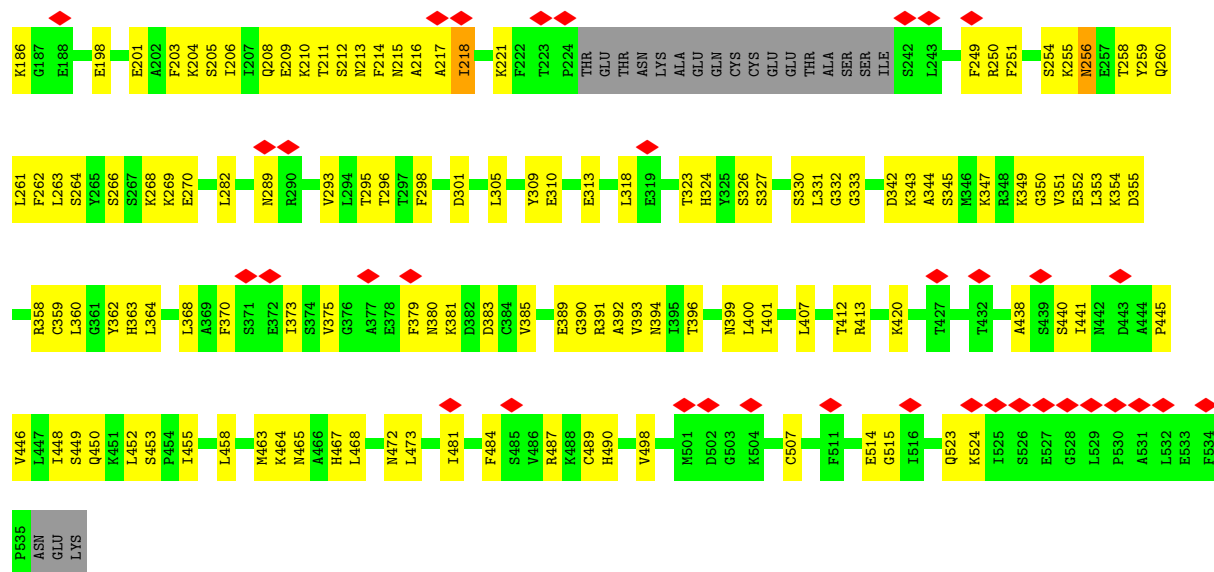
Chain K: 67% 25% 7%



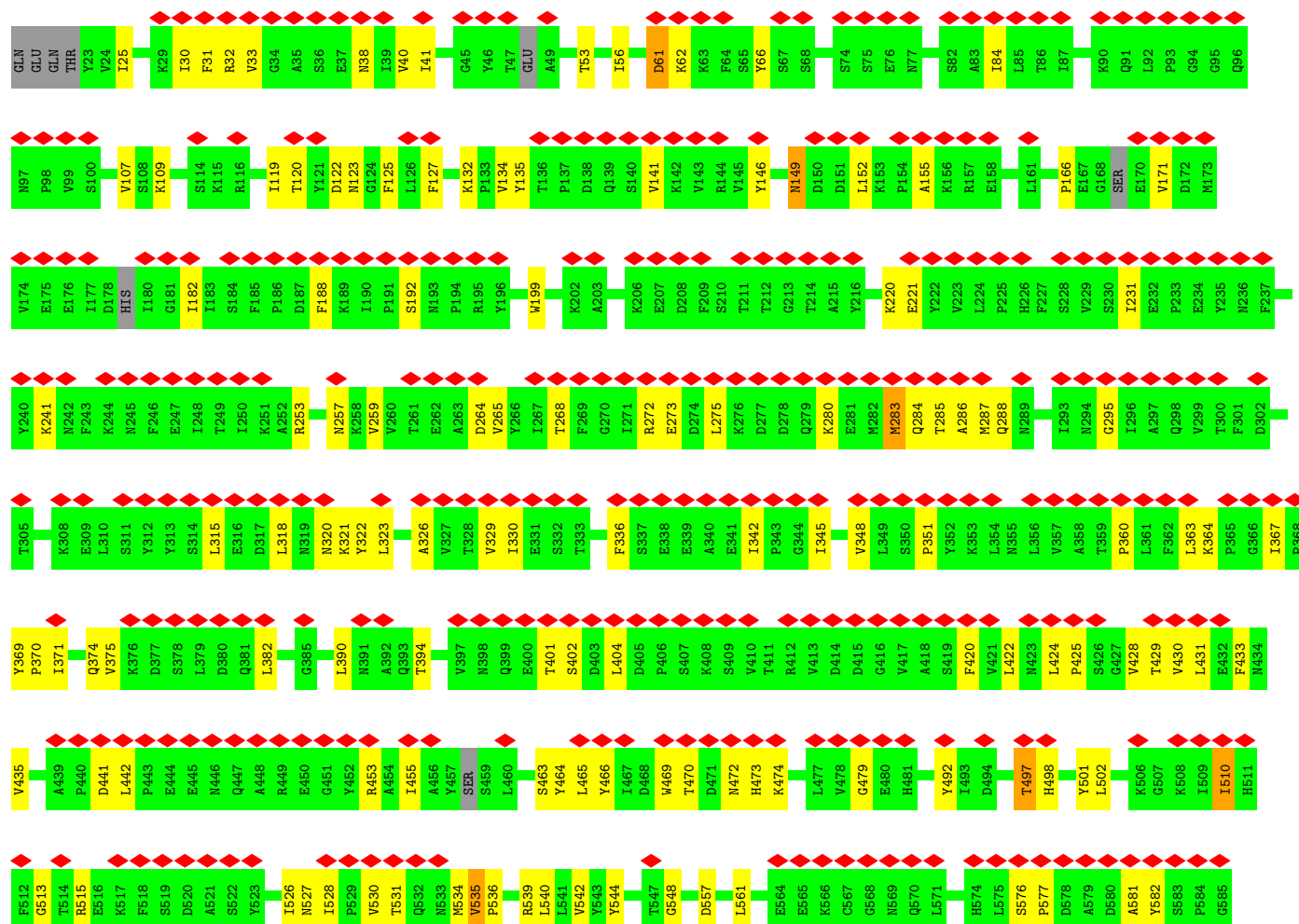
• Molecule 1: Complement component C9

Chain G: 11% 61% 31% 7%





• Molecule 2: Complement C5, Complement C5

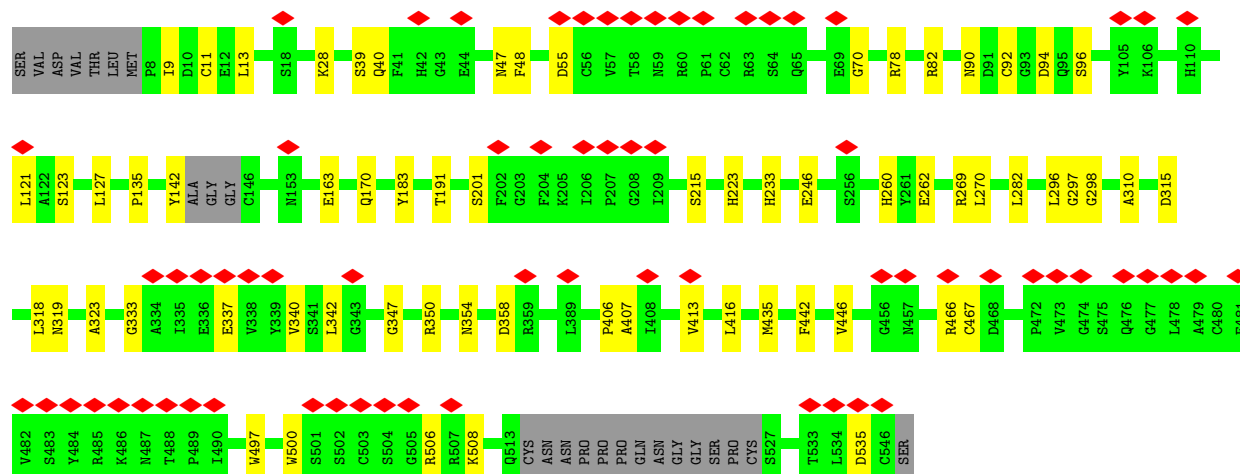




PHE SER PHE ASP ARG TYR ILE TYR PRO LEU ASP SER LEU THR TRP ILE GLU TYR TRP TRP PRO ARG ASP THR CYS SER SER CYS GLN ALA PHE LEU LEU ALA ASN LEU ASP PHE LEU ASP ILE PHE LEU ASN GLY CYS

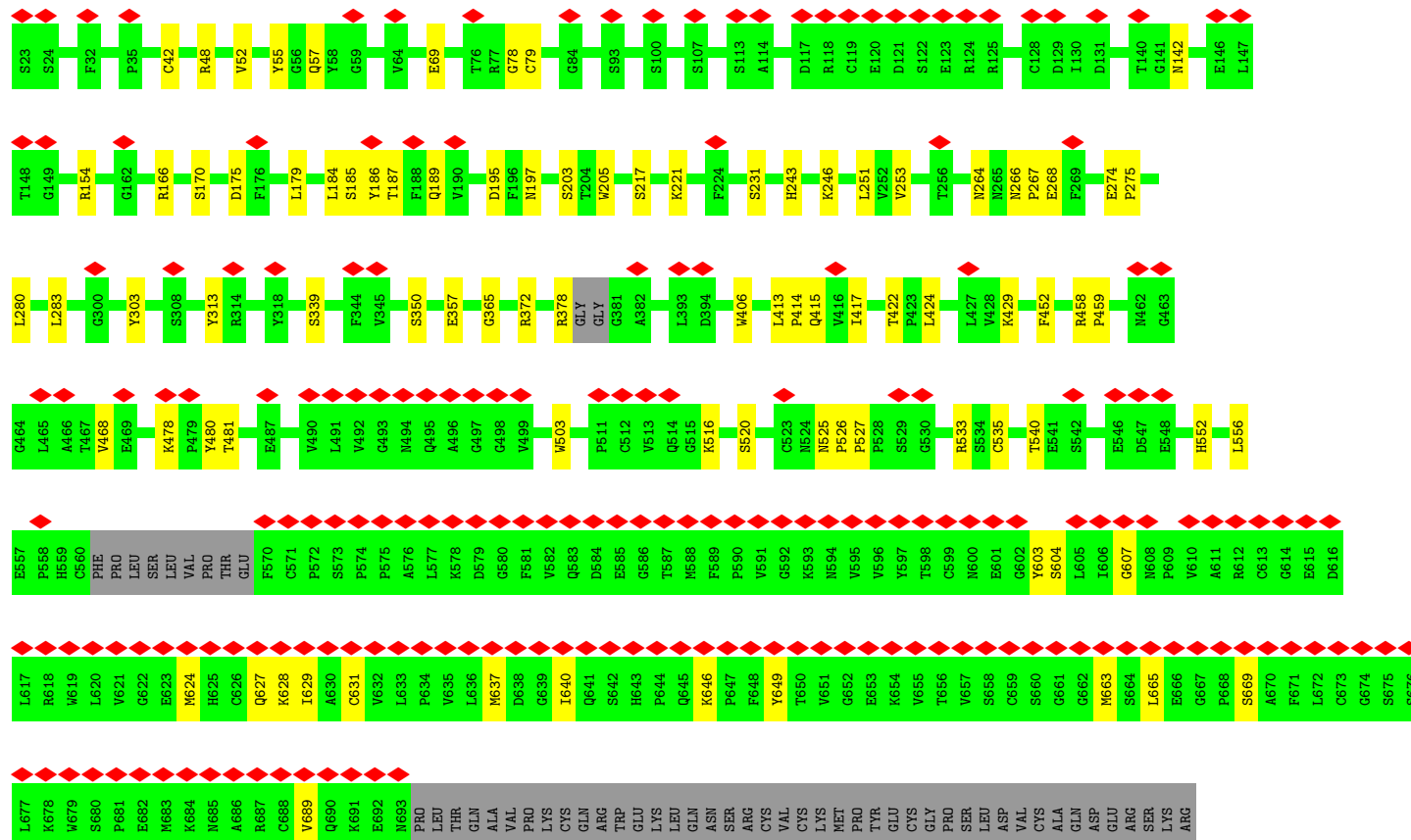
• Molecule 3: Complement component C8 beta chain

Chain C: 13% 83% 12%



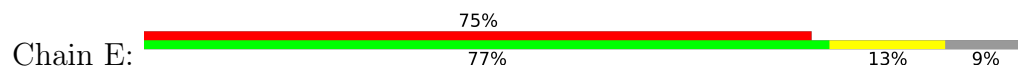
• Molecule 4: Complement component C7

Chain D: 24% 70% 11% 20%



ILE	LEU	PRO	LEU	THR	VAL	CYS	LYS	MET	GLN	VAL	VAL	LEU	ILE	ASN	THR	THR	LEU	THR	GLY	GLY	ASP	SER	SER	CYS	THR	LEU	PRO	PRO	ALA	ALA	SER	GLN	ALA	LEU	THR	ILE	LYS	VAL	ALA	CYS	THR	THR	GLY	GLY	ASP	ASP	ALA	GLU	GLU	GLU	GLN	GLY	THR	GLN	CYS
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• Molecule 5: Complement component C8 gamma chain



Q125	L126	K129	L130	Y131	A132	R133	S134	L135	P136	V137	S138	D139	V141	L142	S143	G144	F145	E146	Q147	R148	V149	Q150	E151	A152	H153	L154	T155	E156	D157	Q158	I159	F160	Y161	P162	K164	G165	C168	E169	A170	A171	D172	Q173	F174	H175	V176	L177	D178	E179	V180	ARG	ARG						
T62	A63	M64	A65	V66	F69	R70	K71	L72	D73	G74	T75	C76	W77	S78	P79	R80	Q81	L82	V83	C84	D85	T86	G87	V88	L89	G90	R91	F92	L93	L94	G95	ALA	ARG	ASP	A99	R100	G101	F102	P103	G104	V105	C106	E107	A108	D111	Y112	Q113	S114	F115	A116	V117	L118	L119	E121	R122	A123	Q124
GLN	LYS	PRO	GLN	ARG	PRO	ARG	ARG	ARG	PRO	ALA	SER	PRO	ILE	ASN	THR	THR	LEU	THR	GLY	GLY	ASP	SER	SER	CYS	THR	LEU	PRO	PRO	ALA	ALA	SER	GLN	ALA	LEU	THR	ILE	LYS	VAL	ALA	CYS	THR	THR	GLY	GLY	ASP	ASP	ALA	GLU	GLU	GLU	GLN	GLY	THR	GLN	CYS		

• Molecule 6: Complement component C8 alpha chain



C498	E499	GLN	THR	GLN	THR	GLU	GLY	LYS	A508	S513	C514	W515	S516	S517	W518	S519	VAL	CYS	ARG	ALA	GLY	ILE	Q526	E527	R528	R529	R530	E531	C532	ASP	ASN	PRO	ALA	PRO	GLN	ASN	GLY	GLY	ALA	SER	C544	K548	V549	Q550	T551	Q552	ALA	CYS		
G362	G363	L364	S365	G366	D367	H368	C369	K370	K371	G375	K376	T377	E378	R379	A380	R381	K382	R394	G395	G399	W416	P433	I434	H435	M452	L453	R454	R455	C467	G470	P471	C472	PHE	ASN	ASN	GLY	V477	C485	R486	C487	Q488	C489	L490	L491	G492	S493	L494	G495	A496	A497
G234	V235	G236	S240	Q241	T242	T243	S244	F245	L246	T247	E248	L249	N250	K251	L262	V266	M273	R274	D277	L278	Q286	E290	Y300	E333	S334	L335	G336	T337	T338	S339	R340	D341	T342	T343	T344	C345	G348	S349	L350	G351	L352	Q353	Y354	E355	D356	K357	L358	N359		
R104	A105	I106	D109	P115	L129	D133	A134	Q135	S136	Q146	E157	L158	R159	D161	S162	T163	C164	E165	R166	L167	F182	A191	I195	L206	L207	S208	K212	D213	K214	S217	F218	G219	V220	T221	L222	L224	G225	P226	A227	G228	S229	P230	L231	V232	V233					
ALA	ALA	THR	PRO	ALA	ALA	VAL	VAL	THR	C9	W14	K27	T28	R29	N37	T42	I43	C44	D50	Q51	A52	S53	C54	S55	S56	S57	T58	T59	C60	VAL	ARG	GLN	ALA	GLN	C66	Q71	T75	G76	R77	C78	R81	C85	Q89	L92	D99	C100	E101	D102	V103		

• Molecule 7: Complement component C6



CYS	F23	C24	D25	Q31	S34	T38	H47	ARG	Q49	I50	V51	V52	D53	K54	F60	T70	R71	E72	D86	F87	G88	P89	D92	C93	D94	P95	C96	Q100	S101	K102	S105	VAL	LEU	ARG	PRO	SER	GLN	PHE	GLY	GLN	PRO	C117	L121	V122	Q125
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- Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose





- Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 8: 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, C1	Depositor
Number of particles used	53167	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	59000	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.342	Depositor
Minimum map value	-0.153	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.011	Depositor
Recommended contour level	0.06	Depositor
Map size (Å)	498.24, 498.24, 498.24	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.384, 1.384, 1.384	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	G	0.10	0/3839	0.31	0/5181
1	H	0.10	0/3856	0.29	0/5203
1	I	0.10	0/3856	0.29	0/5203
1	J	0.10	0/3856	0.31	0/5203
1	K	0.10	0/3856	0.29	0/5203
1	L	0.10	0/3856	0.29	0/5203
1	M	0.09	0/3856	0.29	0/5203
1	N	0.09	0/3856	0.30	0/5203
1	O	0.10	0/3856	0.30	0/5203
1	P	0.10	0/3856	0.30	0/5203
1	Q	0.10	0/3856	0.30	0/5203
1	R	0.10	0/3856	0.29	0/5203
1	S	0.10	0/3856	0.30	0/5203
1	T	0.09	0/3856	0.30	0/5203
1	U	0.10	0/3856	0.30	0/5203
1	V	0.10	0/3856	0.30	0/5203
1	W	0.10	0/3856	0.30	0/5203
1	X	0.10	0/3856	0.31	0/5203
2	A	0.10	0/9707	0.33	4/13191 (0.0%)
3	C	0.09	0/3831	0.26	0/5203
4	D	0.10	0/4687	0.31	0/6362
5	E	0.08	0/1314	0.25	0/1782
6	F	0.09	0/3830	0.26	0/5157
7	B	0.10	0/5231	0.29	2/7085 (0.0%)
All	All	0.10	0/97991	0.30	6/132412 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	61	ASP	CA-C-N	7.28	134.81	121.70
2	A	61	ASP	C-N-CA	7.28	134.81	121.70
2	A	283	MET	CA-C-N	5.71	131.98	121.70
2	A	283	MET	C-N-CA	5.71	131.98	121.70
7	B	713	LEU	CA-C-N	5.03	130.75	121.70
7	B	713	LEU	C-N-CA	5.03	130.75	121.70

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	G	3770	0	3478	134	0
1	H	3785	0	3495	88	0
1	I	3785	0	3495	93	0
1	J	3785	0	3495	93	0
1	K	3785	0	3495	99	0
1	L	3785	0	3495	109	0
1	M	3785	0	3495	111	0
1	N	3785	0	3495	114	0
1	O	3785	0	3495	113	0
1	P	3785	0	3495	107	0
1	Q	3785	0	3495	115	0
1	R	3785	0	3495	116	0
1	S	3785	0	3495	114	0
1	T	3785	0	3495	99	0
1	U	3785	0	3495	95	0
1	V	3785	0	3495	91	0
1	W	3785	0	3495	90	0
1	X	3785	0	3495	74	0
2	A	9497	0	9310	161	0
3	C	3752	0	3289	42	0
4	D	4578	0	3862	55	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	E	1286	0	1244	15	0
6	F	3758	0	3313	92	0
7	B	5128	0	4610	71	0
8	Y	28	0	25	2	0
8	Z	28	0	25	2	0
8	a	28	0	25	2	0
8	b	28	0	25	3	0
8	c	28	0	25	3	0
8	d	28	0	25	3	0
8	e	28	0	25	3	0
8	f	28	0	25	2	0
8	g	28	0	25	2	0
8	h	28	0	25	2	0
8	i	28	0	25	2	0
8	j	28	0	25	1	0
8	k	28	0	25	1	0
8	l	28	0	25	2	0
8	m	28	0	25	2	0
8	n	28	0	25	2	0
8	o	28	0	25	2	0
8	p	28	0	25	3	0
8	q	28	0	25	1	0
9	B	14	0	13	1	0
9	D	14	0	13	1	0
9	G	28	0	26	2	0
9	H	28	0	26	2	0
9	I	28	0	26	3	0
9	J	28	0	26	2	0
9	K	28	0	26	2	0
9	L	28	0	26	2	0
9	M	28	0	26	2	0
9	N	28	0	26	2	0
9	O	28	0	26	1	0
9	P	28	0	26	1	0
9	Q	28	0	26	2	0
9	R	28	0	26	2	0
9	S	28	0	26	1	0
9	T	28	0	26	3	0
9	U	28	0	26	3	0
9	V	28	0	26	2	0
9	W	28	0	26	2	0
9	X	28	0	26	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	97178	0	89490	2031	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 11.

All (2031) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:250:ARG:HB2	1:O:363:HIS:HB3	1.60	0.82
1:G:326:SER:HB3	1:G:450:GLN:HE21	1.44	0.81
1:Q:250:ARG:HB2	1:Q:363:HIS:HB3	1.63	0.81
6:F:490:ARG:H	6:F:498:CYS:HB2	1.45	0.81
1:S:326:SER:HB3	1:S:450:GLN:HE21	1.46	0.81
1:I:326:SER:HB3	1:I:450:GLN:HE21	1.46	0.81
1:K:250:ARG:HB2	1:K:363:HIS:HB3	1.63	0.80
1:K:326:SER:HB3	1:K:450:GLN:HE21	1.47	0.80
1:U:326:SER:HB3	1:U:450:GLN:HE21	1.47	0.80
1:T:326:SER:HB3	1:T:450:GLN:HE21	1.46	0.80
1:V:326:SER:HB3	1:V:450:GLN:HE21	1.47	0.80
1:W:326:SER:HB3	1:W:450:GLN:HE21	1.47	0.80
1:O:326:SER:HB3	1:O:450:GLN:HE21	1.47	0.80
1:M:326:SER:HB3	1:M:450:GLN:HE21	1.47	0.79
1:N:326:SER:HB3	1:N:450:GLN:HE21	1.48	0.79
1:S:208:GLN:HB2	1:S:259:TYR:HB2	1.65	0.79
1:T:208:GLN:HB2	1:T:259:TYR:HB2	1.65	0.78
1:L:326:SER:HB3	1:L:450:GLN:HE21	1.47	0.78
1:H:326:SER:HB3	1:H:450:GLN:HE21	1.47	0.78
1:R:326:SER:HB3	1:R:450:GLN:HE21	1.48	0.78
1:P:264:SER:HB3	1:P:349:LYS:HB3	1.66	0.78
1:R:250:ARG:HB2	1:R:363:HIS:HB3	1.65	0.78
1:P:326:SER:HB3	1:P:450:GLN:HE21	1.46	0.77
6:F:242:ASP:HB2	6:F:343:THR:HB	1.66	0.77
1:Q:326:SER:HB3	1:Q:450:GLN:HE21	1.47	0.77
1:X:326:SER:HB3	1:X:450:GLN:HE21	1.48	0.77
1:N:208:GLN:HB2	1:N:259:TYR:HB2	1.65	0.77
1:J:326:SER:HB3	1:J:450:GLN:HE21	1.48	0.77
1:N:250:ARG:HB2	1:N:363:HIS:HB3	1.67	0.77
2:A:535:VAL:HG23	2:A:536:PRO:HD3	1.67	0.77
1:S:264:SER:HB3	1:S:349:LYS:HB3	1.66	0.76
1:T:264:SER:HB3	1:T:349:LYS:HB3	1.66	0.76
1:L:250:ARG:HB2	1:L:363:HIS:HB3	1.66	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:264:SER:HB3	1:R:349:LYS:HB3	1.66	0.76
1:G:250:ARG:HB2	1:G:363:HIS:HB3	1.66	0.76
1:Q:264:SER:HB3	1:Q:349:LYS:HB3	1.67	0.76
1:Q:208:GLN:HB2	1:Q:259:TYR:HB2	1.66	0.76
1:G:216:ALA:HB3	1:G:251:PHE:HB3	1.68	0.75
6:F:493:SER:H	6:F:498:CYS:HB3	1.50	0.75
2:A:61:ASP:HB2	2:A:62:LYS:HB3	1.68	0.75
1:O:208:GLN:HB2	1:O:259:TYR:HB2	1.68	0.75
1:T:218:ILE:HG23	1:T:249:PHE:HB2	1.68	0.75
7:B:701:ARG:HD2	7:B:748:GLY:HA2	1.69	0.74
1:M:208:GLN:HB2	1:M:259:TYR:HB2	1.69	0.74
1:N:264:SER:HB3	1:N:349:LYS:HB3	1.69	0.74
1:G:215:ASN:HB2	6:F:365:SER:HB2	1.66	0.74
1:O:264:SER:HB3	1:O:349:LYS:HB3	1.67	0.74
1:J:250:ARG:HB2	1:J:363:HIS:HB3	1.68	0.74
1:V:264:SER:HB3	1:V:349:LYS:HB3	1.70	0.73
1:L:201:GLU:HB2	1:K:394:ASN:HB2	1.69	0.73
1:M:264:SER:HB3	1:M:349:LYS:HB3	1.70	0.73
1:L:40:MET:HB3	1:L:65:ARG:HB3	1.70	0.73
1:R:208:GLN:HB2	1:R:259:TYR:HB2	1.71	0.73
1:L:264:SER:HB3	1:L:349:LYS:HB3	1.70	0.73
1:U:264:SER:HB3	1:U:349:LYS:HB3	1.70	0.72
1:G:208:GLN:HB2	1:G:259:TYR:HB2	1.71	0.72
1:G:264:SER:HB3	1:G:349:LYS:HB3	1.70	0.72
1:M:212:SER:HB3	1:M:255:LYS:HB3	1.71	0.72
2:A:283:MET:HA	2:A:284:GLN:HB3	1.69	0.72
1:W:264:SER:HB3	1:W:349:LYS:HB3	1.71	0.72
1:N:394:ASN:HB2	1:O:201:GLU:HB2	1.72	0.72
1:X:258:THR:HB	9:X:603:NAG:H82	1.70	0.72
1:S:370:PHE:HB2	1:S:373:ILE:HB	1.71	0.72
1:H:264:SER:HB3	1:H:349:LYS:HB3	1.71	0.72
1:L:354:LYS:HB3	1:L:389:GLU:HB3	1.72	0.71
1:K:264:SER:HB3	1:K:349:LYS:HB3	1.71	0.71
1:Q:354:LYS:HB3	1:Q:389:GLU:HB3	1.72	0.71
1:G:203:PHE:HB2	6:F:377:THR:HB	1.72	0.71
1:U:370:PHE:HB2	1:U:373:ILE:HB	1.73	0.71
1:S:250:ARG:HB2	1:S:363:HIS:HB3	1.73	0.71
1:L:394:ASN:HB2	1:M:201:GLU:HB2	1.72	0.71
1:O:212:SER:HB3	1:O:255:LYS:HB3	1.72	0.71
1:R:370:PHE:HB2	1:R:373:ILE:HB	1.71	0.71
1:J:208:GLN:HB2	1:J:259:TYR:HB2	1.70	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:370:PHE:HB2	1:T:373:ILE:HB	1.72	0.71
1:U:354:LYS:HB3	1:U:389:GLU:HB3	1.72	0.71
1:K:40:MET:HB3	1:K:65:ARG:HB3	1.70	0.71
1:P:208:GLN:HB2	1:P:259:TYR:HB2	1.71	0.70
1:O:394:ASN:HB2	1:Q:201:GLU:HB2	1.73	0.70
1:O:363:HIS:ND1	1:O:380:ASN:OD1	2.24	0.70
1:I:264:SER:HB3	1:I:349:LYS:HB3	1.71	0.70
1:Q:370:PHE:HB2	1:Q:373:ILE:HB	1.72	0.70
1:J:264:SER:HB3	1:J:349:LYS:HB3	1.71	0.70
1:J:354:LYS:HB3	1:J:389:GLU:HB3	1.73	0.70
1:M:380:ASN:HD22	1:N:215:ASN:HD22	1.37	0.70
1:M:394:ASN:HB2	1:N:201:GLU:HB2	1.73	0.70
1:M:354:LYS:HB3	1:M:389:GLU:HB3	1.74	0.70
1:S:262:PHE:HB3	1:S:351:VAL:HB	1.74	0.70
1:S:354:LYS:HB3	1:S:389:GLU:HB3	1.72	0.69
1:K:354:LYS:HB3	1:K:389:GLU:HB3	1.74	0.69
7:B:754:PRO:HB2	7:B:758:SER:HA	1.74	0.69
1:N:354:LYS:HB3	1:N:389:GLU:HB3	1.73	0.69
1:R:262:PHE:HB3	1:R:351:VAL:HB	1.74	0.69
1:V:250:ARG:HB2	1:V:363:HIS:HB3	1.72	0.69
1:X:354:LYS:HB3	1:X:389:GLU:HB3	1.74	0.69
1:M:216:ALA:HB3	1:M:251:PHE:HB3	1.73	0.69
1:O:204:LYS:HB2	1:O:263:LEU:HB3	1.74	0.69
1:O:370:PHE:HB2	1:O:373:ILE:HB	1.74	0.69
1:O:216:ALA:HB3	1:O:251:PHE:HB3	1.74	0.69
1:O:354:LYS:HB3	1:O:389:GLU:HB3	1.74	0.69
1:Q:262:PHE:HB3	1:Q:351:VAL:HB	1.75	0.69
1:R:216:ALA:HB3	1:R:251:PHE:HB3	1.75	0.69
1:P:206:ILE:HB	1:P:261:LEU:HB2	1.72	0.69
1:X:264:SER:HB3	1:X:349:LYS:HB3	1.74	0.69
1:G:102:ASN:ND2	1:G:105:GLY:O	2.26	0.69
1:R:354:LYS:HB3	1:R:389:GLU:HB3	1.73	0.69
7:B:263:HIS:HB3	7:B:307:HIS:HB2	1.74	0.69
1:N:102:ASN:ND2	1:N:105:GLY:O	2.23	0.69
1:T:354:LYS:HB3	1:T:389:GLU:HB3	1.73	0.69
1:R:368:LEU:HB2	1:R:375:VAL:HB	1.75	0.69
1:V:354:LYS:HB3	1:V:389:GLU:HB3	1.75	0.69
1:P:102:ASN:ND2	1:P:105:GLY:O	2.25	0.68
1:P:250:ARG:HB2	1:P:363:HIS:HB3	1.74	0.68
1:V:145:ASP:OD2	1:W:284:ARG:NH1	2.27	0.68
1:W:354:LYS:HB3	1:W:389:GLU:HB3	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:354:LYS:HB3	1:H:389:GLU:HB3	1.75	0.68
1:T:250:ARG:HB2	1:T:363:HIS:HB3	1.75	0.68
1:G:209:GLU:HB2	6:F:371:LYS:HB3	1.76	0.68
1:Q:394:ASN:HB2	1:R:201:GLU:HB2	1.75	0.68
1:P:354:LYS:HB3	1:P:389:GLU:HB3	1.74	0.68
1:I:354:LYS:HB3	1:I:389:GLU:HB3	1.75	0.68
1:O:204:LYS:HD2	1:O:263:LEU:HD23	1.76	0.68
1:Q:216:ALA:HB3	1:Q:251:PHE:HB3	1.75	0.68
1:T:368:LEU:HB2	1:T:375:VAL:HB	1.74	0.68
5:E:94:LEU:HB3	5:E:103:VAL:HB	1.76	0.68
1:V:208:GLN:HB2	1:V:259:TYR:HB2	1.76	0.68
1:H:102:ASN:ND2	1:H:105:GLY:O	2.25	0.68
1:S:368:LEU:HB2	1:S:375:VAL:HB	1.75	0.67
2:A:860:SER:HB3	2:A:911:ASN:HB2	1.76	0.67
1:J:394:ASN:HB2	1:K:201:GLU:HB2	1.74	0.67
1:N:216:ALA:HB3	1:N:251:PHE:HB3	1.77	0.67
1:R:102:ASN:ND2	1:R:105:GLY:O	2.27	0.67
1:L:363:HIS:ND1	1:L:380:ASN:OD1	2.27	0.67
1:P:196:TYR:HB2	1:P:271:LYS:HB3	1.77	0.67
1:P:370:PHE:HB2	1:P:373:ILE:HB	1.76	0.67
1:R:145:ASP:OD2	1:S:284:ARG:NH1	2.28	0.67
1:S:204:LYS:HD2	1:S:263:LEU:HD23	1.77	0.67
1:V:370:PHE:HB2	1:V:373:ILE:HB	1.75	0.67
1:M:370:PHE:HB2	1:M:373:ILE:HB	1.75	0.67
1:S:216:ALA:HB3	1:S:251:PHE:HB3	1.75	0.67
1:P:284:ARG:NH1	1:G:145:ASP:OD2	2.27	0.67
1:G:368:LEU:HB2	1:G:375:VAL:HB	1.76	0.67
1:N:162:ARG:HD3	1:N:164:ARG:HD2	1.77	0.67
1:G:218:ILE:HG23	1:G:249:PHE:HB2	1.76	0.67
1:M:204:LYS:HD2	1:M:263:LEU:HD23	1.78	0.66
1:Q:204:LYS:HB2	1:Q:263:LEU:HB3	1.76	0.66
1:G:360:LEU:HB3	1:G:383:ASP:HB3	1.75	0.66
6:F:530:ARG:HD3	6:F:548:LYS:HA	1.76	0.66
1:X:208:GLN:HB2	1:X:259:TYR:HB2	1.76	0.66
1:K:204:LYS:HD2	1:K:263:LEU:HD23	1.77	0.66
1:O:102:ASN:ND2	1:O:105:GLY:O	2.23	0.66
1:Q:102:ASN:ND2	1:Q:105:GLY:O	2.24	0.66
1:O:262:PHE:HB3	1:O:351:VAL:HB	1.77	0.66
1:U:368:LEU:HB2	1:U:375:VAL:HB	1.77	0.66
1:P:198:GLU:HB3	1:P:269:LYS:HB2	1.76	0.66
1:P:204:LYS:HD2	1:P:263:LEU:HD23	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:204:LYS:HD2	1:U:263:LEU:HD23	1.77	0.66
6:F:27:LYS:HB2	6:F:52:ALA:HB3	1.77	0.66
1:T:105:GLY:HA2	1:U:159:LEU:HD22	1.77	0.66
1:T:262:PHE:HB3	1:T:351:VAL:HB	1.75	0.66
1:W:208:GLN:HB2	1:W:259:TYR:HB2	1.77	0.66
6:F:226:PRO:HD2	6:F:231:LEU:HB3	1.78	0.66
1:S:105:GLY:HA2	1:T:159:LEU:HD22	1.77	0.66
1:P:262:PHE:HB3	1:P:351:VAL:HB	1.75	0.66
1:G:206:ILE:HB	1:G:261:LEU:HB2	1.75	0.66
1:M:204:LYS:HB2	1:M:263:LEU:HB3	1.78	0.66
1:V:262:PHE:HB3	1:V:351:VAL:HB	1.78	0.66
1:N:204:LYS:HB2	1:N:263:LEU:HB3	1.78	0.66
1:Q:204:LYS:HD2	1:Q:263:LEU:HD23	1.77	0.66
1:T:206:ILE:HB	1:T:261:LEU:HB2	1.78	0.66
1:I:394:ASN:HB2	1:J:201:GLU:HB2	1.78	0.66
1:G:342:ASP:HB3	1:G:401:ILE:HB	1.78	0.66
1:L:102:ASN:ND2	1:L:105:GLY:O	2.24	0.66
1:L:162:ARG:HD3	1:L:164:ARG:HD2	1.78	0.66
1:Q:162:ARG:HD3	1:Q:164:ARG:HD2	1.77	0.66
1:G:262:PHE:HB3	1:G:351:VAL:HB	1.75	0.66
1:N:363:HIS:ND1	1:N:380:ASN:OD1	2.26	0.65
1:Q:145:ASP:OD2	1:R:284:ARG:NH1	2.29	0.65
1:R:204:LYS:HD2	1:R:263:LEU:HD23	1.77	0.65
1:L:208:GLN:HB2	1:L:259:TYR:HB2	1.76	0.65
1:J:145:ASP:OD2	1:K:284:ARG:NH1	2.29	0.65
2:A:336:PHE:HE2	2:A:844:THR:HG22	1.60	0.65
1:U:105:GLY:HA2	1:V:159:LEU:HD22	1.79	0.65
1:P:459:VAL:O	1:G:64:ARG:NH2	2.30	0.65
1:G:370:PHE:HB2	1:G:373:ILE:HB	1.79	0.65
2:A:1176:LEU:HD22	2:A:1204:GLN:HB3	1.78	0.65
1:M:86:CYS:SG	1:M:87:SER:N	2.70	0.65
1:N:145:ASP:OD2	1:O:284:ARG:NH1	2.30	0.65
4:D:142:ASN:HA	4:D:154:ARG:HA	1.79	0.65
1:L:204:LYS:HD2	1:L:263:LEU:HD23	1.77	0.65
1:M:162:ARG:HD3	1:M:164:ARG:HD2	1.78	0.65
1:R:105:GLY:HA2	1:S:159:LEU:HD22	1.79	0.65
1:S:102:ASN:ND2	1:S:105:GLY:O	2.29	0.65
1:P:145:ASP:OD2	1:H:284:ARG:NH1	2.29	0.65
1:J:102:ASN:ND2	1:J:105:GLY:O	2.24	0.65
1:K:162:ARG:HD3	1:K:164:ARG:HD2	1.78	0.65
1:O:145:ASP:OD2	1:Q:284:ARG:NH1	2.30	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:368:LEU:HB2	1:Q:375:VAL:HB	1.77	0.65
1:J:204:LYS:HD2	1:J:263:LEU:HD23	1.77	0.65
1:N:204:LYS:HD2	1:N:263:LEU:HD23	1.78	0.65
1:I:145:ASP:OD2	1:J:284:ARG:NH1	2.30	0.65
1:N:86:CYS:SG	1:N:87:SER:N	2.70	0.65
1:U:262:PHE:HB3	1:U:351:VAL:HB	1.79	0.65
1:X:357:LYS:HD2	9:X:603:NAG:H61	1.78	0.65
6:F:240:SER:HB3	6:F:345:CYS:HB3	1.78	0.65
1:L:86:CYS:SG	1:L:87:SER:N	2.70	0.65
1:Q:86:CYS:SG	1:Q:87:SER:N	2.70	0.65
1:R:204:LYS:HB2	1:R:263:LEU:HB3	1.76	0.65
1:S:204:LYS:HB2	1:S:263:LEU:HB3	1.78	0.65
1:V:204:LYS:HD2	1:V:263:LEU:HD23	1.78	0.65
1:P:362:TYR:HB3	1:P:381:LYS:HB3	1.79	0.65
1:J:162:ARG:HD3	1:J:164:ARG:HD2	1.77	0.65
1:J:218:ILE:HG23	1:J:249:PHE:HB2	1.79	0.65
1:G:333:GLY:H	1:G:448:ILE:HD11	1.61	0.65
1:M:342:ASP:HB3	1:M:401:ILE:HB	1.79	0.64
1:N:370:PHE:HB2	1:N:373:ILE:HB	1.78	0.64
1:U:102:ASN:ND2	1:U:105:GLY:O	2.29	0.64
3:C:319:ASN:HB3	3:C:354:ASN:HB3	1.79	0.64
6:F:9:CYS:N	6:F:42:THR:O	2.30	0.64
6:F:71:GLN:HE21	6:F:76:GLY:HA2	1.62	0.64
1:O:368:LEU:HB2	1:O:375:VAL:HB	1.78	0.64
1:W:145:ASP:OD2	1:X:284:ARG:NH1	2.30	0.64
1:G:39:GLN:NE2	1:G:310:GLU:OE2	2.31	0.64
3:C:183:TYR:HB2	4:D:365:GLY:H	1.60	0.64
1:L:204:LYS:HB2	1:L:263:LEU:HB3	1.79	0.64
1:L:216:ALA:HB3	1:L:251:PHE:HB3	1.79	0.64
1:L:342:ASP:HB3	1:L:401:ILE:HB	1.79	0.64
1:W:64:ARG:NH2	1:X:459:VAL:O	2.31	0.64
1:W:99:ASN:ND2	1:W:118:ARG:O	2.31	0.64
1:W:102:ASN:ND2	1:W:105:GLY:O	2.31	0.64
1:H:204:LYS:HD2	1:H:263:LEU:HD23	1.79	0.64
2:A:1087:GLY:HA2	2:A:1090:ASN:HD22	1.62	0.64
1:L:370:PHE:HB2	1:L:373:ILE:HB	1.78	0.64
1:P:218:ILE:HG23	1:P:249:PHE:HB2	1.79	0.64
1:G:86:CYS:SG	1:G:87:SER:N	2.70	0.64
1:G:213:ASN:HB2	6:F:367:ASP:HB3	1.77	0.64
1:N:262:PHE:HB3	1:N:351:VAL:HB	1.80	0.64
1:O:162:ARG:HD3	1:O:164:ARG:HD2	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:105:GLY:HA2	1:R:159:LEU:HD22	1.79	0.64
1:U:145:ASP:OD2	1:V:284:ARG:NH1	2.31	0.64
1:W:301:ASP:OD1	1:X:288:ARG:NH2	2.31	0.64
1:H:145:ASP:OD2	1:I:284:ARG:NH1	2.30	0.64
1:L:145:ASP:OD2	1:M:284:ARG:NH1	2.30	0.64
1:U:64:ARG:NH2	1:V:459:VAL:O	2.30	0.64
1:X:204:LYS:HD2	1:X:263:LEU:HD23	1.79	0.64
1:H:99:ASN:ND2	1:H:118:ARG:O	2.31	0.64
1:K:216:ALA:HB3	1:K:251:PHE:HB3	1.80	0.64
1:G:99:ASN:ND2	1:G:118:ARG:O	2.31	0.64
1:L:459:VAL:O	1:K:64:ARG:NH2	2.31	0.64
1:M:280:ILE:HG21	1:M:437:TRP:HE1	1.63	0.64
1:S:86:CYS:SG	1:S:87:SER:N	2.71	0.64
1:S:342:ASP:HB3	1:S:401:ILE:HB	1.80	0.64
1:P:99:ASN:ND2	1:P:118:ARG:O	2.31	0.64
1:I:250:ARG:HB2	1:I:363:HIS:HB3	1.79	0.64
1:G:174:ARG:NH2	1:G:179:ALA:O	2.31	0.64
1:S:99:ASN:ND2	1:S:118:ARG:O	2.31	0.64
1:V:64:ARG:NH2	1:W:459:VAL:O	2.31	0.64
1:K:208:GLN:HB2	1:K:259:TYR:HB2	1.79	0.64
1:G:309:TYR:H	1:G:472:ASN:HD21	1.45	0.64
5:E:72:LEU:HG	6:F:167:LEU:HD23	1.78	0.64
6:F:244:SER:HB3	6:F:341:ASP:HB2	1.79	0.64
1:M:262:PHE:HB3	1:M:351:VAL:HB	1.80	0.64
1:T:102:ASN:ND2	1:T:105:GLY:O	2.31	0.64
1:W:174:ARG:NH2	1:W:179:ALA:O	2.31	0.64
1:H:86:CYS:SG	1:H:87:SER:N	2.71	0.64
1:I:204:LYS:HD2	1:I:263:LEU:HD23	1.78	0.64
3:C:123:SER:HA	3:C:135:PRO:HA	1.78	0.64
1:L:413:ARG:HG2	1:M:438:ALA:HB1	1.80	0.64
1:U:250:ARG:HB2	1:U:363:HIS:HB3	1.79	0.64
1:X:174:ARG:NH2	1:X:179:ALA:O	2.31	0.64
1:I:86:CYS:SG	1:I:87:SER:N	2.71	0.64
1:I:162:ARG:HD3	1:I:164:ARG:HD2	1.80	0.64
1:K:342:ASP:HB3	1:K:401:ILE:HB	1.80	0.64
1:U:86:CYS:SG	1:U:87:SER:N	2.71	0.63
1:X:102:ASN:ND2	1:X:105:GLY:O	2.30	0.63
1:H:364:LEU:HB3	1:H:379:PHE:HB2	1.80	0.63
1:G:266:SER:HB3	1:G:347:LYS:HB2	1.81	0.63
1:M:413:ARG:HG2	1:N:438:ALA:HB1	1.79	0.63
1:Q:342:ASP:HB3	1:Q:401:ILE:HB	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:394:ASN:HB2	1:S:201:GLU:HB2	1.78	0.63
1:S:218:ILE:HG23	1:S:249:PHE:HB2	1.80	0.63
1:U:206:ILE:HB	1:U:261:LEU:HB2	1.81	0.63
1:I:64:ARG:NH2	1:J:459:VAL:O	2.31	0.63
1:J:86:CYS:SG	1:J:87:SER:N	2.70	0.63
1:K:86:CYS:SG	1:K:87:SER:N	2.70	0.63
1:M:386:LYS:HB3	1:N:209:GLU:HB3	1.80	0.63
1:O:86:CYS:SG	1:O:87:SER:N	2.70	0.63
1:T:99:ASN:ND2	1:T:118:ARG:O	2.32	0.63
1:U:208:GLN:HB2	1:U:259:TYR:HB2	1.79	0.63
1:V:206:ILE:HB	1:V:261:LEU:HB2	1.81	0.63
1:K:364:LEU:HB3	1:K:379:PHE:HB2	1.81	0.63
1:L:262:PHE:HB3	1:L:351:VAL:HB	1.80	0.63
1:M:145:ASP:OD2	1:N:284:ARG:NH1	2.31	0.63
1:T:362:TYR:HB3	1:T:381:LYS:HB3	1.81	0.63
1:P:86:CYS:SG	1:P:87:SER:N	2.70	0.63
1:L:284:ARG:NH1	1:K:145:ASP:OD2	2.31	0.63
1:R:342:ASP:HB3	1:R:401:ILE:HB	1.79	0.63
1:W:262:PHE:HB3	1:W:351:VAL:HB	1.79	0.63
1:H:64:ARG:NH2	1:I:459:VAL:O	2.31	0.63
1:O:342:ASP:HB3	1:O:401:ILE:HB	1.79	0.63
1:R:86:CYS:SG	1:R:87:SER:N	2.71	0.63
1:U:333:GLY:H	1:U:448:ILE:HD11	1.64	0.63
1:N:99:ASN:ND2	1:N:118:ARG:O	2.32	0.63
1:R:333:GLY:H	1:R:448:ILE:HD11	1.63	0.63
1:T:145:ASP:OD2	1:U:284:ARG:NH1	2.32	0.63
1:V:99:ASN:ND2	1:V:118:ARG:O	2.31	0.63
6:F:214:LYS:HB3	6:F:243:THR:HB	1.80	0.63
1:L:212:SER:HB3	1:L:255:LYS:HB3	1.81	0.63
1:V:86:CYS:SG	1:V:87:SER:N	2.72	0.63
1:W:333:GLY:H	1:W:448:ILE:HD11	1.62	0.63
1:I:99:ASN:ND2	1:I:118:ARG:O	2.32	0.63
2:A:1153:ARG:HG2	2:A:1197:LEU:HB3	1.81	0.63
1:T:333:GLY:H	1:T:448:ILE:HD11	1.64	0.63
1:X:333:GLY:H	1:X:448:ILE:HD11	1.63	0.63
1:H:262:PHE:HB3	1:H:351:VAL:HB	1.81	0.63
1:K:370:PHE:HB2	1:K:373:ILE:HB	1.80	0.63
1:G:330:SER:HB2	1:G:449:SER:H	1.64	0.63
1:R:99:ASN:ND2	1:R:118:ARG:O	2.32	0.62
1:V:102:ASN:ND2	1:V:105:GLY:O	2.31	0.62
1:V:174:ARG:NH2	1:V:179:ALA:O	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:B:328:LYS:NZ	7:B:330:LYS:O	2.32	0.62
1:O:99:ASN:ND2	1:O:118:ARG:O	2.32	0.62
1:T:86:CYS:SG	1:T:87:SER:N	2.72	0.62
6:F:212:LYS:HB3	6:F:245:PHE:HB3	1.81	0.62
1:Q:280:ILE:HG21	1:Q:437:TRP:HE1	1.64	0.62
1:S:333:GLY:H	1:S:448:ILE:HD11	1.64	0.62
1:U:99:ASN:ND2	1:U:118:ARG:O	2.32	0.62
1:V:333:GLY:H	1:V:448:ILE:HD11	1.64	0.62
1:W:204:LYS:HD2	1:W:263:LEU:HD23	1.79	0.62
1:N:342:ASP:HB3	1:N:401:ILE:HB	1.79	0.62
1:S:174:ARG:NH2	1:S:179:ALA:O	2.32	0.62
1:J:99:ASN:ND2	1:J:118:ARG:O	2.32	0.62
1:J:262:PHE:HB3	1:J:351:VAL:HB	1.82	0.62
1:L:64:ARG:NH2	1:M:459:VAL:O	2.31	0.62
1:L:280:ILE:HG21	1:L:437:TRP:HE1	1.64	0.62
1:R:218:ILE:HG23	1:R:249:PHE:HB2	1.80	0.62
1:T:64:ARG:NH2	1:U:459:VAL:O	2.33	0.62
1:T:342:ASP:HB3	1:T:401:ILE:HB	1.80	0.62
1:U:174:ARG:NH2	1:U:179:ALA:O	2.32	0.62
1:W:342:ASP:HB3	1:W:401:ILE:HB	1.81	0.62
1:I:102:ASN:ND2	1:I:105:GLY:O	2.21	0.62
1:Q:99:ASN:ND2	1:Q:118:ARG:O	2.32	0.62
1:R:359:CYS:HA	1:R:384:CYS:HA	1.81	0.62
1:T:174:ARG:NH2	1:T:179:ALA:O	2.32	0.62
1:X:262:PHE:HB3	1:X:351:VAL:HB	1.82	0.62
1:P:64:ARG:NH2	1:H:459:VAL:O	2.31	0.62
1:I:280:ILE:HG21	1:I:437:TRP:HE1	1.63	0.62
1:J:280:ILE:HG21	1:J:437:TRP:HE1	1.63	0.62
4:D:166:ARG:NH2	7:B:207:GLU:OE1	2.32	0.62
6:F:206:LEU:HB3	6:F:251:LYS:HB2	1.82	0.62
1:M:99:ASN:ND2	1:M:118:ARG:O	2.32	0.62
1:M:102:ASN:ND2	1:M:105:GLY:O	2.21	0.62
1:O:256:ASN:OD1	1:O:256:ASN:N	2.33	0.62
1:P:174:ARG:NH2	1:P:179:ALA:O	2.32	0.62
1:R:174:ARG:NH2	1:R:179:ALA:O	2.33	0.62
1:R:400:LEU:HB2	1:S:195:HIS:HB2	1.82	0.62
1:T:204:LYS:HD2	1:T:263:LEU:HD23	1.80	0.62
1:V:105:GLY:HA2	1:W:159:LEU:HD22	1.81	0.62
1:W:86:CYS:SG	1:W:87:SER:N	2.73	0.62
1:K:204:LYS:HB2	1:K:263:LEU:HB3	1.81	0.62
1:L:99:ASN:ND2	1:L:118:ARG:O	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:368:LEU:HB2	1:M:375:VAL:HB	1.82	0.62
1:S:145:ASP:OD2	1:T:284:ARG:NH1	2.32	0.62
1:J:64:ARG:NH2	1:K:459:VAL:O	2.32	0.62
1:N:174:ARG:NH2	1:N:179:ALA:O	2.33	0.61
1:N:333:GLY:H	1:N:448:ILE:HD11	1.65	0.61
1:Q:333:GLY:H	1:Q:448:ILE:HD11	1.64	0.61
1:U:342:ASP:HB3	1:U:401:ILE:HB	1.80	0.61
1:V:368:LEU:HB2	1:V:375:VAL:HB	1.81	0.61
1:I:342:ASP:HB3	1:I:401:ILE:HB	1.80	0.61
2:A:53:THR:HB	2:A:107:VAL:HB	1.82	0.61
1:L:174:ARG:NH2	1:L:179:ALA:O	2.33	0.61
1:Q:359:CYS:HA	1:Q:384:CYS:HA	1.82	0.61
1:I:208:GLN:HB2	1:I:259:TYR:HB2	1.80	0.61
1:M:64:ARG:NH2	1:N:459:VAL:O	2.33	0.61
1:N:280:ILE:HG21	1:N:437:TRP:HE1	1.64	0.61
1:O:174:ARG:NH2	1:O:179:ALA:O	2.33	0.61
1:T:280:ILE:HG21	1:T:437:TRP:HE1	1.66	0.61
1:J:342:ASP:HB3	1:J:401:ILE:HB	1.82	0.61
1:G:354:LYS:HB3	1:G:389:GLU:HB3	1.81	0.61
6:F:337:ILE:HG12	6:F:377:THR:HG23	1.80	0.61
1:S:206:ILE:HB	1:S:261:LEU:HB2	1.82	0.61
1:U:280:ILE:HG21	1:U:437:TRP:HE1	1.65	0.61
1:V:256:ASN:N	1:V:256:ASN:OD1	2.33	0.61
1:X:324:HIS:HA	1:X:455:ILE:HG13	1.81	0.61
1:P:333:GLY:H	1:P:448:ILE:HD11	1.64	0.61
1:H:370:PHE:HB2	1:H:373:ILE:HB	1.82	0.61
7:B:703:GLU:HG2	7:B:721:LEU:HD13	1.80	0.61
9:N:604:NAG:H3	9:N:604:NAG:H83	1.83	0.61
1:O:333:GLY:H	1:O:448:ILE:HD11	1.65	0.61
1:V:280:ILE:HG21	1:V:437:TRP:HE1	1.64	0.61
1:V:342:ASP:HB3	1:V:401:ILE:HB	1.82	0.61
1:V:362:TYR:HB3	1:V:381:LYS:HB3	1.82	0.61
4:D:185:SER:HB2	7:B:207:GLU:H	1.64	0.61
1:P:368:LEU:HB2	1:P:375:VAL:HB	1.82	0.61
1:K:99:ASN:ND2	1:K:118:ARG:O	2.32	0.61
1:K:262:PHE:HB3	1:K:351:VAL:HB	1.81	0.61
1:Q:174:ARG:NH2	1:Q:179:ALA:O	2.34	0.61
1:S:362:TYR:HB3	1:S:381:LYS:HB3	1.81	0.61
1:X:99:ASN:ND2	1:X:118:ARG:O	2.34	0.61
1:H:174:ARG:NH2	1:H:179:ALA:O	2.33	0.61
1:I:262:PHE:HB3	1:I:351:VAL:HB	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:174:ARG:NH2	1:J:179:ALA:O	2.34	0.61
1:K:256:ASN:N	1:K:256:ASN:OD1	2.33	0.61
1:M:174:ARG:NH2	1:M:179:ALA:O	2.33	0.61
1:O:280:ILE:HG21	1:O:437:TRP:HE1	1.66	0.61
1:W:370:PHE:HB2	1:W:373:ILE:HB	1.82	0.61
1:H:280:ILE:HG21	1:H:437:TRP:HE1	1.66	0.61
1:I:256:ASN:N	1:I:256:ASN:OD1	2.34	0.61
2:A:152:LEU:HB3	2:A:808:GLY:HA2	1.82	0.61
2:A:320:ASN:HD21	2:A:348:VAL:HG22	1.64	0.61
2:A:854:GLN:HB3	2:A:885:ARG:HB3	1.83	0.61
2:A:1288:GLN:O	2:A:1292:ASN:ND2	2.34	0.61
1:L:333:GLY:H	1:L:448:ILE:HD11	1.66	0.61
1:L:438:ALA:HB1	1:K:413:ARG:HG2	1.82	0.61
1:W:256:ASN:OD1	1:W:256:ASN:N	2.33	0.61
1:K:102:ASN:ND2	1:K:105:GLY:O	2.20	0.61
2:A:286:ALA:HB1	2:A:288:GLN:HG3	1.82	0.61
1:L:368:LEU:HB2	1:L:375:VAL:HB	1.82	0.61
1:M:333:GLY:H	1:M:448:ILE:HD11	1.65	0.61
1:N:368:LEU:HB2	1:N:375:VAL:HB	1.81	0.61
1:R:280:ILE:HG21	1:R:437:TRP:HE1	1.65	0.61
1:X:280:ILE:HG21	1:X:437:TRP:HE1	1.65	0.61
1:X:305:LEU:HD23	1:X:469:LYS:HD3	1.83	0.61
1:H:208:GLN:HB2	1:H:259:TYR:HB2	1.82	0.61
1:I:174:ARG:NH2	1:I:179:ALA:O	2.34	0.61
1:K:174:ARG:NH2	1:K:179:ALA:O	2.34	0.61
1:M:256:ASN:OD1	1:M:256:ASN:N	2.34	0.60
1:O:413:ARG:HG2	1:Q:438:ALA:HB1	1.83	0.60
1:X:364:LEU:HB3	1:X:379:PHE:HB2	1.83	0.60
1:I:386:LYS:HB3	1:J:209:GLU:HB3	1.83	0.60
1:L:105:GLY:HA2	1:M:159:LEU:HD22	1.83	0.60
1:N:105:GLY:HA2	1:O:159:LEU:HD22	1.82	0.60
1:T:364:LEU:HB3	1:T:379:PHE:HB2	1.83	0.60
1:P:189:LYS:HA	1:P:278:GLY:HA2	1.83	0.60
1:P:105:GLY:HA2	1:H:159:LEU:HD22	1.83	0.60
1:P:330:SER:HB2	1:P:449:SER:H	1.65	0.60
1:J:204:LYS:HB2	1:J:263:LEU:HB3	1.82	0.60
1:G:254:SER:HB3	1:G:359:CYS:HB3	1.82	0.60
2:A:364:LYS:NZ	2:A:557:ASP:OD2	2.35	0.60
1:K:362:TYR:HB3	1:K:381:LYS:HB3	1.83	0.60
1:G:324:HIS:HA	1:G:455:ILE:HG13	1.84	0.60
2:A:253:ARG:HH22	2:A:257:ASN:HD22	1.49	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:260:GLN:HB3	1:R:353:LEU:HB3	1.83	0.60
1:W:280:ILE:HG21	1:W:437:TRP:HE1	1.67	0.60
1:I:333:GLY:H	1:I:448:ILE:HD11	1.66	0.60
5:E:69:PHE:HB3	5:E:168:CYS:HB2	1.84	0.60
7:B:306:SER:HB3	7:B:387:LYS:HD2	1.82	0.60
1:S:400:LEU:HB2	1:T:195:HIS:HB2	1.83	0.60
1:P:288:ARG:NH2	1:G:301:ASP:OD1	2.35	0.60
1:K:330:SER:HB2	1:K:449:SER:H	1.67	0.60
1:K:368:LEU:HB2	1:K:375:VAL:HB	1.84	0.60
2:A:40:VAL:HG11	2:A:502:LEU:HD21	1.82	0.60
1:N:64:ARG:NH2	1:O:459:VAL:O	2.35	0.60
1:N:413:ARG:HG2	1:O:438:ALA:HB1	1.84	0.60
1:W:206:ILE:HB	1:W:261:LEU:HB2	1.84	0.60
1:I:204:LYS:HB2	1:I:263:LEU:HB3	1.83	0.60
1:J:330:SER:HB2	1:J:449:SER:H	1.67	0.60
3:C:78:ARG:NH1	3:C:142:TYR:OH	2.34	0.60
1:L:256:ASN:N	1:L:256:ASN:OD1	2.34	0.60
9:M:604:NAG:H83	9:M:604:NAG:H3	1.84	0.60
1:Q:64:ARG:NH2	1:R:459:VAL:O	2.35	0.60
1:Q:218:ILE:HG23	1:Q:249:PHE:HB2	1.83	0.60
1:V:330:SER:HB2	1:V:449:SER:H	1.67	0.60
1:W:364:LEU:HB3	1:W:379:PHE:HB2	1.84	0.60
1:P:280:ILE:HG21	1:P:437:TRP:HE1	1.65	0.60
1:H:256:ASN:OD1	1:H:256:ASN:N	2.33	0.60
6:F:246:LEU:HB3	6:F:339:SER:HB3	1.84	0.60
1:M:206:ILE:HB	1:M:261:LEU:HB2	1.82	0.60
1:S:359:CYS:HA	1:S:384:CYS:HA	1.83	0.60
1:K:333:GLY:H	1:K:448:ILE:HD11	1.66	0.60
1:O:64:ARG:NH2	1:Q:459:VAL:O	2.33	0.60
1:P:364:LEU:HB3	1:P:379:PHE:HB2	1.84	0.60
1:H:305:LEU:HD23	1:H:469:LYS:HD3	1.84	0.60
1:J:333:GLY:H	1:J:448:ILE:HD11	1.66	0.60
1:G:260:GLN:HB3	1:G:353:LEU:HB3	1.83	0.60
2:A:1228:TRP:H	2:A:1251:THR:HG22	1.67	0.60
7:B:501:VAL:HB	7:B:624:ILE:HG21	1.84	0.60
1:R:64:ARG:NH2	1:S:459:VAL:O	2.35	0.59
1:X:206:ILE:HB	1:X:261:LEU:HB2	1.83	0.59
1:I:364:LEU:HB3	1:I:379:PHE:HB2	1.83	0.59
1:K:206:ILE:HB	1:K:261:LEU:HB2	1.84	0.59
2:A:539:ARG:NH2	2:A:635:GLY:O	2.34	0.59
7:B:87:PHE:HB3	7:B:102:LYS:HE2	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:330:SER:HB2	1:S:449:SER:H	1.67	0.59
1:U:258:THR:HB	9:U:603:NAG:H82	1.83	0.59
1:P:204:LYS:HB2	1:P:263:LEU:HB3	1.84	0.59
1:P:465:ASN:HD21	1:P:468:LEU:HD23	1.68	0.59
1:H:206:ILE:HB	1:H:261:LEU:HB2	1.83	0.59
1:G:164:ARG:HD2	6:F:115:PRO:HD2	1.84	0.59
1:L:206:ILE:HB	1:L:261:LEU:HB2	1.84	0.59
1:S:64:ARG:NH2	1:T:459:VAL:O	2.35	0.59
1:P:305:LEU:HD23	1:P:469:LYS:HD3	1.84	0.59
1:P:342:ASP:HB3	1:P:401:ILE:HB	1.83	0.59
1:H:204:LYS:HB2	1:H:263:LEU:HB3	1.84	0.59
1:H:330:SER:HB2	1:H:449:SER:H	1.66	0.59
9:K:604:NAG:H83	9:K:604:NAG:H3	1.85	0.59
2:A:1313:ILE:HB	2:A:1326:TYR:HB2	1.83	0.59
3:C:350:ARG:HG3	6:F:214:LYS:HE3	1.85	0.59
1:M:218:ILE:HG23	1:M:249:PHE:HB2	1.83	0.59
1:H:342:ASP:HB3	1:H:401:ILE:HB	1.84	0.59
1:K:280:ILE:HG21	1:K:437:TRP:HE1	1.64	0.59
1:G:362:TYR:HB3	1:G:381:LYS:HB3	1.85	0.59
1:G:412:THR:N	1:G:440:SER:OG	2.34	0.59
6:F:452:ASN:OD1	6:F:455:ARG:NH2	2.36	0.59
1:N:359:CYS:HA	1:N:384:CYS:HA	1.84	0.59
9:R:604:NAG:H3	9:R:604:NAG:H83	1.84	0.59
1:I:206:ILE:HB	1:I:261:LEU:HB2	1.84	0.59
9:O:604:NAG:H3	9:O:604:NAG:H83	1.84	0.59
1:V:204:LYS:HB2	1:V:263:LEU:HB3	1.85	0.59
1:X:85:GLN:HE21	1:X:89:GLY:HA2	1.66	0.59
1:X:342:ASP:HB3	1:X:401:ILE:HB	1.84	0.59
2:A:315:LEU:HD23	2:A:318:LEU:HG	1.84	0.59
1:M:330:SER:HB2	1:M:449:SER:H	1.68	0.59
1:N:330:SER:HB2	1:N:449:SER:H	1.68	0.59
1:Q:198:GLU:HB3	1:Q:269:LYS:HB2	1.85	0.59
9:S:604:NAG:H83	9:S:604:NAG:H3	1.84	0.59
1:P:190:ASN:N	1:P:277:LYS:O	2.36	0.59
1:I:330:SER:HB2	1:I:449:SER:H	1.66	0.59
1:J:206:ILE:HB	1:J:261:LEU:HB2	1.84	0.59
1:G:354:LYS:O	1:G:389:GLU:N	2.35	0.59
1:S:280:ILE:HG21	1:S:437:TRP:HE1	1.66	0.59
1:U:301:ASP:OD1	1:V:288:ARG:NH2	2.36	0.59
1:W:90:ARG:NH1	1:W:103:ASP:OD1	2.36	0.59
1:H:333:GLY:H	1:H:448:ILE:HD11	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:330:SER:HB2	1:T:449:SER:H	1.68	0.59
1:H:250:ARG:HB2	1:H:363:HIS:HB3	1.84	0.59
3:C:223:HIS:HD2	3:C:318:LEU:HD22	1.67	0.59
9:Q:604:NAG:H3	9:Q:604:NAG:H83	1.84	0.58
1:S:371:SER:HA	1:T:224:PRO:HA	1.85	0.58
1:T:198:GLU:HB3	1:T:269:LYS:HB2	1.84	0.58
1:U:204:LYS:HB2	1:U:263:LEU:HB3	1.83	0.58
1:W:330:SER:HB2	1:W:449:SER:H	1.68	0.58
1:G:350:GLY:O	1:G:393:VAL:N	2.34	0.58
1:O:206:ILE:HB	1:O:261:LEU:HB2	1.84	0.58
1:W:250:ARG:HB2	1:W:363:HIS:HB3	1.84	0.58
1:X:162:ARG:HD3	1:X:164:ARG:HD2	1.85	0.58
1:G:204:LYS:HD2	1:G:263:LEU:HD23	1.85	0.58
3:C:163:GLU:HG3	4:D:275:PRO:HG2	1.85	0.58
8:q:1:NAG:H83	8:q:1:NAG:H3	1.85	0.58
1:M:349:LYS:HB2	8:Z:1:NAG:H83	1.84	0.58
1:Q:364:LEU:HD23	1:Q:379:PHE:HB2	1.85	0.58
1:R:364:LEU:HD23	1:R:379:PHE:HB2	1.85	0.58
2:A:259:VAL:HB	2:A:295:GLY:HA3	1.83	0.58
2:A:1286:SER:HB2	2:A:1287:THR:HA	1.85	0.58
9:L:604:NAG:H3	9:L:604:NAG:H83	1.84	0.58
1:N:380:ASN:HD22	1:O:215:ASN:HD22	1.51	0.58
1:J:368:LEU:HB2	1:J:375:VAL:HB	1.86	0.58
1:Q:380:ASN:HD22	1:R:215:ASN:HD22	1.49	0.58
1:S:198:GLU:HB3	1:S:269:LYS:HB2	1.85	0.58
1:U:364:LEU:HB3	1:U:379:PHE:HB2	1.85	0.58
1:X:330:SER:HB2	1:X:449:SER:H	1.69	0.58
9:G:604:NAG:H3	9:G:604:NAG:H83	1.84	0.58
1:R:198:GLU:HB3	1:R:269:LYS:HB2	1.85	0.58
1:T:400:LEU:HB2	1:U:195:HIS:HB2	1.84	0.58
1:U:330:SER:HB2	1:U:449:SER:H	1.68	0.58
1:V:394:ASN:HB2	1:W:201:GLU:HB2	1.86	0.58
1:R:206:ILE:HB	1:R:261:LEU:HB2	1.84	0.58
1:T:204:LYS:HB2	1:T:263:LEU:HB3	1.86	0.58
1:U:394:ASN:HB2	1:V:201:GLU:HB2	1.86	0.58
1:X:204:LYS:HB2	1:X:263:LEU:HB3	1.86	0.58
1:X:344:ALA:HB3	1:X:399:ASN:HB2	1.86	0.58
3:C:269:ARG:NH1	6:F:277:ASP:OD2	2.36	0.58
1:L:330:SER:HB2	1:L:449:SER:H	1.68	0.58
1:N:206:ILE:HB	1:N:261:LEU:HB2	1.86	0.58
1:V:90:ARG:NH1	1:V:103:ASP:OD1	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:364:LEU:HB3	1:V:379:PHE:HB2	1.85	0.58
1:I:305:LEU:HD23	1:I:469:LYS:HD3	1.84	0.58
1:G:363:HIS:ND1	1:G:380:ASN:OD1	2.24	0.58
4:D:452:PHE:HB2	4:D:468:VAL:HG11	1.86	0.58
1:O:386:LYS:HB3	1:Q:209:GLU:HB3	1.85	0.57
1:Q:371:SER:HA	1:R:224:PRO:HA	1.86	0.57
1:R:386:LYS:HB3	1:S:209:GLU:HB3	1.85	0.57
1:X:324:HIS:CE1	1:X:452:LEU:HD21	2.38	0.57
1:H:105:GLY:HA2	1:I:159:LEU:HD22	1.86	0.57
1:G:140:ASN:HA	1:G:323:THR:HG22	1.86	0.57
1:Q:260:GLN:HB3	1:Q:353:LEU:HB3	1.86	0.57
1:R:330:SER:HB2	1:R:449:SER:H	1.69	0.57
1:S:137:TYR:HB3	1:S:146:PRO:HB3	1.86	0.57
1:T:58:THR:HG21	1:U:452:LEU:HD23	1.86	0.57
1:W:204:LYS:HB2	1:W:263:LEU:HB3	1.86	0.57
1:O:105:GLY:HA2	1:Q:159:LEU:HD22	1.85	0.57
1:O:330:SER:HB2	1:O:449:SER:H	1.68	0.57
1:W:305:LEU:HD23	1:W:469:LYS:HD3	1.87	0.57
1:G:364:LEU:HB3	1:G:379:PHE:HB2	1.86	0.57
2:A:182:ILE:HD13	2:A:601:ALA:HB2	1.86	0.57
1:V:301:ASP:OD1	1:W:288:ARG:NH2	2.37	0.57
1:I:413:ARG:HG2	1:J:438:ALA:HB1	1.85	0.57
1:J:105:GLY:HA2	1:K:159:LEU:HD22	1.84	0.57
2:A:171:VAL:HG21	2:A:199:TRP:HZ3	1.70	0.57
6:F:206:LEU:HD23	6:F:251:LYS:HD2	1.85	0.57
1:N:349:LYS:HB2	8:a:1:NAG:H83	1.86	0.57
1:Q:330:SER:HB2	1:Q:449:SER:H	1.68	0.57
1:I:368:LEU:HB2	1:I:375:VAL:HB	1.86	0.57
2:A:540:LEU:HD23	2:A:561:LEU:HD11	1.85	0.57
2:A:781:PRO:HD2	2:A:784:LYS:HB2	1.87	0.57
1:Q:413:ARG:HG2	1:R:438:ALA:HB1	1.86	0.57
1:P:277:LYS:HA	1:P:336:GLU:HA	1.87	0.57
1:J:370:PHE:HB2	1:J:373:ILE:HB	1.86	0.57
1:G:90:ARG:NH1	1:G:103:ASP:OD1	2.35	0.57
6:F:435:HIS:HB3	6:F:453:LEU:HD22	1.85	0.57
1:O:198:GLU:HB3	1:O:269:LYS:HB2	1.87	0.57
1:Q:206:ILE:HB	1:Q:261:LEU:HB2	1.85	0.57
1:S:90:ARG:NH1	1:S:103:ASP:OD1	2.38	0.57
1:T:349:LYS:HB2	8:f:1:NAG:H83	1.86	0.57
1:P:309:TYR:H	1:P:472:ASN:HD21	1.51	0.57
1:T:394:ASN:HB2	1:U:201:GLU:HB2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:159:LEU:HD22	1:G:105:GLY:HA2	1.87	0.57
1:P:467:HIS:CD2	1:G:65:ARG:HD2	2.40	0.57
1:J:305:LEU:HD23	1:J:469:LYS:HD3	1.86	0.57
2:A:283:MET:HA	2:A:284:GLN:CB	2.35	0.57
1:L:137:TYR:HB3	1:L:146:PRO:HB3	1.87	0.57
1:N:324:HIS:HA	1:N:455:ILE:HG13	1.87	0.57
1:I:370:PHE:HB2	1:I:373:ILE:HB	1.87	0.57
2:A:25:ILE:HB	2:A:654:LEU:HB2	1.86	0.57
5:E:107:VAL:HG22	5:E:118:LEU:HG	1.87	0.57
1:M:137:TYR:HB3	1:M:146:PRO:HB3	1.87	0.56
1:N:362:TYR:HB3	1:N:381:LYS:HB3	1.85	0.56
1:U:324:HIS:CE1	1:U:452:LEU:HD21	2.40	0.56
1:U:362:TYR:HB3	1:U:381:LYS:HB3	1.87	0.56
1:P:256:ASN:OD1	1:P:256:ASN:N	2.36	0.56
1:P:324:HIS:HA	1:P:455:ILE:HG13	1.87	0.56
1:G:211:THR:N	6:F:369:CYS:O	2.36	0.56
7:B:581:TYR:HD1	7:B:610:ASP:HB2	1.70	0.56
1:L:305:LEU:HD23	1:L:469:LYS:HD3	1.87	0.56
1:S:324:HIS:HA	1:S:455:ILE:HG13	1.87	0.56
1:T:90:ARG:NH1	1:T:103:ASP:OD1	2.37	0.56
3:C:337:GLU:HB3	6:F:228:GLY:HA3	1.85	0.56
6:F:248:GLU:HB3	6:F:337:ILE:HB	1.87	0.56
1:L:349:LYS:HB2	8:Y:1:NAG:H83	1.86	0.56
1:M:359:CYS:HA	1:M:384:CYS:HA	1.87	0.56
1:N:90:ARG:NH1	1:N:103:ASP:OD1	2.39	0.56
1:N:198:GLU:HB3	1:N:269:LYS:HB2	1.87	0.56
1:N:324:HIS:CE1	1:N:452:LEU:HD21	2.40	0.56
1:O:137:TYR:HB3	1:O:146:PRO:HB3	1.88	0.56
1:O:362:TYR:HB3	1:O:381:LYS:HB3	1.87	0.56
1:T:324:HIS:HA	1:T:455:ILE:HG13	1.86	0.56
9:T:604:NAG:H3	9:T:604:NAG:H83	1.88	0.56
1:V:324:HIS:CE1	1:V:452:LEU:HD21	2.40	0.56
1:W:324:HIS:CE1	1:W:452:LEU:HD21	2.40	0.56
1:J:413:ARG:HG2	1:K:438:ALA:HB1	1.88	0.56
9:J:604:NAG:H3	9:J:604:NAG:H83	1.88	0.56
1:K:90:ARG:NH1	1:K:103:ASP:OD1	2.39	0.56
1:G:327:SER:HB2	1:G:453:SER:HB2	1.87	0.56
2:A:286:ALA:HA	2:A:287:MET:HB2	1.86	0.56
2:A:1277:GLU:HG3	2:A:1278:GLN:H	1.69	0.56
1:R:324:HIS:HA	1:R:455:ILE:HG13	1.87	0.56
1:U:137:TYR:HB3	1:U:146:PRO:HB3	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:B:94:ASP:N	7:B:95:PRO:HD3	2.20	0.56
7:B:490:ILE:HG13	7:B:493:LEU:HD12	1.88	0.56
1:L:324:HIS:CE1	1:L:452:LEU:HD21	2.40	0.56
1:Q:400:LEU:HB2	1:R:195:HIS:HB2	1.87	0.56
1:S:386:LYS:HB3	1:T:209:GLU:HB3	1.88	0.56
1:T:324:HIS:CE1	1:T:452:LEU:HD21	2.40	0.56
1:U:324:HIS:HA	1:U:455:ILE:HG13	1.86	0.56
9:U:604:NAG:H83	9:U:604:NAG:H3	1.88	0.56
9:V:604:NAG:H83	9:V:604:NAG:H3	1.88	0.56
1:J:137:TYR:HB3	1:J:146:PRO:HB3	1.87	0.56
1:O:90:ARG:NH1	1:O:103:ASP:OD1	2.39	0.56
1:S:350:GLY:O	1:S:393:VAL:N	2.39	0.56
1:P:474:GLU:OE2	1:G:44:ARG:NH2	2.39	0.56
1:H:137:TYR:HB3	1:H:146:PRO:HB3	1.88	0.56
1:T:196:TYR:HB2	1:T:271:LYS:HB3	1.87	0.56
1:I:105:GLY:HA2	1:J:159:LEU:HD22	1.88	0.56
1:T:301:ASP:OD1	1:U:288:ARG:NH2	2.38	0.56
1:P:39:GLN:NE2	1:P:310:GLU:OE2	2.39	0.56
1:P:137:TYR:HB3	1:P:146:PRO:HB3	1.88	0.56
1:P:201:GLU:HB2	1:G:394:ASN:HB2	1.88	0.56
1:P:324:HIS:CE1	1:P:452:LEU:HD21	2.40	0.56
1:H:465:ASN:HD21	1:H:468:LEU:HD23	1.71	0.56
1:K:305:LEU:HD23	1:K:469:LYS:HD3	1.87	0.56
7:B:746:CYS:HB3	7:B:751:TRP:CZ2	2.41	0.56
1:M:90:ARG:NH1	1:M:103:ASP:OD1	2.39	0.56
1:M:105:GLY:HA2	1:N:159:LEU:HD22	1.87	0.56
1:M:324:HIS:HA	1:M:455:ILE:HG13	1.88	0.56
1:T:295:THR:HG23	1:T:298:PHE:H	1.69	0.56
2:A:273:GLU:HA	2:A:321:LYS:HB2	1.88	0.56
1:O:324:HIS:CE1	1:O:452:LEU:HD21	2.41	0.56
1:O:359:CYS:HA	1:O:384:CYS:HA	1.87	0.56
1:R:523:GLN:O	1:R:524:LYS:N	2.38	0.56
1:T:59:ASP:OD1	1:U:456:TYR:OH	2.24	0.56
1:V:523:GLN:O	1:V:524:LYS:N	2.39	0.56
9:X:604:NAG:H83	9:X:604:NAG:H3	1.88	0.56
2:A:268:THR:HB	2:A:326:ALA:HB3	1.88	0.56
3:C:28:LYS:NZ	3:C:55:ASP:OD1	2.39	0.56
1:R:137:TYR:HB3	1:R:146:PRO:HB3	1.88	0.55
1:R:324:HIS:CE1	1:R:452:LEU:HD21	2.41	0.55
1:U:523:GLN:O	1:U:524:LYS:N	2.39	0.55
9:W:604:NAG:H3	9:W:604:NAG:H83	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:604:NAG:H3	9:I:604:NAG:H83	1.88	0.55
2:A:363:LEU:HD13	2:A:431:LEU:HD23	1.88	0.55
1:N:378:GLU:HB3	1:O:217:ALA:HB3	1.88	0.55
1:S:523:GLN:O	1:S:524:LYS:N	2.39	0.55
1:T:523:GLN:O	1:T:524:LYS:N	2.39	0.55
1:W:324:HIS:HA	1:W:455:ILE:HG13	1.88	0.55
1:X:415:TYR:HD2	1:X:440:SER:HB2	1.70	0.55
1:P:195:HIS:HB2	1:G:400:LEU:HB2	1.88	0.55
4:D:221:LYS:HG2	7:B:416:VAL:H	1.71	0.55
1:O:324:HIS:HA	1:O:455:ILE:HG13	1.88	0.55
1:O:380:ASN:HB2	1:Q:215:ASN:HB2	1.87	0.55
1:W:413:ARG:HD3	1:X:280:ILE:HD11	1.89	0.55
9:H:604:NAG:H83	9:H:604:NAG:H3	1.88	0.55
1:Q:324:HIS:CE1	1:Q:452:LEU:HD21	2.41	0.55
1:R:380:ASN:HB2	1:S:215:ASN:HB2	1.87	0.55
1:S:394:ASN:HB2	1:T:201:GLU:HB2	1.87	0.55
1:U:90:ARG:NH1	1:U:103:ASP:OD1	2.37	0.55
1:I:324:HIS:CE1	1:I:452:LEU:HD21	2.42	0.55
1:I:324:HIS:HA	1:I:455:ILE:HG13	1.87	0.55
1:J:523:GLN:O	1:J:524:LYS:N	2.40	0.55
9:B:1001:NAG:H83	9:B:1001:NAG:H3	1.87	0.55
1:Q:137:TYR:HB3	1:Q:146:PRO:HB3	1.88	0.55
1:R:59:ASP:OD1	1:S:456:TYR:OH	2.23	0.55
1:U:400:LEU:HB2	1:V:195:HIS:HB2	1.89	0.55
1:I:465:ASN:HD21	1:I:468:LEU:HD23	1.71	0.55
1:J:465:ASN:HD21	1:J:468:LEU:HD23	1.72	0.55
1:K:324:HIS:CE1	1:K:452:LEU:HD21	2.41	0.55
1:K:523:GLN:O	1:K:524:LYS:N	2.39	0.55
1:G:344:ALA:HB3	1:G:399:ASN:HB2	1.88	0.55
1:Q:324:HIS:HA	1:Q:455:ILE:HG13	1.87	0.55
1:S:295:THR:HG23	1:S:298:PHE:H	1.72	0.55
1:U:295:THR:HG23	1:U:298:PHE:H	1.72	0.55
2:A:394:THR:O	2:A:401:THR:OG1	2.25	0.55
2:A:844:THR:OG1	2:A:893:SER:OG	2.21	0.55
2:A:1279:ARG:HG2	2:A:1281:GLY:HA3	1.86	0.55
1:O:350:GLY:O	1:O:393:VAL:N	2.39	0.55
1:V:59:ASP:OD1	1:W:456:TYR:OH	2.23	0.55
9:P:604:NAG:H83	9:P:604:NAG:H3	1.88	0.55
1:K:324:HIS:HA	1:K:455:ILE:HG13	1.88	0.55
2:A:604:ALA:O	2:A:772:SER:OG	2.21	0.55
1:O:371:SER:HA	1:Q:224:PRO:HA	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:523:GLN:O	1:O:524:LYS:N	2.40	0.55
1:S:324:HIS:CE1	1:S:452:LEU:HD21	2.41	0.55
1:V:324:HIS:HA	1:V:455:ILE:HG13	1.88	0.55
1:X:137:TYR:HB3	1:X:146:PRO:HB3	1.87	0.55
2:A:132:LYS:NZ	2:A:134:VAL:O	2.40	0.55
6:F:222:ILE:HB	6:F:235:VAL:HB	1.89	0.55
7:B:23:PHE:HB2	7:B:388:ASN:HD22	1.72	0.55
1:L:324:HIS:HA	1:L:455:ILE:HG13	1.88	0.55
1:M:324:HIS:CE1	1:M:452:LEU:HD21	2.41	0.55
1:Q:212:SER:HB3	1:Q:255:LYS:HB3	1.89	0.55
1:Q:270:GLU:HB3	1:Q:343:LYS:HB2	1.89	0.55
1:V:295:THR:HG23	1:V:298:PHE:H	1.72	0.55
2:A:31:PHE:HB2	2:A:119:ILE:HG22	1.89	0.55
4:D:525:ASN:O	4:D:527:PRO:HD3	2.07	0.55
1:M:270:GLU:HB3	1:M:343:LYS:HB2	1.89	0.55
1:V:137:TYR:HB3	1:V:146:PRO:HB3	1.89	0.55
1:P:65:ARG:HD2	1:H:467:HIS:CD2	2.42	0.55
1:G:204:LYS:HB2	1:G:263:LEU:HB3	1.88	0.55
1:G:215:ASN:N	6:F:365:SER:O	2.39	0.55
1:L:159:LEU:HD22	1:K:105:GLY:HA2	1.88	0.54
1:N:137:TYR:HB3	1:N:146:PRO:HB3	1.88	0.54
1:T:137:TYR:HB3	1:T:146:PRO:HB3	1.90	0.54
1:V:305:LEU:HD23	1:V:469:LYS:HD3	1.89	0.54
1:P:295:THR:HG23	1:P:298:PHE:H	1.72	0.54
1:H:368:LEU:HB2	1:H:375:VAL:HB	1.89	0.54
1:J:295:THR:HG23	1:J:298:PHE:H	1.72	0.54
1:J:380:ASN:HD22	1:K:215:ASN:HD22	1.55	0.54
1:K:137:TYR:HB3	1:K:146:PRO:HB3	1.87	0.54
7:B:713:LEU:HA	7:B:714:THR:OG1	2.07	0.54
1:L:90:ARG:NH1	1:L:103:ASP:OD1	2.39	0.54
1:N:523:GLN:O	1:N:524:LYS:N	2.41	0.54
1:O:295:THR:HG23	1:O:298:PHE:H	1.72	0.54
1:Q:523:GLN:O	1:Q:524:LYS:N	2.40	0.54
1:L:295:THR:HG23	1:L:298:PHE:H	1.73	0.54
1:M:198:GLU:HB3	1:M:269:LYS:HB2	1.89	0.54
1:M:523:GLN:O	1:M:524:LYS:N	2.40	0.54
1:R:90:ARG:NH1	1:R:103:ASP:OD1	2.39	0.54
1:U:270:GLU:HB3	1:U:343:LYS:HB2	1.90	0.54
1:H:295:THR:HG23	1:H:298:PHE:H	1.72	0.54
1:I:295:THR:HG23	1:I:298:PHE:H	1.72	0.54
2:A:1360:HIS:NE2	7:B:667:ASP:OD2	2.39	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:B:198:HIS:N	7:B:204:PRO:O	2.34	0.54
7:B:654:PHE:HB2	7:B:673:LEU:HD23	1.89	0.54
1:L:523:GLN:O	1:L:524:LYS:N	2.40	0.54
1:M:378:GLU:HB3	1:N:217:ALA:HB3	1.89	0.54
1:O:380:ASN:HD22	1:Q:215:ASN:HD22	1.55	0.54
1:O:400:LEU:HB2	1:Q:195:HIS:HB2	1.88	0.54
1:R:350:GLY:O	1:R:393:VAL:N	2.40	0.54
1:S:260:GLN:HB3	1:S:353:LEU:HB3	1.89	0.54
1:W:523:GLN:O	1:W:524:LYS:N	2.40	0.54
1:H:324:HIS:CE1	1:H:452:LEU:HD21	2.42	0.54
6:F:356:ASP:O	6:F:358:ILE:N	2.41	0.54
7:B:233:PRO:HD2	7:B:236:LEU:HD12	1.88	0.54
1:O:270:GLU:HB3	1:O:343:LYS:HB2	1.89	0.54
1:T:270:GLU:HB3	1:T:343:LYS:HB2	1.89	0.54
1:U:349:LYS:HB2	8:g:1:NAG:H83	1.90	0.54
1:P:90:ARG:NH1	1:P:103:ASP:OD1	2.38	0.54
1:G:256:ASN:OD1	1:G:256:ASN:N	2.41	0.54
1:G:270:GLU:HB3	1:G:343:LYS:HB2	1.89	0.54
3:C:466:ARG:NH1	3:C:467:CYS:O	2.41	0.54
1:L:359:CYS:HA	1:L:384:CYS:HA	1.90	0.54
1:M:305:LEU:HD23	1:M:469:LYS:HD3	1.89	0.54
1:N:270:GLU:HB3	1:N:343:LYS:HB2	1.89	0.54
1:N:305:LEU:HD23	1:N:469:LYS:HD3	1.88	0.54
1:S:58:THR:HG21	1:T:452:LEU:HD23	1.89	0.54
1:S:270:GLU:HB3	1:S:343:LYS:HB2	1.90	0.54
1:X:433:ASP:OD1	1:X:434:PHE:N	2.41	0.54
1:J:324:HIS:CE1	1:J:452:LEU:HD21	2.42	0.54
2:A:430:VAL:HG12	2:A:455:ILE:HA	1.89	0.54
3:C:416:LEU:HD23	3:C:435:MET:HE2	1.89	0.54
1:Q:295:THR:HG23	1:Q:298:PHE:H	1.73	0.54
1:X:523:GLN:O	1:X:524:LYS:N	2.40	0.54
1:I:309:TYR:H	1:I:472:ASN:HD21	1.56	0.54
1:J:324:HIS:HA	1:J:455:ILE:HG13	1.89	0.54
7:B:713:LEU:HB2	7:B:715:ILE:HB	1.89	0.54
1:L:380:ASN:HD22	1:M:215:ASN:HD22	1.53	0.54
1:M:364:LEU:HB3	1:M:379:PHE:HB2	1.90	0.54
1:N:295:THR:HG23	1:N:298:PHE:H	1.72	0.54
1:W:295:THR:HG23	1:W:298:PHE:H	1.71	0.54
1:H:324:HIS:HA	1:H:455:ILE:HG13	1.89	0.54
1:I:137:TYR:HB3	1:I:146:PRO:HB3	1.88	0.54
1:R:371:SER:HA	1:S:224:PRO:HA	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:371:ILE:HD12	2:A:422:LEU:HD13	1.88	0.54
3:C:246:GLU:HA	3:C:297:GLY:HA2	1.89	0.54
7:B:649:PRO:HB2	7:B:653:GLY:HA2	1.90	0.54
1:M:295:THR:HG23	1:M:298:PHE:H	1.73	0.54
1:R:413:ARG:HG2	1:S:438:ALA:HB1	1.89	0.54
1:S:196:TYR:HB2	1:S:271:LYS:HB3	1.89	0.54
1:X:92:ILE:HB	1:X:96:LEU:HB3	1.90	0.54
1:J:255:LYS:HA	1:J:358:ARG:HA	1.90	0.54
1:J:359:CYS:HA	1:J:384:CYS:HA	1.90	0.54
1:G:137:TYR:HB3	1:G:146:PRO:HB3	1.90	0.54
1:O:305:LEU:HD23	1:O:469:LYS:HD3	1.89	0.53
1:R:270:GLU:HB3	1:R:343:LYS:HB2	1.90	0.53
1:V:58:THR:HG21	1:W:452:LEU:HD23	1.90	0.53
1:X:256:ASN:ND2	9:X:603:NAG:O7	2.41	0.53
1:J:90:ARG:NH1	1:J:103:ASP:OD1	2.38	0.53
2:A:429:THR:HG22	2:A:430:VAL:HG13	1.91	0.53
1:P:270:GLU:HB3	1:P:343:LYS:HB2	1.89	0.53
1:H:514:GLU:HG2	1:H:515:GLY:H	1.73	0.53
4:D:205:TRP:HB2	4:D:243:HIS:HB2	1.90	0.53
1:L:514:GLU:HG2	1:L:515:GLY:H	1.74	0.53
1:M:344:ALA:HB3	1:M:399:ASN:HB2	1.90	0.53
1:N:380:ASN:HB2	1:O:215:ASN:HB2	1.91	0.53
1:Q:392:ALA:HB3	1:R:203:PHE:H	1.73	0.53
1:W:394:ASN:HB2	1:X:201:GLU:HB2	1.89	0.53
1:K:295:THR:HG23	1:K:298:PHE:H	1.73	0.53
2:A:1287:THR:HB	2:A:1290:THR:HB	1.91	0.53
3:C:298:GLY:HA2	3:C:407:ALA:HB3	1.88	0.53
1:L:270:GLU:HB3	1:L:343:LYS:HB2	1.91	0.53
1:N:400:LEU:HB2	1:O:195:HIS:HB2	1.89	0.53
1:Q:386:LYS:HB3	1:R:209:GLU:HB3	1.91	0.53
1:R:58:THR:HG21	1:S:452:LEU:HD23	1.90	0.53
1:S:59:ASP:OD1	1:T:456:TYR:OH	2.23	0.53
1:X:514:GLU:HG2	1:X:515:GLY:H	1.74	0.53
1:H:282:LEU:HD11	1:H:442:ASN:HA	1.90	0.53
1:K:465:ASN:HD21	1:K:468:LEU:HD23	1.72	0.53
1:G:487:ARG:NH2	6:F:42:THR:OG1	2.38	0.53
2:A:430:VAL:HG21	2:A:453:ARG:HH21	1.73	0.53
7:B:200:LEU:O	7:B:533:THR:OG1	2.25	0.53
1:L:465:ASN:HD21	1:L:468:LEU:HD23	1.73	0.53
1:O:309:TYR:H	1:O:472:ASN:HD21	1.57	0.53
1:S:301:ASP:OD1	1:T:288:ARG:NH2	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:270:GLU:HB3	1:W:343:LYS:HB2	1.91	0.53
1:P:514:GLU:HG2	1:P:515:GLY:H	1.73	0.53
3:C:315:ASP:HB3	3:C:358:ASP:HB3	1.90	0.53
1:M:318:LEU:HD11	1:M:323:THR:HB	1.91	0.53
1:V:270:GLU:HB3	1:V:343:LYS:HB2	1.90	0.53
1:V:514:GLU:HG2	1:V:515:GLY:H	1.74	0.53
1:P:523:GLN:O	1:P:524:LYS:N	2.41	0.53
1:H:523:GLN:O	1:H:524:LYS:N	2.41	0.53
1:I:523:GLN:O	1:I:524:LYS:N	2.41	0.53
2:A:275:LEU:HB3	2:A:322:TYR:HE2	1.74	0.53
2:A:531:THR:HG22	2:A:534:MET:HE2	1.91	0.53
1:R:295:THR:HG23	1:R:298:PHE:H	1.73	0.53
1:T:318:LEU:HD11	1:T:323:THR:HB	1.91	0.53
1:T:413:ARG:HD3	1:U:280:ILE:HD11	1.90	0.53
1:U:196:TYR:HB2	1:U:271:LYS:HB3	1.91	0.53
1:I:514:GLU:HG2	1:I:515:GLY:H	1.74	0.53
7:B:724:ILE:HG23	7:B:747:GLN:HA	1.90	0.53
1:K:514:GLU:HG2	1:K:515:GLY:H	1.74	0.52
1:G:210:LYS:HG3	6:F:370:LYS:HG2	1.90	0.52
1:G:523:GLN:O	1:G:524:LYS:N	2.41	0.52
1:M:514:GLU:HG2	1:M:515:GLY:H	1.74	0.52
1:V:309:TYR:H	1:V:472:ASN:HD21	1.57	0.52
1:V:318:LEU:HD11	1:V:323:THR:HB	1.91	0.52
1:G:96:LEU:HD11	1:G:103:ASP:HB2	1.92	0.52
1:R:309:TYR:H	1:R:472:ASN:HD21	1.57	0.52
1:U:363:HIS:ND1	1:U:380:ASN:OD1	2.29	0.52
1:H:309:TYR:H	1:H:472:ASN:HD21	1.57	0.52
2:A:1175:LEU:O	2:A:1179:THR:OG1	2.15	0.52
1:N:344:ALA:HB3	1:N:399:ASN:HB2	1.90	0.52
1:R:196:TYR:HB2	1:R:271:LYS:HB3	1.91	0.52
1:R:514:GLU:HG2	1:R:515:GLY:H	1.75	0.52
1:U:260:GLN:HB3	1:U:353:LEU:HB3	1.92	0.52
1:X:96:LEU:HD11	1:X:103:ASP:HB2	1.91	0.52
1:M:465:ASN:HD21	1:M:468:LEU:HD23	1.75	0.52
1:N:309:TYR:H	1:N:472:ASN:HD21	1.58	0.52
1:W:39:GLN:NE2	1:W:310:GLU:OE2	2.43	0.52
1:H:318:LEU:HD11	1:H:323:THR:HB	1.92	0.52
1:I:90:ARG:NH1	1:I:103:ASP:OD1	2.39	0.52
1:G:264:SER:N	1:G:349:LYS:O	2.37	0.52
2:A:473:HIS:N	2:A:474:LYS:HA	2.25	0.52
3:C:11:CYS:HB2	3:C:39:SER:HB3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:514:GLU:HG2	1:T:515:GLY:H	1.74	0.52
1:X:370:PHE:HB2	1:X:373:ILE:HB	1.90	0.52
1:H:310:GLU:HG2	1:H:313:GLU:H	1.75	0.52
1:G:438:ALA:HB2	6:F:399:GLY:HA3	1.90	0.52
4:D:205:TRP:N	4:D:243:HIS:O	2.38	0.52
1:U:222:PHE:O	1:U:245:GLY:N	2.42	0.52
1:U:514:GLU:HG2	1:U:515:GLY:H	1.74	0.52
1:W:514:GLU:HG2	1:W:515:GLY:H	1.74	0.52
1:H:90:ARG:NH1	1:H:103:ASP:OD1	2.39	0.52
1:G:514:GLU:HG2	1:G:515:GLY:H	1.74	0.52
2:A:975:ARG:HB2	2:A:1340:VAL:HB	1.90	0.52
1:P:199:GLN:HB3	1:G:396:THR:HB	1.92	0.52
1:P:301:ASP:OD1	1:H:288:ARG:NH2	2.43	0.52
1:K:270:GLU:HB3	1:K:343:LYS:HB2	1.92	0.52
4:D:520:SER:HA	4:D:540:THR:HG22	1.92	0.52
1:M:309:TYR:H	1:M:472:ASN:HD21	1.58	0.52
1:N:514:GLU:HG2	1:N:515:GLY:H	1.75	0.52
1:Q:309:TYR:H	1:Q:472:ASN:HD21	1.58	0.52
1:Q:380:ASN:HB2	1:R:215:ASN:HB2	1.91	0.52
1:S:514:GLU:HG2	1:S:515:GLY:H	1.74	0.52
1:U:318:LEU:HD11	1:U:323:THR:HB	1.92	0.52
1:W:83:ASP:HB3	1:W:92:ILE:HG23	1.92	0.52
1:W:137:TYR:HB3	1:W:146:PRO:HB3	1.92	0.52
3:C:233:HIS:H	3:C:310:ALA:HB3	1.75	0.52
1:O:378:GLU:HB3	1:Q:217:ALA:HB3	1.91	0.52
1:R:380:ASN:HD22	1:S:215:ASN:HD22	1.57	0.52
1:U:58:THR:HG21	1:V:452:LEU:HD23	1.92	0.52
1:X:270:GLU:HB3	1:X:343:LYS:HB2	1.92	0.52
2:A:283:MET:HB2	2:A:285:THR:N	2.25	0.52
2:A:798:GLU:HG2	2:A:816:LYS:HG3	1.91	0.52
1:M:400:LEU:HB2	1:N:195:HIS:HB2	1.92	0.51
1:Q:59:ASP:OD1	1:R:456:TYR:OH	2.23	0.51
1:Q:90:ARG:NH1	1:Q:103:ASP:OD1	2.38	0.51
1:P:470:LYS:HZ3	1:G:64:ARG:H	1.58	0.51
1:L:378:GLU:HB3	1:M:217:ALA:HB3	1.90	0.51
1:N:218:ILE:HG23	1:N:249:PHE:HB2	1.90	0.51
1:O:318:LEU:HD11	1:O:323:THR:HB	1.92	0.51
1:V:83:ASP:HB3	1:V:92:ILE:HG23	1.92	0.51
1:I:463:MET:HG2	1:I:464:LYS:H	1.76	0.51
1:G:358:ARG:N	1:G:385:VAL:O	2.42	0.51
2:A:767:SER:HB2	2:A:768:TYR:HB3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:309:TYR:H	1:L:472:ASN:HD21	1.57	0.51
1:L:463:MET:HG2	1:L:464:LYS:H	1.76	0.51
1:M:463:MET:HG2	1:M:464:LYS:H	1.76	0.51
1:Q:264:SER:N	1:Q:349:LYS:O	2.36	0.51
1:U:413:ARG:HD3	1:V:280:ILE:HD11	1.90	0.51
1:H:413:ARG:HG2	1:I:438:ALA:HB1	1.92	0.51
1:I:270:GLU:HB3	1:I:343:LYS:HB2	1.93	0.51
1:K:344:ALA:HB3	1:K:399:ASN:HB2	1.93	0.51
4:D:339:SER:OG	4:D:350:SER:O	2.28	0.51
1:L:344:ALA:HB3	1:L:399:ASN:HB2	1.92	0.51
1:T:65:ARG:HD2	1:U:467:HIS:CE1	2.45	0.51
1:U:218:ILE:HG23	1:U:249:PHE:HB2	1.92	0.51
1:P:463:MET:HG2	1:P:464:LYS:H	1.76	0.51
1:G:295:THR:HG23	1:G:298:PHE:H	1.75	0.51
2:A:192:SER:HB3	2:A:976:ILE:HD11	1.93	0.51
2:A:1079:THR:HG21	2:A:1107:LEU:HD11	1.92	0.51
4:D:42:CYS:N	4:D:79:CYS:SG	2.83	0.51
7:B:712:VAL:HG21	7:B:759:LEU:HD11	1.91	0.51
1:L:362:TYR:HB3	1:L:381:LYS:HB3	1.92	0.51
1:N:465:ASN:HD21	1:N:468:LEU:HD23	1.75	0.51
1:O:514:GLU:HG2	1:O:515:GLY:H	1.75	0.51
1:T:359:CYS:HA	1:T:384:CYS:HA	1.91	0.51
1:U:64:ARG:H	1:V:470:LYS:HZ3	1.58	0.51
1:H:270:GLU:HB3	1:H:343:LYS:HB2	1.92	0.51
1:T:463:MET:HG2	1:T:464:LYS:H	1.75	0.51
1:U:359:CYS:HA	1:U:384:CYS:HA	1.93	0.51
1:V:222:PHE:O	1:V:245:GLY:N	2.43	0.51
1:W:386:LYS:HD3	1:X:209:GLU:HB3	1.91	0.51
1:J:463:MET:HG2	1:J:464:LYS:H	1.76	0.51
4:D:631:CYS:HB2	4:D:649:TYR:HB2	1.93	0.51
1:N:260:GLN:HB3	1:N:353:LEU:HB3	1.93	0.51
1:K:309:TYR:H	1:K:472:ASN:HD21	1.57	0.51
1:G:332:GLY:N	1:G:446:VAL:O	2.44	0.51
3:C:170:GLN:H	4:D:378:ARG:HG3	1.76	0.51
4:D:48:ARG:HH11	4:D:69:GLU:HB3	1.75	0.51
1:L:96:LEU:HD11	1:L:103:ASP:HB2	1.93	0.51
1:Q:196:TYR:HB2	1:Q:271:LYS:HB3	1.92	0.51
1:V:400:LEU:HB2	1:W:195:HIS:HB2	1.92	0.51
1:V:413:ARG:HD3	1:W:280:ILE:HD11	1.92	0.51
1:W:310:GLU:HG2	1:W:313:GLU:H	1.76	0.51
1:P:203:PHE:H	1:G:392:ALA:HB3	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:344:ALA:HB3	1:P:399:ASN:HB2	1.92	0.51
2:A:1249:GLU:HG2	2:A:1289:ASP:HB2	1.93	0.51
1:L:371:SER:HA	1:M:224:PRO:HA	1.92	0.51
1:L:400:LEU:HB2	1:M:195:HIS:HB2	1.93	0.51
1:O:463:MET:HG2	1:O:464:LYS:H	1.76	0.51
1:Q:305:LEU:HD23	1:Q:469:LYS:HD3	1.93	0.51
1:Q:318:LEU:HD11	1:Q:323:THR:HB	1.92	0.51
1:T:83:ASP:HB3	1:T:92:ILE:HG23	1.93	0.51
1:U:83:ASP:HB3	1:U:92:ILE:HG23	1.92	0.51
1:P:199:GLN:HG3	1:P:268:LYS:HG2	1.92	0.51
1:I:282:LEU:HD11	1:I:442:ASN:HA	1.93	0.51
1:I:363:HIS:ND1	1:I:380:ASN:OD1	2.37	0.51
1:K:463:MET:HG2	1:K:464:LYS:H	1.76	0.51
1:G:83:ASP:HB3	1:G:92:ILE:HG23	1.93	0.51
1:G:324:HIS:CE1	1:G:452:LEU:HD11	2.46	0.51
2:A:640:LEU:HG	2:A:641:ASN:H	1.75	0.51
2:A:1112:GLN:HE22	2:A:1167:ALA:HA	1.75	0.51
7:B:223:SER:HB3	7:B:226:THR:HB	1.91	0.51
1:Q:514:GLU:HG2	1:Q:515:GLY:H	1.75	0.51
1:J:282:LEU:HD11	1:J:442:ASN:HA	1.93	0.51
1:J:318:LEU:HD11	1:J:323:THR:HB	1.93	0.51
1:G:258:THR:N	1:G:355:ASP:O	2.44	0.51
5:E:91:ARG:HG2	5:E:106:VAL:HG22	1.93	0.51
1:U:463:MET:HG2	1:U:464:LYS:H	1.76	0.50
1:X:282:LEU:HD11	1:X:442:ASN:HA	1.93	0.50
1:P:44:ARG:NH2	1:H:474:GLU:OE2	2.44	0.50
1:I:318:LEU:HD11	1:I:323:THR:HB	1.92	0.50
2:A:141:VAL:HB	2:A:188:PHE:HB3	1.93	0.50
3:C:47:ASN:HB2	6:F:433:PRO:HG2	1.93	0.50
7:B:676:PHE:HB3	7:B:699:CYS:HB3	1.93	0.50
1:N:96:LEU:HD11	1:N:103:ASP:HB2	1.93	0.50
1:N:382:ASP:HB3	1:O:213:ASN:HB2	1.92	0.50
1:W:309:TYR:H	1:W:472:ASN:HD21	1.59	0.50
1:X:463:MET:HG2	1:X:464:LYS:H	1.76	0.50
2:A:464:TYR:O	2:A:544:TYR:OH	2.29	0.50
1:L:282:LEU:HD11	1:L:442:ASN:HA	1.94	0.50
1:N:463:MET:HG2	1:N:464:LYS:H	1.76	0.50
1:R:349:LYS:HB2	8:d:1:NAG:H83	1.92	0.50
1:S:396:THR:HB	1:T:199:GLN:HB3	1.93	0.50
1:G:370:PHE:N	1:G:373:ILE:O	2.37	0.50
2:A:272:ARG:HA	2:A:280:LYS:HG3	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:380:ASN:HB2	1:M:215:ASN:HB2	1.93	0.50
1:N:318:LEU:HD11	1:N:323:THR:HB	1.94	0.50
1:O:96:LEU:HD11	1:O:103:ASP:HB2	1.93	0.50
1:P:83:ASP:HB3	1:P:92:ILE:HG23	1.93	0.50
1:P:318:LEU:HD11	1:P:323:THR:HB	1.93	0.50
1:K:318:LEU:HD11	1:K:323:THR:HB	1.93	0.50
6:F:513:SER:OG	6:F:531:GLU:N	2.43	0.50
1:Q:214:PHE:HB3	1:Q:253:TYR:HB3	1.93	0.50
1:S:318:LEU:HD11	1:S:323:THR:HB	1.92	0.50
1:W:196:TYR:HB2	1:W:271:LYS:HB3	1.93	0.50
1:P:266:SER:O	1:P:347:LYS:N	2.43	0.50
1:J:514:GLU:HG2	1:J:515:GLY:H	1.74	0.50
3:C:90:ASN:ND2	3:C:94:ASP:O	2.36	0.50
1:N:282:LEU:HD11	1:N:442:ASN:HA	1.94	0.50
1:R:463:MET:HG2	1:R:464:LYS:H	1.76	0.50
1:Q:463:MET:HG2	1:Q:464:LYS:H	1.76	0.50
1:T:309:TYR:H	1:T:472:ASN:HD21	1.58	0.50
1:P:280:ILE:HD11	1:G:413:ARG:HD3	1.92	0.50
1:J:310:GLU:HG2	1:J:313:GLU:H	1.77	0.50
2:A:283:MET:SD	2:A:283:MET:N	2.82	0.50
1:Q:350:GLY:O	1:Q:393:VAL:N	2.40	0.50
1:S:392:ALA:HB3	1:T:203:PHE:H	1.77	0.50
1:S:463:MET:HG2	1:S:464:LYS:H	1.76	0.50
1:T:305:LEU:HD23	1:T:469:LYS:HD3	1.93	0.50
1:W:463:MET:HG2	1:W:464:LYS:H	1.76	0.50
1:J:96:LEU:HD11	1:J:103:ASP:HB2	1.94	0.50
2:A:32:ARG:NH2	2:A:630:SER:O	2.45	0.50
2:A:1231:ASN:HB2	2:A:1246:ARG:HH21	1.77	0.50
7:B:293:ILE:HA	7:B:400:VAL:HG12	1.93	0.50
1:L:318:LEU:HD11	1:L:323:THR:HB	1.94	0.50
1:H:39:GLN:NE2	1:H:310:GLU:OE2	2.45	0.50
1:K:359:CYS:HA	1:K:384:CYS:HA	1.94	0.50
1:G:305:LEU:HD21	1:G:473:LEU:HD11	1.94	0.50
1:G:465:ASN:HD21	1:G:468:LEU:HD23	1.76	0.50
3:C:70:GLY:HA2	3:C:82:ARG:HH11	1.76	0.50
1:R:162:ARG:HD3	1:R:164:ARG:HD2	1.94	0.49
1:R:305:LEU:HD23	1:R:469:LYS:HD3	1.93	0.49
1:R:318:LEU:HD11	1:R:323:THR:HB	1.94	0.49
1:S:83:ASP:HB3	1:S:92:ILE:HG23	1.94	0.49
1:V:463:MET:HG2	1:V:464:LYS:H	1.76	0.49
1:P:282:LEU:HD11	1:P:442:ASN:HA	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:270:GLU:HB3	1:J:343:LYS:HB2	1.92	0.49
1:K:282:LEU:HD11	1:K:442:ASN:HA	1.94	0.49
1:U:305:LEU:HD23	1:U:469:LYS:HD3	1.94	0.49
1:W:105:GLY:HA2	1:X:159:LEU:HD13	1.94	0.49
1:P:222:PHE:O	1:P:245:GLY:N	2.45	0.49
1:H:362:TYR:HB3	1:H:381:LYS:HB3	1.94	0.49
1:I:310:GLU:HG2	1:I:313:GLU:H	1.76	0.49
1:J:309:TYR:H	1:J:472:ASN:HD21	1.57	0.49
1:G:254:SER:O	1:G:359:CYS:N	2.41	0.49
1:G:463:MET:HG2	1:G:464:LYS:H	1.76	0.49
6:F:233:VAL:HG22	6:F:352:ILE:HG12	1.93	0.49
6:F:470:GLY:N	6:F:485:CYS:SG	2.77	0.49
1:M:96:LEU:HD11	1:M:103:ASP:HB2	1.93	0.49
1:R:83:ASP:HB3	1:R:92:ILE:HG23	1.95	0.49
1:S:309:TYR:H	1:S:472:ASN:HD21	1.59	0.49
1:S:364:LEU:HB3	1:S:379:PHE:HB2	1.93	0.49
1:T:260:GLN:HB3	1:T:353:LEU:HB3	1.93	0.49
1:W:65:ARG:HD2	1:X:467:HIS:CE1	2.46	0.49
1:J:64:ARG:H	1:K:470:LYS:HZ3	1.60	0.49
4:D:246:LYS:HD3	9:D:901:NAG:H82	1.93	0.49
1:N:371:SER:HA	1:O:224:PRO:HA	1.93	0.49
1:O:260:GLN:HB3	1:O:353:LEU:HB3	1.93	0.49
1:Q:465:ASN:HD21	1:Q:468:LEU:HD23	1.77	0.49
1:V:196:TYR:HB2	1:V:271:LYS:HB3	1.92	0.49
1:V:310:GLU:HG2	1:V:313:GLU:H	1.77	0.49
1:I:256:ASN:HB3	9:I:603:NAG:HN2	1.77	0.49
2:A:463:SER:OG	2:A:544:TYR:OH	2.24	0.49
2:A:1185:THR:HB	2:A:1230:ASP:HA	1.93	0.49
7:B:704:CYS:SG	7:B:722:TYR:HB2	2.52	0.49
1:M:310:GLU:HG2	1:M:313:GLU:H	1.78	0.49
1:P:260:GLN:HB3	1:P:353:LEU:HB3	1.94	0.49
1:L:215:ASN:HB2	1:K:380:ASN:HB2	1.95	0.49
1:S:349:LYS:HB2	8:e:1:NAG:H83	1.93	0.49
1:X:131:LEU:HG	1:X:132:ALA:H	1.78	0.49
1:K:256:ASN:HB3	9:K:603:NAG:HN2	1.78	0.49
2:A:577:PRO:O	2:A:582:TYR:OH	2.29	0.49
2:A:1259:LEU:HD13	2:A:1299:GLU:HB2	1.94	0.49
6:F:490:ARG:N	6:F:498:CYS:HB2	2.23	0.49
1:N:59:ASP:OD1	1:O:456:TYR:OH	2.25	0.49
1:R:96:LEU:HD11	1:R:103:ASP:HB2	1.94	0.49
1:S:310:GLU:HG2	1:S:313:GLU:H	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:363:HIS:ND1	1:V:380:ASN:OD1	2.31	0.49
1:H:83:ASP:HB3	1:H:92:ILE:HG23	1.94	0.49
1:H:256:ASN:HB3	9:H:603:NAG:HN2	1.77	0.49
1:H:463:MET:HG2	1:H:464:LYS:H	1.76	0.49
1:G:349:LYS:HB2	8:p:1:NAG:H83	1.94	0.49
1:G:364:LEU:N	1:G:379:PHE:O	2.42	0.49
2:A:323:LEU:H	2:A:345:ILE:H	1.61	0.49
2:A:943:THR:HA	2:A:1358:THR:HA	1.93	0.49
2:A:1255:LEU:HB2	2:A:1270:VAL:HG11	1.95	0.49
1:L:41:PHE:CD1	1:L:310:GLU:HG3	2.47	0.49
1:O:92:ILE:HB	1:O:96:LEU:HB3	1.95	0.49
1:U:310:GLU:HG2	1:U:313:GLU:H	1.77	0.49
1:P:310:GLU:HG2	1:P:313:GLU:H	1.77	0.49
1:J:59:ASP:OD1	1:K:456:TYR:OH	2.25	0.49
1:K:96:LEU:HD11	1:K:103:ASP:HB2	1.94	0.49
1:G:347:LYS:HG2	1:G:396:THR:HG23	1.95	0.49
2:A:581:ALA:HB1	2:A:820:PHE:HB3	1.94	0.49
6:F:528:ARG:HD3	6:F:550:GLN:HB3	1.94	0.49
1:L:131:LEU:HG	1:L:132:ALA:H	1.78	0.49
1:O:310:GLU:HG2	1:O:313:GLU:H	1.78	0.49
1:Q:310:GLU:HG2	1:Q:313:GLU:H	1.78	0.49
1:R:88:THR:OG1	1:R:296:THR:OG1	2.26	0.49
1:R:301:ASP:OD1	1:S:288:ARG:NH2	2.46	0.49
1:T:310:GLU:HG2	1:T:313:GLU:H	1.78	0.49
1:U:350:GLY:O	1:U:393:VAL:N	2.46	0.49
1:V:465:ASN:HD21	1:V:468:LEU:HD23	1.78	0.49
1:K:41:PHE:CD1	1:K:310:GLU:HG3	2.47	0.49
1:G:201:GLU:N	6:F:379:ARG:O	2.37	0.49
2:A:955:ARG:NH2	2:A:1350:THR:O	2.45	0.49
1:M:83:ASP:HB3	1:M:92:ILE:HG23	1.95	0.49
1:X:295:THR:HG23	1:X:298:PHE:H	1.78	0.49
1:P:332:GLY:O	1:P:446:VAL:N	2.46	0.49
1:I:96:LEU:HD11	1:I:103:ASP:HB2	1.94	0.49
1:G:186:LYS:HG3	6:F:394:ARG:HA	1.95	0.49
4:D:665:LEU:HD23	4:D:669:SER:HA	1.95	0.49
1:N:131:LEU:HG	1:N:132:ALA:H	1.78	0.48
1:Q:96:LEU:HD11	1:Q:103:ASP:HB2	1.94	0.48
1:T:96:LEU:HD11	1:T:103:ASP:HB2	1.95	0.48
1:W:58:THR:HG21	1:X:452:LEU:HD23	1.95	0.48
1:W:318:LEU:HD11	1:W:323:THR:HB	1.93	0.48
1:X:90:ARG:NH1	1:X:103:ASP:OD1	2.45	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:301:ASP:OD1	1:I:288:ARG:NH2	2.46	0.48
1:I:83:ASP:HB3	1:I:92:ILE:HG23	1.94	0.48
6:F:14:TRP:HB3	6:F:29:ARG:HD2	1.95	0.48
1:N:83:ASP:HB3	1:N:92:ILE:HG23	1.95	0.48
1:N:206:ILE:O	1:N:261:LEU:N	2.44	0.48
1:O:131:LEU:HG	1:O:132:ALA:H	1.79	0.48
1:O:349:LYS:HB2	8:b:1:NAG:H83	1.95	0.48
1:W:59:ASP:OD1	1:X:456:TYR:OH	2.28	0.48
1:P:131:LEU:HG	1:P:132:ALA:H	1.78	0.48
1:G:282:LEU:HD13	1:G:445:PRO:HB3	1.95	0.48
2:A:501:TYR:CZ	2:A:513:GLY:HA3	2.48	0.48
1:O:264:SER:N	1:O:349:LYS:O	2.36	0.48
1:R:282:LEU:HD11	1:R:442:ASN:HA	1.96	0.48
1:I:332:GLY:O	1:I:446:VAL:N	2.46	0.48
1:J:131:LEU:HG	1:J:132:ALA:H	1.78	0.48
1:J:222:PHE:O	1:J:245:GLY:N	2.45	0.48
1:G:159:LEU:HD13	6:F:89:GLN:HG3	1.96	0.48
2:A:1176:LEU:HD13	2:A:1202:HIS:CE1	2.48	0.48
3:C:127:LEU:HD22	3:C:413:VAL:HG11	1.95	0.48
6:F:160:TYR:HD1	6:F:167:LEU:HD13	1.78	0.48
7:B:369:GLY:HA3	7:B:485:PHE:HA	1.95	0.48
7:B:744:TYR:HE2	7:B:751:TRP:CD1	2.32	0.48
8:n:1:NAG:H4	8:n:2:NAG:H2	1.60	0.48
1:Q:92:ILE:HB	1:Q:96:LEU:HB3	1.96	0.48
1:S:305:LEU:HD23	1:S:469:LYS:HD3	1.95	0.48
1:S:413:ARG:HD3	1:T:280:ILE:HD11	1.95	0.48
1:X:30:TRP:CH2	1:X:42:ARG:HD2	2.49	0.48
1:J:92:ILE:HB	1:J:96:LEU:HB3	1.95	0.48
1:G:270:GLU:O	1:G:343:LYS:N	2.42	0.48
1:M:282:LEU:HD11	1:M:442:ASN:HA	1.95	0.48
1:M:332:GLY:O	1:M:446:VAL:N	2.47	0.48
1:O:83:ASP:HB3	1:O:92:ILE:HG23	1.95	0.48
1:O:465:ASN:HD21	1:O:468:LEU:HD23	1.78	0.48
1:V:349:LYS:HB2	8:h:1:NAG:H83	1.94	0.48
1:X:147:LEU:HG	1:X:148:SER:H	1.77	0.48
1:H:58:THR:HG21	1:I:452:LEU:HD23	1.95	0.48
1:J:83:ASP:HB3	1:J:92:ILE:HG23	1.95	0.48
1:K:83:ASP:HB3	1:K:92:ILE:HG23	1.95	0.48
1:G:331:LEU:HD23	1:G:445:PRO:HG2	1.95	0.48
2:A:370:PRO:HG2	2:A:470:THR:HG21	1.96	0.48
2:A:1279:ARG:O	2:A:1281:GLY:HA2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:b:1:NAG:H4	8:b:2:NAG:H2	1.59	0.48
1:L:83:ASP:HB3	1:L:92:ILE:HG23	1.95	0.48
1:U:96:LEU:HD11	1:U:103:ASP:HB2	1.95	0.48
1:P:224:PRO:HG3	1:P:243:LEU:HD23	1.96	0.48
1:P:415:TYR:HD2	1:P:440:SER:HB2	1.79	0.48
2:A:1342:LEU:HD23	2:A:1342:LEU:H	1.78	0.48
1:Q:349:LYS:HB2	8:c:1:NAG:H83	1.94	0.48
1:V:198:GLU:HB3	1:V:269:LYS:HB2	1.96	0.48
1:V:421:GLU:HB3	1:W:434:PHE:HD2	1.78	0.48
1:W:400:LEU:HB2	1:X:195:HIS:HB2	1.96	0.48
2:A:1227:PHE:HE2	2:A:1229:LYS:HE3	1.78	0.48
7:B:291:GLU:HA	7:B:402:ILE:HG22	1.96	0.48
1:L:59:ASP:OD1	1:M:456:TYR:OH	2.25	0.48
1:M:131:LEU:HG	1:M:132:ALA:H	1.78	0.48
1:N:92:ILE:HB	1:N:96:LEU:HB3	1.96	0.48
1:N:366:VAL:O	1:N:377:ALA:N	2.45	0.48
1:Q:83:ASP:HB3	1:Q:92:ILE:HG23	1.95	0.48
1:S:220:LEU:O	1:S:247:GLY:N	2.38	0.48
1:W:92:ILE:HB	1:W:96:LEU:HB3	1.96	0.48
5:E:122:ARG:NH1	6:F:161:ASP:OD1	2.46	0.48
1:N:214:PHE:HB3	1:N:253:TYR:HB3	1.94	0.48
1:S:266:SER:O	1:S:347:LYS:N	2.44	0.48
1:H:162:ARG:HD3	1:H:164:ARG:HD2	1.96	0.48
1:G:40:MET:HB2	1:G:65:ARG:HB3	1.96	0.48
3:C:260:HIS:HD2	3:C:262:GLU:HB2	1.79	0.48
1:R:131:LEU:HG	1:R:132:ALA:H	1.79	0.48
1:W:362:TYR:HB3	1:W:381:LYS:HB3	1.95	0.48
1:I:39:GLN:NE2	1:I:310:GLU:OE2	2.47	0.48
1:I:64:ARG:H	1:J:470:LYS:HZ3	1.62	0.48
1:J:332:GLY:O	1:J:446:VAL:N	2.47	0.48
1:K:310:GLU:HG2	1:K:313:GLU:H	1.78	0.48
1:G:198:GLU:HB3	1:G:269:LYS:HB2	1.95	0.48
2:A:424:LEU:HD23	2:A:428:VAL:HG21	1.96	0.48
2:A:995:GLU:HG2	2:A:1021:VAL:HG21	1.96	0.48
6:F:85:CYS:HB3	6:F:103:VAL:HG11	1.95	0.48
1:L:256:ASN:HB3	9:L:603:NAG:HN2	1.79	0.47
1:N:372:GLU:N	1:O:223:THR:O	2.46	0.47
1:O:282:LEU:HD11	1:O:442:ASN:HA	1.95	0.47
1:O:332:GLY:O	1:O:446:VAL:N	2.47	0.47
1:R:220:LEU:O	1:R:247:GLY:N	2.41	0.47
1:T:350:GLY:O	1:T:393:VAL:N	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:224:PRO:HG3	1:U:243:LEU:HD23	1.96	0.47
1:H:131:LEU:HG	1:H:132:ALA:H	1.79	0.47
1:K:92:ILE:HB	1:K:96:LEU:HB3	1.96	0.47
2:A:61:ASP:HB2	2:A:62:LYS:CB	2.43	0.47
4:D:413:LEU:HD12	4:D:414:PRO:HD2	1.96	0.47
4:D:478:LYS:O	4:D:481:THR:OG1	2.22	0.47
8:e:1:NAG:H4	8:e:2:NAG:H2	1.60	0.47
1:L:92:ILE:HB	1:L:96:LEU:HB3	1.95	0.47
1:M:92:ILE:HB	1:M:96:LEU:HB3	1.96	0.47
1:U:92:ILE:HB	1:U:96:LEU:HB3	1.97	0.47
1:V:332:GLY:O	1:V:446:VAL:N	2.48	0.47
1:W:40:MET:HB2	1:W:65:ARG:HB3	1.96	0.47
1:I:349:LYS:HB2	8:m:1:NAG:H83	1.96	0.47
1:G:332:GLY:O	1:G:446:VAL:N	2.46	0.47
2:A:472:ASN:HA	2:A:474:LYS:HD2	1.96	0.47
3:C:323:ALA:HB3	3:C:350:ARG:HB3	1.96	0.47
6:F:236:GLY:N	6:F:349:SER:O	2.47	0.47
1:O:59:ASP:OD1	1:Q:456:TYR:OH	2.24	0.47
1:U:309:TYR:H	1:U:472:ASN:HD21	1.60	0.47
1:P:413:ARG:HG2	1:H:438:ALA:HB1	1.96	0.47
1:K:131:LEU:HG	1:K:132:ALA:H	1.78	0.47
1:M:264:SER:N	1:M:349:LYS:O	2.39	0.47
1:N:310:GLU:HG2	1:N:313:GLU:H	1.78	0.47
1:S:162:ARG:HD3	1:S:164:ARG:HD2	1.96	0.47
1:T:92:ILE:HB	1:T:96:LEU:HB3	1.97	0.47
1:W:465:ASN:HD21	1:W:468:LEU:HD23	1.80	0.47
1:K:332:GLY:O	1:K:446:VAL:N	2.46	0.47
1:N:332:GLY:O	1:N:446:VAL:N	2.47	0.47
1:Q:332:GLY:O	1:Q:446:VAL:N	2.48	0.47
1:R:92:ILE:HB	1:R:96:LEU:HB3	1.96	0.47
1:P:96:LEU:HD11	1:P:103:ASP:HB2	1.95	0.47
1:J:349:LYS:HB2	8:n:1:NAG:H83	1.97	0.47
1:G:131:LEU:HG	1:G:132:ALA:H	1.78	0.47
1:G:209:GLU:N	6:F:371:LYS:O	2.46	0.47
1:G:268:LYS:O	1:G:345:SER:N	2.48	0.47
2:A:56:ILE:O	2:A:66:TYR:N	2.43	0.47
7:B:483:ILE:HG13	7:B:484:ASP:H	1.79	0.47
7:B:674:THR:HA	7:B:675:GLY:HA2	1.62	0.47
1:M:371:SER:HA	1:N:224:PRO:HA	1.95	0.47
1:R:357:LYS:HD2	9:R:603:NAG:H62	1.95	0.47
1:R:465:ASN:HD21	1:R:468:LEU:HD23	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:96:LEU:HD11	1:S:103:ASP:HB2	1.96	0.47
1:H:415:TYR:HD2	1:H:440:SER:HB2	1.79	0.47
2:A:109:LYS:HG2	4:D:78:GLY:HA3	1.97	0.47
2:A:773:TRP:CE3	2:A:774:LEU:HB2	2.49	0.47
1:N:350:GLY:O	1:N:393:VAL:N	2.47	0.47
1:Q:58:THR:HG21	1:R:452:LEU:HD23	1.97	0.47
1:R:212:SER:HB3	1:R:255:LYS:HB3	1.97	0.47
1:R:264:SER:N	1:R:349:LYS:O	2.36	0.47
1:R:310:GLU:HG2	1:R:313:GLU:H	1.79	0.47
1:S:131:LEU:HG	1:S:132:ALA:H	1.79	0.47
1:X:83:ASP:HB3	1:X:92:ILE:HG23	1.97	0.47
1:P:468:LEU:O	1:P:472:ASN:HB2	2.15	0.47
1:H:332:GLY:O	1:H:446:VAL:N	2.47	0.47
1:J:147:LEU:HG	1:J:148:SER:H	1.80	0.47
1:G:349:LYS:HD2	8:p:1:NAG:HN2	1.79	0.47
1:G:360:LEU:O	1:G:383:ASP:N	2.43	0.47
2:A:364:LYS:HG2	2:A:466:TYR:CD1	2.50	0.47
2:A:371:ILE:HB	2:A:420:PHE:HB2	1.96	0.47
7:B:715:ILE:HG12	7:B:728:ILE:HG12	1.97	0.47
1:U:332:GLY:O	1:U:446:VAL:N	2.47	0.47
1:V:131:LEU:HG	1:V:132:ALA:H	1.80	0.47
1:V:350:GLY:O	1:V:393:VAL:N	2.48	0.47
1:W:131:LEU:HG	1:W:132:ALA:H	1.80	0.47
1:I:92:ILE:HB	1:I:96:LEU:HB3	1.96	0.47
1:I:131:LEU:HG	1:I:132:ALA:H	1.79	0.47
2:A:220:LYS:HG2	2:A:221:GLU:H	1.79	0.47
2:A:1218:VAL:HB	2:A:1223:PRO:HB3	1.97	0.47
4:D:52:VAL:HB	4:D:55:TYR:HE1	1.79	0.47
4:D:195:ASP:N	4:D:253:VAL:O	2.48	0.47
1:L:40:MET:SD	1:L:65:ARG:HD3	2.54	0.47
1:R:266:SER:O	1:R:347:LYS:N	2.44	0.47
3:C:500:TRP:CE3	3:C:506:ARG:HB3	2.49	0.47
1:L:30:TRP:CH2	1:L:42:ARG:HD2	2.50	0.47
1:L:310:GLU:HG2	1:L:313:GLU:H	1.80	0.47
1:W:256:ASN:HB3	9:W:603:NAG:HN2	1.80	0.47
1:X:41:PHE:CD1	1:X:310:GLU:HG3	2.49	0.47
1:X:86:CYS:SG	1:X:87:SER:N	2.87	0.47
1:P:92:ILE:HB	1:P:96:LEU:HB3	1.96	0.47
1:H:96:LEU:HD11	1:H:103:ASP:HB2	1.95	0.47
1:I:147:LEU:HG	1:I:148:SER:H	1.80	0.47
1:K:349:LYS:HB2	8:o:1:NAG:H83	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:500:TRP:HE3	3:C:506:ARG:HB3	1.80	0.47
6:F:231:LEU:HG	6:F:354:TYR:HB3	1.97	0.47
1:L:218:ILE:HG23	1:L:249:PHE:HB2	1.97	0.46
1:L:332:GLY:O	1:L:446:VAL:N	2.47	0.46
1:N:358:ARG:O	1:N:385:VAL:N	2.42	0.46
1:Q:131:LEU:HG	1:Q:132:ALA:H	1.79	0.46
1:T:28:SER:HB2	1:T:43:SER:HB3	1.96	0.46
1:V:92:ILE:HB	1:V:96:LEU:HB3	1.97	0.46
1:P:220:LEU:N	1:P:247:GLY:O	2.38	0.46
1:I:359:CYS:HA	1:I:384:CYS:HA	1.97	0.46
6:F:395:GLY:HA3	6:F:416:TRP:HE1	1.81	0.46
7:B:491:VAL:HG23	7:B:507:LEU:HD23	1.96	0.46
8:p:1:NAG:H4	8:p:2:NAG:H2	1.61	0.46
1:M:206:ILE:O	1:M:261:LEU:N	2.44	0.46
1:N:360:LEU:N	1:N:383:ASP:O	2.40	0.46
1:R:360:LEU:N	1:R:383:ASP:O	2.41	0.46
1:S:92:ILE:HB	1:S:96:LEU:HB3	1.97	0.46
1:T:131:LEU:HG	1:T:132:ALA:H	1.80	0.46
2:A:149:ASN:HB2	2:A:155:ALA:HB2	1.97	0.46
2:A:1279:ARG:C	2:A:1281:GLY:HA2	2.41	0.46
1:L:58:THR:HG21	1:M:452:LEU:HD23	1.97	0.46
1:L:147:LEU:HG	1:L:148:SER:H	1.81	0.46
1:M:366:VAL:O	1:M:377:ALA:N	2.46	0.46
1:Q:255:LYS:HA	1:Q:358:ARG:HA	1.96	0.46
1:Q:282:LEU:HD11	1:Q:442:ASN:HA	1.97	0.46
1:R:362:TYR:HB3	1:R:381:LYS:HB3	1.97	0.46
1:W:332:GLY:O	1:W:446:VAL:N	2.47	0.46
1:P:202:ALA:N	1:P:265:TYR:O	2.46	0.46
4:D:372:ARG:HH22	4:D:480:TYR:HA	1.80	0.46
4:D:604:SER:HB3	4:D:629:ILE:HA	1.97	0.46
5:E:116:ALA:HB3	5:E:131:TYR:HB2	1.97	0.46
1:M:41:PHE:CD1	1:M:310:GLU:HG3	2.51	0.46
1:Q:266:SER:O	1:Q:347:LYS:N	2.47	0.46
1:R:41:PHE:CD1	1:R:310:GLU:HG3	2.51	0.46
1:S:41:PHE:CD1	1:S:310:GLU:HG3	2.51	0.46
1:S:282:LEU:HD11	1:S:442:ASN:HA	1.96	0.46
1:U:39:GLN:NE2	1:U:310:GLU:OE2	2.48	0.46
1:W:332:GLY:N	1:W:446:VAL:O	2.49	0.46
1:I:362:TYR:HB3	1:I:381:LYS:HB3	1.97	0.46
1:J:41:PHE:CD1	1:J:310:GLU:HG3	2.51	0.46
2:A:1016:VAL:HG21	2:A:1081:PHE:HE2	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:280:LEU:HD12	4:D:283:LEU:HD12	1.98	0.46
8:j:1:NAG:H4	8:j:2:NAG:H2	1.61	0.46
1:O:196:TYR:HB2	1:O:271:LYS:HB3	1.97	0.46
1:Q:380:ASN:HD22	1:R:215:ASN:ND2	2.13	0.46
1:P:64:ARG:H	1:H:470:LYS:HZ3	1.62	0.46
1:H:92:ILE:HB	1:H:96:LEU:HB3	1.96	0.46
1:M:372:GLU:N	1:N:223:THR:O	2.48	0.46
1:S:147:LEU:HG	1:S:148:SER:H	1.80	0.46
1:X:28:SER:HB2	1:X:43:SER:HB3	1.98	0.46
1:P:147:LEU:HG	1:P:148:SER:H	1.80	0.46
1:K:30:TRP:CH2	1:K:42:ARG:HD2	2.50	0.46
1:K:40:MET:SD	1:K:65:ARG:HD3	2.55	0.46
2:A:127:PHE:HB2	2:A:146:TYR:HB2	1.97	0.46
1:N:58:THR:HG21	1:O:452:LEU:HD23	1.97	0.46
1:R:147:LEU:HG	1:R:148:SER:H	1.81	0.46
3:C:40:GLN:HG3	3:C:466:ARG:HH12	1.79	0.46
5:E:111:ASP:OD2	5:E:114:SER:OG	2.24	0.46
7:B:655:ILE:HG12	7:B:670:ILE:HG22	1.98	0.46
1:L:470:LYS:HZ3	1:K:64:ARG:H	1.64	0.46
1:M:64:ARG:H	1:N:470:LYS:HZ3	1.63	0.46
1:R:332:GLY:O	1:R:446:VAL:N	2.48	0.46
1:R:332:GLY:N	1:R:446:VAL:O	2.49	0.46
1:T:332:GLY:O	1:T:446:VAL:N	2.48	0.46
1:T:465:ASN:HD21	1:T:468:LEU:HD23	1.81	0.46
1:U:131:LEU:HG	1:U:132:ALA:H	1.80	0.46
1:X:359:CYS:HA	1:X:384:CYS:HA	1.98	0.46
1:L:382:ASP:HB3	1:M:213:ASN:HB2	1.98	0.46
1:O:58:THR:HG21	1:Q:452:LEU:HD23	1.98	0.46
1:O:332:GLY:N	1:O:446:VAL:O	2.49	0.46
1:U:198:GLU:HB3	1:U:269:LYS:HB2	1.98	0.46
7:B:706:LYS:HG2	7:B:707:PRO:HD2	1.98	0.46
1:N:41:PHE:CD1	1:N:310:GLU:HG3	2.51	0.46
1:O:41:PHE:CD1	1:O:310:GLU:HG3	2.51	0.46
1:S:349:LYS:HD2	8:e:1:NAG:HN2	1.81	0.46
1:G:204:LYS:HG2	6:F:376:LYS:HG2	1.98	0.46
2:A:253:ARG:HE	2:A:259:VAL:HG12	1.81	0.46
2:A:799:ILE:HD11	2:A:815:VAL:HB	1.97	0.46
2:A:873:ILE:HA	2:A:874:ASP:HA	1.60	0.46
4:D:203:SER:HA	7:B:433:PHE:HB2	1.97	0.46
7:B:180:CYS:HB2	7:B:218:CYS:HB2	1.81	0.46
1:N:356:ILE:O	1:N:387:ARG:N	2.43	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:147:LEU:HG	1:Q:148:SER:H	1.81	0.45
1:J:260:GLN:HB3	1:J:353:LEU:HB3	1.98	0.45
1:J:301:ASP:OD1	1:K:288:ARG:NH2	2.49	0.45
3:C:497:TRP:HB2	3:C:508:LYS:HD2	1.98	0.45
7:B:345:LEU:HD11	7:B:357:ILE:HD13	1.99	0.45
1:L:366:VAL:HB	1:L:377:ALA:HB3	1.97	0.45
1:M:147:LEU:HG	1:M:148:SER:H	1.81	0.45
1:N:301:ASP:OD1	1:O:288:ARG:NH2	2.49	0.45
1:Q:489:CYS:SG	1:Q:490:HIS:N	2.89	0.45
1:S:264:SER:N	1:S:349:LYS:O	2.35	0.45
1:S:413:ARG:HG2	1:T:438:ALA:HB1	1.98	0.45
1:V:39:GLN:NE2	1:V:310:GLU:OE2	2.49	0.45
1:P:349:LYS:HB2	8:k:1:NAG:H83	1.98	0.45
1:K:366:VAL:O	1:K:377:ALA:N	2.49	0.45
2:A:617:LYS:HE2	2:A:617:LYS:HB3	1.79	0.45
3:C:9:ILE:HD11	3:C:40:GLN:HB3	1.98	0.45
1:N:147:LEU:HG	1:N:148:SER:H	1.81	0.45
1:N:255:LYS:HA	1:N:358:ARG:HA	1.99	0.45
1:O:364:LEU:HD23	1:O:379:PHE:HB2	1.98	0.45
1:Q:41:PHE:CD1	1:Q:310:GLU:HG3	2.51	0.45
1:I:41:PHE:CD1	1:I:310:GLU:HG3	2.51	0.45
1:K:147:LEU:HG	1:K:148:SER:H	1.81	0.45
1:G:152:ASP:HB2	1:G:295:THR:HA	1.98	0.45
2:A:360:PRO:HG3	2:A:636:ALA:HB3	1.98	0.45
2:A:658:ASN:HD22	2:A:659:ALA:H	1.62	0.45
7:B:717:PRO:HD2	7:B:728:ILE:HG13	1.98	0.45
1:L:198:GLU:HB3	1:L:269:LYS:HB2	1.99	0.45
1:Q:360:LEU:N	1:Q:383:ASP:O	2.43	0.45
1:S:270:GLU:O	1:S:343:LYS:N	2.47	0.45
1:H:147:LEU:HG	1:H:148:SER:H	1.80	0.45
1:J:58:THR:HG21	1:K:452:LEU:HD23	1.96	0.45
2:A:363:LEU:HD21	2:A:428:VAL:HG13	1.97	0.45
2:A:465:LEU:HD11	2:A:542:VAL:HB	1.99	0.45
2:A:923:LEU:HD12	2:A:925:LYS:HD3	1.98	0.45
1:N:357:LYS:HD2	9:N:603:NAG:H62	1.98	0.45
1:Q:362:TYR:HB3	1:Q:381:LYS:HB3	1.99	0.45
1:T:357:LYS:HD2	9:T:603:NAG:H62	1.99	0.45
1:X:309:TYR:H	1:X:472:ASN:HD21	1.64	0.45
1:K:350:GLY:O	1:K:393:VAL:N	2.50	0.45
2:A:351:PRO:HG3	2:A:442:LEU:HD22	1.99	0.45
2:A:515:ARG:HG3	2:A:526:ILE:HG22	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:637:MET:HB2	4:D:640:ILE:HG12	1.98	0.45
1:L:364:LEU:HD23	1:L:379:PHE:HB2	1.98	0.45
1:M:260:GLN:HB3	1:M:353:LEU:HB3	1.99	0.45
1:O:366:VAL:HB	1:O:377:ALA:HB3	1.99	0.45
1:V:282:LEU:HD11	1:V:442:ASN:HA	1.98	0.45
4:D:179:LEU:HD21	4:D:186:TYR:HB2	1.98	0.45
4:D:607:GLY:HA3	4:D:624:MET:HG2	1.98	0.45
1:U:332:GLY:N	1:U:446:VAL:O	2.50	0.45
1:U:492:CYS:SG	1:U:493:GLN:N	2.89	0.45
1:I:374:SER:HB3	1:J:221:LYS:H	1.81	0.45
1:I:502:ASP:OD2	1:J:452:LEU:N	2.47	0.45
1:J:344:ALA:HB3	1:J:399:ASN:HB2	1.99	0.45
1:G:147:LEU:HG	1:G:148:SER:H	1.82	0.45
1:G:159:LEU:HD22	6:F:89:GLN:HB2	1.99	0.45
2:A:1090:ASN:OD1	2:A:1095:GLN:HB2	2.16	0.45
3:C:296:LEU:HB3	3:C:406:PRO:HB2	1.99	0.45
4:D:646:LYS:HB2	4:D:649:TYR:HE1	1.81	0.45
6:F:241:GLN:HE22	6:F:344:THR:HG23	1.81	0.45
6:F:333:GLU:HG2	6:F:381:ARG:HG3	1.98	0.45
1:M:255:LYS:HA	1:M:358:ARG:HA	1.98	0.45
1:M:350:GLY:O	1:M:393:VAL:N	2.46	0.45
1:O:147:LEU:HG	1:O:148:SER:H	1.81	0.45
1:T:282:LEU:HD11	1:T:442:ASN:HA	1.99	0.45
1:H:64:ARG:H	1:I:470:LYS:HZ3	1.62	0.45
1:K:332:GLY:N	1:K:446:VAL:O	2.50	0.45
7:B:399:CYS:HA	7:B:420:CYS:HA	1.98	0.45
8:c:1:NAG:H4	8:c:2:NAG:H2	1.59	0.45
8:g:1:NAG:H4	8:g:2:NAG:H2	1.60	0.45
8:o:1:NAG:H4	8:o:2:NAG:H2	1.60	0.45
1:R:349:LYS:HD2	8:d:1:NAG:HN2	1.82	0.45
1:S:224:PRO:HG3	1:S:243:LEU:HD23	1.98	0.45
1:U:147:LEU:HG	1:U:148:SER:H	1.81	0.45
1:U:282:LEU:HD11	1:U:442:ASN:HA	1.98	0.45
1:V:28:SER:HB2	1:V:43:SER:HB3	1.98	0.45
1:W:41:PHE:CD1	1:W:310:GLU:HG3	2.51	0.45
1:P:502:ASP:OD2	1:H:452:LEU:N	2.47	0.45
1:H:41:PHE:CD1	1:H:310:GLU:HG3	2.51	0.45
1:G:28:SER:HB2	1:G:43:SER:HB3	1.99	0.45
1:G:407:LEU:H	1:G:420:LYS:HZ1	1.64	0.45
2:A:25:ILE:HG13	2:A:41:ILE:HG13	1.99	0.45
1:Q:327:SER:HB2	1:Q:453:SER:HB2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:332:GLY:N	1:T:446:VAL:O	2.50	0.45
1:V:489:CYS:SG	1:V:490:HIS:N	2.90	0.45
1:W:364:LEU:HD23	1:W:379:PHE:HD2	1.82	0.45
1:I:218:ILE:HG23	1:I:249:PHE:HB2	1.99	0.45
1:I:332:GLY:N	1:I:446:VAL:O	2.50	0.45
1:K:39:GLN:NE2	1:K:310:GLU:OE2	2.50	0.45
2:A:30:ILE:H	2:A:632:LEU:HD13	1.82	0.45
6:F:191:ALA:HA	6:F:266:VAL:HA	1.99	0.45
7:B:205:ARG:HG3	7:B:361:PHE:C	2.41	0.45
8:Z:1:NAG:H4	8:Z:2:NAG:H2	1.61	0.45
1:Q:349:LYS:HD2	8:c:1:NAG:HN2	1.82	0.44
1:U:256:ASN:OD1	1:U:256:ASN:C	2.60	0.44
1:W:489:CYS:SG	1:W:490:HIS:N	2.88	0.44
2:A:253:ARG:HH22	2:A:257:ASN:ND2	2.13	0.44
2:A:265:VAL:HG13	2:A:329:VAL:HG22	1.98	0.44
5:E:81:GLN:HE22	6:F:162:SER:HB2	1.81	0.44
8:Y:1:NAG:H4	8:Y:2:NAG:H2	1.61	0.44
1:M:347:LYS:HG2	1:M:396:THR:HG23	1.99	0.44
1:M:366:VAL:HB	1:M:377:ALA:HB3	1.99	0.44
1:N:492:CYS:SG	1:N:493:GLN:N	2.91	0.44
1:O:255:LYS:HA	1:O:358:ARG:HA	1.98	0.44
1:T:147:LEU:HG	1:T:148:SER:H	1.82	0.44
1:T:386:LYS:HB3	1:U:209:GLU:HB3	1.98	0.44
1:V:332:GLY:N	1:V:446:VAL:O	2.50	0.44
1:X:96:LEU:HD13	1:X:155:PHE:HE1	1.81	0.44
3:C:191:THR:HB	4:D:357:GLU:HB3	1.99	0.44
7:B:187:ILE:HD11	7:B:232:VAL:HG22	1.99	0.44
1:Q:357:LYS:HD2	9:Q:603:NAG:H62	1.99	0.44
1:W:282:LEU:HD11	1:W:442:ASN:HA	1.99	0.44
1:X:297:THR:HG23	7:B:605:LYS:HE2	2.00	0.44
1:H:489:CYS:SG	1:H:490:HIS:N	2.90	0.44
1:G:352:GLU:O	1:G:391:ARG:N	2.46	0.44
6:F:9:CYS:HB3	6:F:44:CYS:HB3	1.90	0.44
1:L:332:GLY:N	1:L:446:VAL:O	2.50	0.44
1:M:59:ASP:OD1	1:N:456:TYR:OH	2.25	0.44
1:N:347:LYS:HG2	1:N:396:THR:HG23	1.99	0.44
1:U:41:PHE:CD1	1:U:310:GLU:HG3	2.52	0.44
1:V:256:ASN:HB3	9:V:603:NAG:HN2	1.83	0.44
1:W:28:SER:HB2	1:W:43:SER:HB3	1.99	0.44
1:X:492:CYS:SG	1:X:493:GLN:N	2.90	0.44
1:J:489:CYS:SG	1:J:490:HIS:N	2.90	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:347:GLY:O	6:F:218:PHE:HB3	2.17	0.44
3:C:442:PHE:O	3:C:446:VAL:HG22	2.17	0.44
8:a:1:NAG:H4	8:a:2:NAG:H2	1.61	0.44
8:f:1:NAG:H4	8:f:2:NAG:H2	1.61	0.44
1:L:288:ARG:NH2	1:K:301:ASP:OD1	2.50	0.44
1:M:489:CYS:SG	1:M:490:HIS:N	2.89	0.44
1:O:257:GLU:HA	1:O:356:ILE:HA	2.00	0.44
1:R:392:ALA:HB3	1:S:203:PHE:H	1.82	0.44
1:T:421:GLU:HB3	1:U:434:PHE:HD2	1.83	0.44
1:V:96:LEU:HD11	1:V:103:ASP:HB2	1.98	0.44
1:P:359:CYS:HA	1:P:384:CYS:HA	1.99	0.44
1:P:400:LEU:HD12	1:H:195:HIS:HB2	2.00	0.44
2:A:62:LYS:HD3	7:B:128:ILE:HD12	2.00	0.44
2:A:374:GLN:HE21	2:A:382:LEU:HB3	1.83	0.44
2:A:497:THR:HG23	2:A:498:HIS:H	1.82	0.44
2:A:872:VAL:HG12	2:A:879:LYS:HG3	1.99	0.44
4:D:303:TYR:HD1	4:D:424:LEU:HA	1.83	0.44
7:B:667:ASP:OD1	7:B:667:ASP:N	2.51	0.44
1:N:224:PRO:HG3	1:N:243:LEU:HD23	1.98	0.44
1:R:255:LYS:HA	1:R:358:ARG:HA	1.99	0.44
1:S:354:LYS:O	1:S:389:GLU:N	2.45	0.44
1:I:489:CYS:SG	1:I:490:HIS:N	2.90	0.44
1:G:205:SER:O	6:F:375:GLY:N	2.50	0.44
2:A:536:PRO:HG3	2:A:624:PHE:HD1	1.83	0.44
1:S:358:ARG:O	1:S:385:VAL:N	2.42	0.44
1:V:147:LEU:HG	1:V:148:SER:H	1.83	0.44
1:G:211:THR:HB	6:F:369:CYS:HB3	2.00	0.44
3:C:121:LEU:HD11	3:C:296:LEU:HD21	1.99	0.44
4:D:268:GLU:O	4:D:429:LYS:NZ	2.40	0.44
6:F:195:ILE:HA	6:F:262:ILE:HA	1.99	0.44
1:L:492:CYS:SG	1:L:493:GLN:N	2.90	0.44
1:S:360:LEU:N	1:S:383:ASP:O	2.42	0.44
1:T:222:PHE:O	1:T:245:GLY:N	2.51	0.44
1:W:368:LEU:HB2	1:W:375:VAL:HB	2.00	0.44
1:X:256:ASN:OD1	1:X:256:ASN:C	2.60	0.44
1:X:332:GLY:N	1:X:446:VAL:O	2.51	0.44
1:P:41:PHE:CD1	1:P:310:GLU:HG3	2.53	0.44
1:J:332:GLY:N	1:J:446:VAL:O	2.51	0.44
1:G:221:LYS:O	6:F:359:ASN:ND2	2.35	0.44
2:A:855:PHE:HA	2:A:916:THR:HG23	1.99	0.44
6:F:274:ARG:HG3	6:F:278:ILE:HG12	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:380:ASN:HD22	1:M:215:ASN:ND2	2.16	0.44
1:M:96:LEU:HD13	1:M:155:PHE:HE1	1.83	0.44
1:Q:301:ASP:OD1	1:R:288:ARG:NH2	2.50	0.44
1:T:41:PHE:CD1	1:T:310:GLU:HG3	2.53	0.44
1:T:266:SER:O	1:T:347:LYS:N	2.42	0.44
1:U:255:LYS:HA	1:U:358:ARG:HA	1.98	0.44
1:X:318:LEU:HD11	1:X:323:THR:HB	2.00	0.44
1:X:332:GLY:O	1:X:446:VAL:N	2.47	0.44
1:I:301:ASP:OD1	1:J:288:ARG:NH2	2.51	0.44
1:G:489:CYS:SG	1:G:490:HIS:N	2.89	0.44
2:A:660:ASP:OD1	2:A:660:ASP:N	2.50	0.44
4:D:663:MET:HB3	4:D:689:VAL:HG21	2.00	0.44
1:L:211:THR:O	1:K:383:ASP:HA	2.18	0.43
1:N:332:GLY:N	1:N:446:VAL:O	2.51	0.43
1:Q:366:VAL:HB	1:Q:377:ALA:HB3	2.00	0.43
1:S:206:ILE:O	1:S:261:LEU:N	2.44	0.43
1:X:310:GLU:HG2	1:X:313:GLU:H	1.83	0.43
1:H:332:GLY:N	1:H:446:VAL:O	2.50	0.43
1:H:363:HIS:ND1	1:H:380:ASN:OD1	2.45	0.43
1:J:415:TYR:HD2	1:J:440:SER:HB2	1.83	0.43
1:K:96:LEU:HD13	1:K:155:PHE:HE1	1.83	0.43
6:F:349:SER:HA	6:F:365:SER:HA	2.00	0.43
1:L:489:CYS:SG	1:L:490:HIS:N	2.89	0.43
1:M:372:GLU:HB3	1:N:223:THR:HB	2.00	0.43
1:M:492:CYS:SG	1:M:493:GLN:N	2.90	0.43
1:O:218:ILE:HG23	1:O:249:PHE:HB2	2.01	0.43
1:Q:220:LEU:O	1:Q:247:GLY:N	2.45	0.43
1:S:332:GLY:N	1:S:446:VAL:O	2.50	0.43
1:V:41:PHE:CD1	1:V:310:GLU:HG3	2.53	0.43
1:X:498:VAL:HA	1:X:507:CYS:HA	2.00	0.43
1:G:481:ILE:HD13	6:F:43:ILE:HD11	2.00	0.43
2:A:767:SER:HA	2:A:768:TYR:HA	1.70	0.43
3:C:201:SER:HA	3:C:215:SER:HA	2.00	0.43
8:d:1:NAG:H4	8:d:2:NAG:H2	1.59	0.43
1:L:64:ARG:H	1:M:470:LYS:HZ3	1.67	0.43
1:L:452:LEU:HD23	1:K:58:THR:HG21	1.99	0.43
1:Q:332:GLY:N	1:Q:446:VAL:O	2.50	0.43
1:T:40:MET:HB2	1:T:65:ARG:HB3	2.01	0.43
1:P:165:ASP:HA	1:G:130:GLU:HG3	1.99	0.43
1:P:251:PHE:HD1	1:P:362:TYR:HD1	1.67	0.43
1:I:58:THR:HG21	1:J:452:LEU:HD23	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:198:GLU:HB3	1:J:269:LYS:HB2	1.99	0.43
1:G:212:SER:HB3	1:G:255:LYS:HB3	1.99	0.43
2:A:166:PRO:HD3	2:A:199:TRP:CD2	2.54	0.43
2:A:390:LEU:HB3	2:A:435:VAL:HG22	2.00	0.43
2:A:1023:HIS:ND1	2:A:1298:THR:HG21	2.33	0.43
7:B:253:ASP:HB3	7:B:317:HIS:HB3	2.00	0.43
1:M:332:GLY:N	1:M:446:VAL:O	2.51	0.43
1:O:96:LEU:HD13	1:O:155:PHE:HE1	1.84	0.43
1:W:30:TRP:CZ2	1:W:42:ARG:HD2	2.53	0.43
1:P:346:MET:N	1:P:397:SER:O	2.42	0.43
1:G:44:ARG:HG2	1:G:45:SER:H	1.82	0.43
1:G:155:PHE:HD2	1:G:293:VAL:HG21	1.83	0.43
2:A:576:SER:HB3	2:A:577:PRO:HD3	2.01	0.43
4:D:459:PRO:HG3	4:D:526:PRO:HB3	1.99	0.43
1:L:301:ASP:OD1	1:M:288:ARG:NH2	2.52	0.43
1:M:301:ASP:OD1	1:N:288:ARG:NH2	2.52	0.43
1:Q:244:HIS:HB2	1:Q:369:ALA:HB3	2.01	0.43
1:R:244:HIS:HB2	1:R:369:ALA:HB3	2.00	0.43
1:R:489:CYS:SG	1:R:490:HIS:N	2.90	0.43
1:S:421:GLU:HB3	1:T:434:PHE:HD2	1.83	0.43
1:I:152:ASP:HB2	1:I:295:THR:HA	2.01	0.43
2:A:945:ASP:N	2:A:954:SER:O	2.44	0.43
7:B:399:CYS:HB2	7:B:420:CYS:HB3	1.83	0.43
7:B:409:LEU:HD13	7:B:410:PHE:HA	2.01	0.43
1:T:30:TRP:CZ2	1:T:42:ARG:HD2	2.53	0.43
1:T:251:PHE:HD1	1:T:362:TYR:HD1	1.66	0.43
1:T:347:LYS:HG2	1:T:396:THR:HG23	2.00	0.43
1:W:433:ASP:OD1	1:W:434:PHE:N	2.52	0.43
1:H:359:CYS:HA	1:H:384:CYS:HA	2.00	0.43
1:K:198:GLU:HB3	1:K:269:LYS:HB2	2.01	0.43
1:K:492:CYS:SG	1:K:493:GLN:N	2.89	0.43
1:L:215:ASN:HD22	1:K:380:ASN:HD22	1.65	0.43
1:L:350:GLY:O	1:L:393:VAL:N	2.50	0.43
1:M:380:ASN:ND2	1:N:215:ASN:HD22	2.11	0.43
1:O:30:TRP:CZ2	1:O:42:ARG:HD2	2.54	0.43
1:O:366:VAL:O	1:O:377:ALA:N	2.51	0.43
1:S:332:GLY:O	1:S:446:VAL:N	2.48	0.43
1:V:40:MET:HB2	1:V:65:ARG:HB3	2.00	0.43
1:H:344:ALA:HB3	1:H:399:ASN:HB2	2.00	0.43
2:A:120:THR:HG22	2:A:122:ASP:H	1.84	0.43
2:A:1019:PHE:CD1	2:A:1049:LEU:HG	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:170:SER:HB2	4:D:175:ASP:O	2.18	0.43
6:F:493:SER:N	6:F:498:CYS:HB3	2.27	0.43
1:S:382:ASP:HB3	1:T:213:ASN:HB2	2.00	0.43
1:I:350:GLY:O	1:I:393:VAL:N	2.49	0.43
1:L:255:LYS:HA	1:L:358:ARG:HA	2.00	0.43
1:L:347:LYS:HG2	1:L:396:THR:HG23	2.01	0.43
1:L:452:LEU:N	1:K:502:ASP:OD2	2.50	0.43
1:N:489:CYS:SG	1:N:490:HIS:N	2.90	0.43
1:O:380:ASN:ND2	1:Q:215:ASN:HD22	2.15	0.43
1:W:332:GLY:C	1:W:441:ILE:HD11	2.44	0.43
1:P:40:MET:HB2	1:P:65:ARG:HB3	2.00	0.43
3:C:270:LEU:HD11	3:C:282:LEU:HD22	2.01	0.43
4:D:197:ASN:N	4:D:251:LEU:O	2.48	0.43
4:D:268:GLU:H	4:D:429:LYS:NZ	2.17	0.43
1:N:96:LEU:HD13	1:N:155:PHE:HE1	1.84	0.43
1:Q:206:ILE:O	1:Q:261:LEU:N	2.48	0.43
1:R:224:PRO:HG3	1:R:243:LEU:HD23	2.00	0.43
1:S:64:ARG:H	1:T:470:LYS:HZ3	1.66	0.43
1:S:244:HIS:HB2	1:S:369:ALA:HB3	2.01	0.43
1:U:140:ASN:HD22	1:U:141:ILE:N	2.17	0.43
1:W:492:CYS:SG	1:W:493:GLN:N	2.92	0.43
1:H:152:ASP:HB2	1:H:295:THR:HA	2.01	0.43
1:H:468:LEU:O	1:H:472:ASN:HB2	2.19	0.43
1:J:328:SER:O	1:J:451:LYS:N	2.43	0.43
1:G:467:HIS:HB2	6:F:52:ALA:HA	2.01	0.43
2:A:469:TRP:HE1	2:A:473:HIS:HA	1.83	0.43
1:Q:46:ILE:O	1:Q:488:LYS:NZ	2.50	0.42
1:J:502:ASP:OD2	1:K:452:LEU:N	2.51	0.42
1:K:489:CYS:SG	1:K:490:HIS:N	2.89	0.42
1:G:198:GLU:HG3	6:F:382:LYS:HE2	2.01	0.42
1:G:213:ASN:N	6:F:367:ASP:O	2.44	0.42
4:D:503:TRP:CD1	4:D:535:CYS:HB2	2.54	0.42
6:F:515:TRP:HB3	6:F:528:ARG:NE	2.34	0.42
7:B:497:ILE:HB	7:B:498:PRO:HD2	2.01	0.42
1:M:58:THR:HG21	1:N:452:LEU:HD23	2.01	0.42
1:M:502:ASP:OD2	1:N:452:LEU:N	2.48	0.42
1:O:349:LYS:HD2	8:b:1:NAG:HN2	1.84	0.42
1:Q:492:CYS:SG	1:Q:493:GLN:N	2.90	0.42
1:R:152:ASP:HB2	1:R:295:THR:HA	2.02	0.42
1:R:358:ARG:O	1:R:385:VAL:N	2.43	0.42
1:U:413:ARG:HG2	1:V:438:ALA:HB1	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:51:GLN:HA	1:W:505:CYS:HB3	2.02	0.42
1:W:162:ARG:HD3	1:W:164:ARG:HD2	2.01	0.42
1:J:152:ASP:HB2	1:J:295:THR:HA	2.02	0.42
4:D:603:TYR:HA	4:D:628:LYS:HA	2.01	0.42
1:O:364:LEU:N	1:O:379:PHE:O	2.47	0.42
1:S:465:ASN:HD21	1:S:468:LEU:HD23	1.83	0.42
1:U:220:LEU:N	1:U:247:GLY:O	2.37	0.42
1:V:30:TRP:CZ2	1:V:42:ARG:HD2	2.54	0.42
2:A:231:ILE:HB	2:A:342:ILE:HD11	2.01	0.42
2:A:283:MET:HB2	2:A:285:THR:H	1.84	0.42
4:D:184:LEU:H	4:D:264:ASN:HA	1.85	0.42
6:F:50:ASP:OD1	6:F:51:GLN:N	2.52	0.42
7:B:100:GLN:HE21	7:B:125:GLN:HB2	1.84	0.42
1:Q:358:ARG:O	1:Q:385:VAL:N	2.43	0.42
1:S:152:ASP:HB2	1:S:295:THR:HA	2.02	0.42
1:V:260:GLN:HB3	1:V:353:LEU:HB3	2.02	0.42
1:P:489:CYS:SG	1:P:490:HIS:N	2.89	0.42
1:H:327:SER:HB2	1:H:453:SER:HB2	2.02	0.42
1:K:218:ILE:HG23	1:K:249:PHE:HB2	2.00	0.42
1:G:213:ASN:HB3	9:G:604:NAG:HN2	1.84	0.42
2:A:540:LEU:HD23	2:A:561:LEU:HD21	2.02	0.42
2:A:1285:TYR:N	2:A:1286:SER:HA	2.33	0.42
3:C:13:LEU:HD12	3:C:48:PHE:CZ	2.55	0.42
5:E:36:VAL:HG22	5:E:129:LYS:HG2	2.01	0.42
6:F:75:THR:HG22	6:F:286:GLN:HE21	1.85	0.42
6:F:104:ARG:HH11	6:F:106:ILE:HB	1.84	0.42
6:F:250:ASN:HB3	6:F:335:LEU:HD12	2.00	0.42
6:F:300:TYR:CE2	6:F:452:ASN:HB3	2.54	0.42
1:O:152:ASP:HB2	1:O:295:THR:HA	2.01	0.42
1:S:140:ASN:HD22	1:S:141:ILE:N	2.17	0.42
1:T:489:CYS:SG	1:T:490:HIS:N	2.90	0.42
1:P:198:GLU:N	1:P:269:LYS:O	2.48	0.42
1:I:415:TYR:HD2	1:I:440:SER:HB2	1.85	0.42
1:J:30:TRP:CZ2	1:J:42:ARG:HD2	2.54	0.42
1:J:380:ASN:HB2	1:K:215:ASN:HB2	2.01	0.42
1:G:49:PHE:CE2	1:G:484:PHE:HB2	2.55	0.42
6:F:519:SER:HB3	6:F:527:GLU:HB2	2.01	0.42
7:B:122:VAL:HG21	7:B:352:ALA:HB1	2.02	0.42
1:T:433:ASP:OD1	1:T:434:PHE:N	2.53	0.42
1:U:433:ASP:OD1	1:U:434:PHE:N	2.53	0.42
1:I:96:LEU:HD13	1:I:155:PHE:HE1	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:39:GLN:NE2	1:J:310:GLU:OE2	2.53	0.42
1:G:92:ILE:HB	1:G:96:LEU:HB3	2.00	0.42
2:A:132:LYS:HB2	2:A:135:TYR:CE1	2.55	0.42
2:A:768:TYR:HA	2:A:769:PHE:HA	1.78	0.42
1:L:96:LEU:HD13	1:L:155:PHE:HE1	1.84	0.42
1:L:260:GLN:HB3	1:L:353:LEU:HB3	2.02	0.42
1:N:364:LEU:HD23	1:N:379:PHE:HB2	2.02	0.42
1:R:214:PHE:HB3	1:R:253:TYR:HB3	2.02	0.42
1:V:151:PHE:HB2	1:V:294:LEU:HA	2.02	0.42
1:V:224:PRO:HG3	1:V:243:LEU:HD23	2.00	0.42
1:W:359:CYS:HA	1:W:384:CYS:HA	2.02	0.42
1:H:364:LEU:HD23	1:H:379:PHE:HD2	1.84	0.42
2:A:394:THR:HG21	2:A:425:PRO:HD2	2.01	0.42
2:A:825:LEU:HD21	2:A:827:MET:HE3	2.01	0.42
3:C:92:CYS:HB3	3:C:96:SER:OG	2.19	0.42
4:D:266:ASN:HD21	4:D:422:THR:HG21	1.85	0.42
5:E:84:GLY:O	5:E:93:LEU:N	2.38	0.42
7:B:571:TRP:CE2	7:B:587:ARG:HD3	2.55	0.42
1:L:151:PHE:HB2	1:L:294:LEU:HA	2.02	0.42
1:N:264:SER:N	1:N:349:LYS:O	2.38	0.42
1:N:380:ASN:HD22	1:O:215:ASN:ND2	2.16	0.42
1:O:301:ASP:OD1	1:Q:288:ARG:NH2	2.53	0.42
1:S:347:LYS:HG2	1:S:396:THR:HG23	2.00	0.42
1:V:359:CYS:HA	1:V:384:CYS:HA	2.02	0.42
1:P:205:SER:O	1:G:390:GLY:N	2.53	0.42
1:I:468:LEU:O	1:I:472:ASN:HB2	2.20	0.42
1:K:364:LEU:HD23	1:K:379:PHE:HD2	1.85	0.42
1:G:41:PHE:O	1:G:41:PHE:CG	2.73	0.42
2:A:360:PRO:O	2:A:369:TYR:OH	2.22	0.42
4:D:217:SER:O	4:D:231:SER:OG	2.31	0.42
1:L:186:LYS:HB3	1:L:281:HIS:HB3	2.02	0.42
1:L:372:GLU:N	1:M:223:THR:O	2.52	0.42
1:L:383:ASP:HA	1:M:211:THR:O	2.20	0.42
1:N:140:ASN:HD22	1:N:141:ILE:N	2.18	0.42
1:Q:96:LEU:HD13	1:Q:155:PHE:HE1	1.85	0.42
1:R:30:TRP:CZ2	1:R:42:ARG:HD2	2.54	0.42
1:U:30:TRP:CZ2	1:U:42:ARG:HD2	2.55	0.42
1:V:64:ARG:H	1:W:470:LYS:HZ3	1.66	0.42
1:X:196:TYR:HB2	1:X:271:LYS:HB3	2.02	0.42
8:I:1:NAG:H4	8:I:2:NAG:H2	1.61	0.42
1:M:256:ASN:HB3	9:M:603:NAG:HN2	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:30:TRP:CZ2	1:Q:42:ARG:HD2	2.55	0.42
1:Q:151:PHE:HB2	1:Q:294:LEU:HA	2.02	0.42
1:R:327:SER:HB2	1:R:453:SER:HB2	2.02	0.42
1:U:347:LYS:HG2	1:U:396:THR:HG23	2.01	0.42
1:J:96:LEU:HD13	1:J:155:PHE:HE1	1.85	0.42
1:J:468:LEU:O	1:J:472:ASN:HB2	2.20	0.42
1:G:88:THR:OG1	1:G:296:THR:OG1	2.29	0.42
7:B:717:PRO:O	7:B:722:TYR:OH	2.24	0.42
1:L:366:VAL:O	1:L:377:ALA:N	2.52	0.41
1:R:347:LYS:HG2	1:R:396:THR:HG23	2.02	0.41
1:T:492:CYS:SG	1:T:493:GLN:N	2.93	0.41
1:W:41:PHE:HE1	1:W:312:GLY:H	1.68	0.41
1:W:147:LEU:HG	1:W:148:SER:H	1.84	0.41
1:X:135:ALA:HB1	1:X:285:PHE:CE2	2.55	0.41
1:P:364:LEU:HD23	1:P:379:PHE:HD2	1.84	0.41
1:J:327:SER:HB2	1:J:453:SER:HB2	2.01	0.41
1:K:44:ARG:HG2	1:K:45:SER:H	1.85	0.41
1:K:415:TYR:HD2	1:K:440:SER:HB2	1.85	0.41
2:A:1158:ILE:H	2:A:1158:ILE:HG13	1.71	0.41
2:A:1264:ILE:HG22	2:A:1268:ASN:HD21	1.85	0.41
6:F:208:SER:O	6:F:249:LEU:N	2.38	0.41
1:L:152:ASP:HB2	1:L:295:THR:HA	2.01	0.41
1:O:344:ALA:HB3	1:O:399:ASN:HB2	2.02	0.41
1:O:489:CYS:SG	1:O:490:HIS:N	2.90	0.41
1:R:41:PHE:HE1	1:R:312:GLY:H	1.68	0.41
1:H:492:CYS:SG	1:H:493:GLN:N	2.93	0.41
1:K:41:PHE:O	1:K:41:PHE:CG	2.73	0.41
1:G:332:GLY:C	1:G:441:ILE:HD11	2.46	0.41
2:A:1026:GLU:HG2	2:A:1092:TYR:HE1	1.85	0.41
1:L:31:SER:OG	1:L:41:PHE:HB3	2.20	0.41
1:L:215:ASN:HD22	1:K:380:ASN:ND2	2.19	0.41
1:S:28:SER:HB2	1:S:43:SER:HB3	2.02	0.41
1:S:88:THR:OG1	1:S:296:THR:OG1	2.25	0.41
1:V:130:GLU:HG3	1:W:165:ASP:HA	2.03	0.41
1:V:433:ASP:OD1	1:V:434:PHE:N	2.54	0.41
1:P:28:SER:HB2	1:P:43:SER:HB3	2.02	0.41
1:P:58:THR:HG21	1:H:452:LEU:HD23	2.01	0.41
1:P:350:GLY:O	1:P:393:VAL:N	2.53	0.41
1:H:502:ASP:OD2	1:I:452:LEU:N	2.50	0.41
1:J:380:ASN:HD22	1:K:215:ASN:ND2	2.18	0.41
1:K:152:ASP:HB2	1:K:295:THR:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:401:THR:OG1	2:A:402:SER:N	2.54	0.41
2:A:1166:THR:HG23	7:B:718:PHE:CE2	2.54	0.41
4:D:415:GLN:O	4:D:417:ILE:N	2.53	0.41
6:F:182:PHE:CE1	6:F:273:MET:HE1	2.55	0.41
7:B:309:LYS:HG2	7:B:384:GLU:HA	2.02	0.41
7:B:583:ARG:NH2	7:B:609:GLU:OE2	2.40	0.41
1:M:186:LYS:HB3	1:M:281:HIS:HB3	2.03	0.41
1:N:327:SER:HB2	1:N:453:SER:HB2	2.01	0.41
1:Q:199:GLN:HG3	1:Q:268:LYS:HG2	2.02	0.41
1:S:492:CYS:SG	1:S:493:GLN:N	2.93	0.41
1:U:256:ASN:ND2	9:U:603:NAG:O7	2.53	0.41
1:V:140:ASN:HD22	1:V:141:ILE:N	2.18	0.41
1:W:154:GLU:OE1	1:X:162:ARG:NH1	2.54	0.41
1:P:46:ILE:O	1:P:488:LYS:NZ	2.52	0.41
1:P:487:ARG:HD2	1:G:19:HIS:NE2	2.35	0.41
1:H:46:ILE:O	1:H:488:LYS:NZ	2.52	0.41
1:I:59:ASP:OD1	1:J:456:TYR:OH	2.26	0.41
1:I:151:PHE:HB2	1:I:294:LEU:HA	2.02	0.41
1:I:347:LYS:HG2	1:I:396:THR:HG23	2.02	0.41
1:I:492:CYS:SG	1:I:493:GLN:N	2.93	0.41
1:J:140:ASN:HD22	1:J:141:ILE:N	2.19	0.41
1:K:347:LYS:HG2	1:K:396:THR:HG23	2.01	0.41
1:G:217:ALA:O	6:F:363:GLY:HA3	2.20	0.41
2:A:501:TYR:CE2	2:A:513:GLY:HA3	2.56	0.41
4:D:187:THR:HG22	4:D:189:GLN:H	1.84	0.41
4:D:274:GLU:HB3	4:D:275:PRO:HD3	2.03	0.41
7:B:60:PHE:HD2	7:B:303:ILE:HD13	1.86	0.41
1:L:41:PHE:O	1:L:41:PHE:CG	2.73	0.41
1:M:30:TRP:CZ2	1:M:42:ARG:HD2	2.55	0.41
1:M:46:ILE:O	1:M:488:LYS:NZ	2.51	0.41
1:O:31:SER:OG	1:O:41:PHE:HB3	2.21	0.41
1:R:28:SER:HB2	1:R:43:SER:HB3	2.02	0.41
1:R:199:GLN:HG3	1:R:268:LYS:HG2	2.02	0.41
1:S:30:TRP:CZ2	1:S:42:ARG:HD2	2.55	0.41
1:S:46:ILE:O	1:S:488:LYS:NZ	2.51	0.41
1:U:28:SER:HB2	1:U:43:SER:HB3	2.01	0.41
1:U:489:CYS:SG	1:U:490:HIS:N	2.90	0.41
1:W:198:GLU:HB3	1:W:269:LYS:HB2	2.03	0.41
1:W:260:GLN:HB3	1:W:353:LEU:HB3	2.02	0.41
1:I:364:LEU:HD23	1:I:379:PHE:HD2	1.86	0.41
1:K:51:GLN:HA	1:K:505:CYS:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:214:PHE:CZ	6:F:364:LEU:HD11	2.55	0.41
2:A:1246:ARG:H	2:A:1246:ARG:HD3	1.85	0.41
4:D:516:LYS:NZ	7:B:86:ASP:OD2	2.54	0.41
8:h:1:NAG:H4	8:h:2:NAG:H2	1.61	0.41
1:O:41:PHE:HE1	1:O:312:GLY:H	1.69	0.41
1:O:220:LEU:O	1:O:247:GLY:N	2.52	0.41
1:R:346:MET:N	1:R:397:SER:O	2.43	0.41
1:R:380:ASN:HD22	1:S:215:ASN:ND2	2.18	0.41
1:S:380:ASN:ND2	9:T:604:NAG:H62	2.35	0.41
1:T:41:PHE:HE1	1:T:312:GLY:H	1.69	0.41
1:H:151:PHE:HB2	1:H:294:LEU:HA	2.03	0.41
1:K:31:SER:OG	1:K:41:PHE:HB3	2.20	0.41
1:G:30:TRP:CZ2	1:G:42:ARG:HD2	2.56	0.41
2:A:367:ILE:HD13	2:A:466:TYR:CD2	2.56	0.41
2:A:1180:LEU:HB2	2:A:1181:PRO:HD3	2.03	0.41
5:E:31:TRP:HB2	5:E:55:LEU:HB3	2.03	0.41
1:N:30:TRP:CZ2	1:N:42:ARG:HD2	2.55	0.41
1:O:46:ILE:O	1:O:488:LYS:NZ	2.52	0.41
1:O:206:ILE:O	1:O:261:LEU:N	2.42	0.41
1:Q:41:PHE:HE1	1:Q:312:GLY:H	1.69	0.41
1:Q:366:VAL:O	1:Q:377:ALA:N	2.53	0.41
1:R:31:SER:OG	1:R:41:PHE:HB3	2.21	0.41
1:S:31:SER:OG	1:S:41:PHE:HB3	2.21	0.41
1:S:364:LEU:HD23	1:S:379:PHE:HB2	2.03	0.41
1:U:151:PHE:HB2	1:U:294:LEU:HA	2.03	0.41
1:V:152:ASP:HB2	1:V:295:THR:HA	2.03	0.41
1:X:489:CYS:SG	1:X:490:HIS:N	2.91	0.41
1:P:354:LYS:O	1:P:389:GLU:N	2.46	0.41
1:H:44:ARG:NH2	1:I:474:GLU:OE2	2.54	0.41
1:H:394:ASN:HB2	1:I:201:GLU:HB2	2.02	0.41
1:G:289:ASN:H	6:F:135:GLN:NE2	2.19	0.41
4:D:533:ARG:HA	7:B:38:THR:HB	2.02	0.41
5:E:116:ALA:N	5:E:131:TYR:O	2.54	0.41
7:B:571:TRP:CE3	7:B:587:ARG:HB2	2.55	0.41
8:m:1:NAG:H4	8:m:2:NAG:H2	1.61	0.41
1:M:152:ASP:HB2	1:M:295:THR:HA	2.02	0.41
1:N:186:LYS:HB3	1:N:281:HIS:HB3	2.03	0.41
1:O:64:ARG:H	1:Q:470:LYS:HZ3	1.69	0.41
1:Q:28:SER:HB2	1:Q:43:SER:HB3	2.02	0.41
1:Q:31:SER:OG	1:Q:41:PHE:HB3	2.21	0.41
1:Q:140:ASN:HD22	1:Q:141:ILE:N	2.18	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:346:MET:N	1:Q:397:SER:O	2.45	0.41
1:Q:347:LYS:HG2	1:Q:396:THR:HG23	2.03	0.41
1:R:382:ASP:HB3	1:S:213:ASN:HB2	2.01	0.41
1:S:41:PHE:HE1	1:S:312:GLY:H	1.69	0.41
1:S:305:LEU:HD12	1:S:306:PRO:HD2	2.03	0.41
1:S:489:CYS:SG	1:S:490:HIS:N	2.91	0.41
1:X:140:ASN:HD22	1:X:141:ILE:N	2.18	0.41
1:X:283:GLY:O	1:X:331:LEU:N	2.53	0.41
1:P:30:TRP:CZ2	1:P:42:ARG:HD2	2.56	0.41
1:I:31:SER:OG	1:I:41:PHE:HB3	2.21	0.41
1:J:206:ILE:O	1:J:261:LEU:N	2.52	0.41
2:A:264:ASP:N	2:A:330:ILE:O	2.52	0.41
2:A:492:TYR:CE2	2:A:548:GLY:HA2	2.55	0.41
3:C:342:LEU:HD12	6:F:224:ILE:HD11	2.03	0.41
7:B:495:ARG:HA	7:B:504:ARG:HH21	1.86	0.41
1:L:264:SER:N	1:L:349:LYS:O	2.43	0.41
1:M:31:SER:OG	1:M:41:PHE:HB3	2.21	0.41
1:M:151:PHE:HB2	1:M:294:LEU:HA	2.02	0.41
1:M:224:PRO:HG3	1:M:243:LEU:HD23	2.02	0.41
1:N:270:GLU:O	1:N:343:LYS:N	2.48	0.41
1:O:492:CYS:SG	1:O:493:GLN:N	2.93	0.41
1:Q:224:PRO:HG3	1:Q:243:LEU:HD23	2.02	0.41
1:R:270:GLU:O	1:R:343:LYS:N	2.45	0.41
1:R:415:TYR:HD2	1:R:440:SER:HB2	1.85	0.41
1:T:46:ILE:O	1:T:488:LYS:NZ	2.51	0.41
1:T:152:ASP:HB2	1:T:295:THR:HA	2.02	0.41
1:T:162:ARG:HD3	1:T:164:ARG:HD2	2.02	0.41
1:U:40:MET:HB2	1:U:65:ARG:HB3	2.02	0.41
1:U:152:ASP:HB2	1:U:295:THR:HA	2.02	0.41
1:U:264:SER:N	1:U:349:LYS:O	2.43	0.41
1:V:492:CYS:SG	1:V:493:GLN:N	2.92	0.41
1:W:270:GLU:O	1:W:343:LYS:N	2.51	0.41
1:P:151:PHE:HB2	1:P:294:LEU:HA	2.02	0.41
1:P:270:GLU:O	1:P:343:LYS:N	2.46	0.41
1:H:96:LEU:HD13	1:H:155:PHE:HE1	1.86	0.41
1:H:140:ASN:HD22	1:H:141:ILE:N	2.19	0.41
1:H:349:LYS:HB2	8:I:1:NAG:H83	2.03	0.41
1:I:224:PRO:HG3	1:I:243:LEU:HD23	2.03	0.41
1:I:357:LYS:HD2	9:I:603:NAG:O5	2.21	0.41
1:J:383:ASP:HA	1:K:211:THR:O	2.20	0.41
1:K:364:LEU:N	1:K:379:PHE:O	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:266:SER:N	1:G:347:LYS:O	2.41	0.41
1:G:310:GLU:HG2	1:G:313:GLU:H	1.86	0.41
2:A:125:PHE:HZ	2:A:630:SER:HB2	1.86	0.41
4:D:552:HIS:CB	4:D:556:LEU:HA	2.51	0.41
4:D:604:SER:N	4:D:627:GLN:O	2.38	0.41
4:D:663:MET:HB3	4:D:689:VAL:HG11	2.03	0.41
5:E:82:LEU:HB2	5:E:180:VAL:HG22	2.03	0.41
6:F:37:ASN:HB3	6:F:43:ILE:HG22	2.03	0.41
7:B:95:PRO:HB3	7:B:346:PRO:HB3	2.02	0.41
8:i:1:NAG:H4	8:i:2:NAG:H2	1.60	0.41
1:N:152:ASP:HB2	1:N:295:THR:HA	2.02	0.41
1:O:140:ASN:HD22	1:O:141:ILE:N	2.18	0.41
1:Q:149:THR:HA	1:Q:150:PRO:HD3	1.93	0.41
1:R:96:LEU:HD13	1:R:155:PHE:HE1	1.86	0.41
1:R:140:ASN:HD22	1:R:141:ILE:N	2.19	0.41
1:R:305:LEU:HD12	1:R:306:PRO:HD2	2.03	0.41
1:R:354:LYS:O	1:R:389:GLU:N	2.49	0.41
1:R:372:GLU:N	1:S:223:THR:O	2.54	0.41
1:S:370:PHE:N	1:S:373:ILE:O	2.48	0.41
1:T:140:ASN:HD22	1:T:141:ILE:N	2.18	0.41
1:V:266:SER:O	1:V:347:LYS:N	2.49	0.41
1:W:349:LYS:HB2	8:i:1:NAG:H83	2.03	0.41
1:P:492:CYS:SG	1:P:493:GLN:N	2.92	0.41
1:H:65:ARG:HD2	1:I:467:HIS:CD2	2.56	0.41
1:H:350:GLY:O	1:H:393:VAL:N	2.54	0.41
1:I:30:TRP:CZ2	1:I:42:ARG:HD2	2.56	0.41
1:J:256:ASN:ND2	9:J:603:NAG:O7	2.52	0.41
1:J:350:GLY:O	1:J:393:VAL:N	2.51	0.41
2:A:515:ARG:HH22	2:A:527:ASN:H	1.69	0.41
2:A:958:GLU:HG3	2:A:1347:ILE:HG12	2.03	0.41
2:A:1117:SER:HB2	2:A:1174:PHE:CZ	2.56	0.41
6:F:75:THR:HG22	6:F:286:GLN:NE2	2.36	0.41
6:F:395:GLY:HA3	6:F:416:TRP:NE1	2.35	0.41
6:F:467:CYS:SG	6:F:514:CYS:N	2.94	0.41
1:L:44:ARG:HG2	1:L:45:SER:H	1.85	0.40
1:M:41:PHE:HE1	1:M:312:GLY:H	1.69	0.40
1:N:305:LEU:HD12	1:N:306:PRO:HD2	2.03	0.40
1:N:415:TYR:HD2	1:N:440:SER:HB2	1.87	0.40
1:O:186:LYS:HB3	1:O:281:HIS:HB3	2.02	0.40
1:U:266:SER:O	1:U:347:LYS:N	2.49	0.40
1:W:222:PHE:O	1:W:245:GLY:N	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:433:ASP:OD1	1:P:434:PHE:N	2.54	0.40
1:P:454:PRO:HG2	1:G:60:ALA:H	1.85	0.40
1:I:222:PHE:O	1:I:245:GLY:N	2.54	0.40
1:K:327:SER:HB2	1:K:453:SER:HB2	2.02	0.40
2:A:38:ASN:HA	2:A:84:ILE:HA	2.03	0.40
2:A:265:VAL:HG22	2:A:329:VAL:HG13	2.03	0.40
4:D:267:PRO:HG3	7:B:356:ARG:HB3	2.03	0.40
4:D:313:TYR:HB2	4:D:406:TRP:CH2	2.56	0.40
6:F:487:CYS:C	6:F:489:CYS:H	2.28	0.40
7:B:210:ASP:HB2	7:B:335:SER:HA	2.02	0.40
1:L:270:GLU:O	1:L:343:LYS:N	2.48	0.40
1:M:140:ASN:HD22	1:M:141:ILE:N	2.18	0.40
1:N:151:PHE:HB2	1:N:294:LEU:HA	2.03	0.40
1:R:46:ILE:O	1:R:488:LYS:NZ	2.50	0.40
1:T:364:LEU:HD23	1:T:379:PHE:HD2	1.86	0.40
1:V:413:ARG:HG2	1:W:438:ALA:HB1	2.02	0.40
1:X:305:LEU:HD12	1:X:306:PRO:HD2	2.02	0.40
1:I:140:ASN:HD22	1:I:141:ILE:N	2.18	0.40
1:I:344:ALA:HB3	1:I:399:ASN:HB2	2.03	0.40
1:G:309:TYR:N	1:G:472:ASN:HD21	2.15	0.40
1:G:498:VAL:HA	1:G:507:CYS:HA	2.03	0.40
2:A:643:ALA:HA	2:A:653:PHE:HE1	1.85	0.40
2:A:1313:ILE:O	2:A:1326:TYR:N	2.44	0.40
6:F:530:ARG:HB2	6:F:548:LYS:HB2	2.02	0.40
7:B:409:LEU:HD22	7:B:410:PHE:HD1	1.86	0.40
1:L:65:ARG:HB2	1:M:467:HIS:ND1	2.36	0.40
1:M:413:ARG:NH1	1:N:282:LEU:HG	2.37	0.40
1:O:354:LYS:O	1:O:389:GLU:N	2.48	0.40
1:T:224:PRO:HG3	1:T:243:LEU:HD23	2.02	0.40
1:V:41:PHE:HE1	1:V:312:GLY:H	1.69	0.40
1:H:30:TRP:CZ2	1:H:42:ARG:HD2	2.57	0.40
1:H:31:SER:OG	1:H:41:PHE:HB3	2.21	0.40
1:I:46:ILE:O	1:I:488:LYS:NZ	2.52	0.40
1:J:28:SER:HB2	1:J:43:SER:HB3	2.03	0.40
1:G:44:ARG:NH2	1:G:59:ASP:OD2	2.54	0.40
2:A:510:ILE:H	2:A:510:ILE:HG13	1.62	0.40
7:B:379:TYR:HA	7:B:440:SER:HA	2.02	0.40
1:L:327:SER:HB2	1:L:453:SER:HB2	2.02	0.40
1:N:266:SER:O	1:N:347:LYS:N	2.51	0.40
1:N:383:ASP:HA	1:O:211:THR:O	2.22	0.40
1:O:266:SER:O	1:O:347:LYS:N	2.53	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:152:ASP:HB2	1:Q:295:THR:HA	2.02	0.40
1:V:347:LYS:HG2	1:V:396:THR:HG23	2.04	0.40
1:W:305:LEU:HD12	1:W:306:PRO:HD2	2.03	0.40
1:P:41:PHE:O	1:P:41:PHE:CG	2.74	0.40
1:P:152:ASP:HB2	1:P:295:THR:HA	2.02	0.40
1:J:31:SER:OG	1:J:41:PHE:HB3	2.21	0.40
1:J:41:PHE:HE1	1:J:312:GLY:H	1.69	0.40
1:G:92:ILE:HG13	1:G:96:LEU:H	1.86	0.40
2:A:479:GLY:H	2:A:530:VAL:HG23	1.86	0.40
2:A:1284:PHE:HB3	2:A:1285:TYR:HA	2.03	0.40
3:C:92:CYS:O	3:C:96:SER:OG	2.39	0.40
3:C:506:ARG:NH2	3:C:535:ASP:O	2.50	0.40
4:D:57:GLN:HE22	4:D:458:ARG:HB2	1.87	0.40
6:F:489:CYS:HB3	6:F:491:LEU:H	1.85	0.40
1:L:415:TYR:HD2	1:L:440:SER:HB2	1.86	0.40
1:M:327:SER:HB2	1:M:453:SER:HB2	2.03	0.40
1:O:151:PHE:HB2	1:O:294:LEU:HA	2.02	0.40
1:O:327:SER:HB2	1:O:453:SER:HB2	2.03	0.40
1:R:492:CYS:SG	1:R:493:GLN:N	2.91	0.40
1:S:327:SER:HB2	1:S:453:SER:HB2	2.03	0.40
1:T:413:ARG:HG2	1:U:438:ALA:HB1	2.03	0.40
1:U:305:LEU:HD12	1:U:306:PRO:HD2	2.03	0.40
1:G:31:SER:OG	1:G:41:PHE:HB3	2.21	0.40
1:G:210:LYS:HA	6:F:370:LYS:HA	2.04	0.40
2:A:33:VAL:O	2:A:123:ASN:ND2	2.50	0.40
2:A:241:LYS:HG3	2:A:441:ASP:HB3	2.02	0.40
2:A:433:PHE:HD2	2:A:435:VAL:HG23	1.86	0.40
3:C:333:GLY:N	3:C:340:VAL:O	2.52	0.40
5:E:19:LYS:N	5:E:107:VAL:O	2.46	0.40
7:B:197:PHE:HD1	7:B:204:PRO:HB3	1.85	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	G	493/538 (92%)	455 (92%)	38 (8%)	0	100	100
1	H	493/538 (92%)	461 (94%)	32 (6%)	0	100	100
1	I	493/538 (92%)	457 (93%)	36 (7%)	0	100	100
1	J	493/538 (92%)	457 (93%)	36 (7%)	0	100	100
1	K	493/538 (92%)	458 (93%)	35 (7%)	0	100	100
1	L	493/538 (92%)	457 (93%)	36 (7%)	0	100	100
1	M	493/538 (92%)	457 (93%)	36 (7%)	0	100	100
1	N	493/538 (92%)	458 (93%)	35 (7%)	0	100	100
1	O	493/538 (92%)	459 (93%)	34 (7%)	0	100	100
1	P	493/538 (92%)	462 (94%)	31 (6%)	0	100	100
1	Q	493/538 (92%)	458 (93%)	35 (7%)	0	100	100
1	R	493/538 (92%)	458 (93%)	35 (7%)	0	100	100
1	S	493/538 (92%)	459 (93%)	34 (7%)	0	100	100
1	T	493/538 (92%)	461 (94%)	32 (6%)	0	100	100
1	U	493/538 (92%)	460 (93%)	33 (7%)	0	100	100
1	V	493/538 (92%)	460 (93%)	33 (7%)	0	100	100
1	W	493/538 (92%)	458 (93%)	35 (7%)	0	100	100
1	X	493/538 (92%)	457 (93%)	36 (7%)	0	100	100
2	A	1201/1580 (76%)	1136 (95%)	65 (5%)	0	100	100
3	C	501/537 (93%)	481 (96%)	20 (4%)	0	100	100
4	D	648/821 (79%)	603 (93%)	45 (7%)	0	100	100
5	E	161/182 (88%)	160 (99%)	1 (1%)	0	100	100
6	F	492/554 (89%)	472 (96%)	20 (4%)	0	100	100
7	B	668/913 (73%)	642 (96%)	25 (4%)	1 (0%)	48	83
All	All	12545/14271 (88%)	11746 (94%)	798 (6%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	B	204	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	G	382/477 (80%)	375 (98%)	7 (2%)	51	67
1	H	385/477 (81%)	380 (99%)	5 (1%)	61	73
1	I	385/477 (81%)	379 (98%)	6 (2%)	55	69
1	J	385/477 (81%)	380 (99%)	5 (1%)	61	73
1	K	385/477 (81%)	379 (98%)	6 (2%)	55	69
1	L	385/477 (81%)	379 (98%)	6 (2%)	55	69
1	M	385/477 (81%)	378 (98%)	7 (2%)	51	67
1	N	385/477 (81%)	380 (99%)	5 (1%)	61	73
1	O	385/477 (81%)	379 (98%)	6 (2%)	55	69
1	P	385/477 (81%)	379 (98%)	6 (2%)	55	69
1	Q	385/477 (81%)	379 (98%)	6 (2%)	55	69
1	R	385/477 (81%)	379 (98%)	6 (2%)	55	69
1	S	385/477 (81%)	379 (98%)	6 (2%)	55	69
1	T	385/477 (81%)	379 (98%)	6 (2%)	55	69
1	U	385/477 (81%)	379 (98%)	6 (2%)	55	69
1	V	385/477 (81%)	380 (99%)	5 (1%)	61	73
1	W	385/477 (81%)	379 (98%)	6 (2%)	55	69
1	X	385/477 (81%)	379 (98%)	6 (2%)	55	69
2	A	1030/1403 (73%)	1017 (99%)	13 (1%)	61	73
3	C	357/473 (76%)	357 (100%)	0	100	100
4	D	411/714 (58%)	411 (100%)	0	100	100
5	E	131/149 (88%)	131 (100%)	0	100	100
6	F	363/466 (78%)	361 (99%)	2 (1%)	78	82
7	B	522/810 (64%)	515 (99%)	7 (1%)	61	73
All	All	9741/12601 (77%)	9613 (99%)	128 (1%)	59	73

All (128) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	92	ILE
1	L	153	ASN
1	L	256	ASN
1	L	318	LEU
1	L	458	LEU
1	L	509	CYS
1	M	92	ILE
1	M	153	ASN
1	M	218	ILE
1	M	256	ASN
1	M	318	LEU
1	M	458	LEU
1	M	509	CYS
1	N	92	ILE
1	N	153	ASN
1	N	318	LEU
1	N	458	LEU
1	N	509	CYS
1	O	92	ILE
1	O	153	ASN
1	O	256	ASN
1	O	318	LEU
1	O	458	LEU
1	O	509	CYS
1	Q	92	ILE
1	Q	153	ASN
1	Q	218	ILE
1	Q	318	LEU
1	Q	458	LEU
1	Q	509	CYS
1	R	92	ILE
1	R	153	ASN
1	R	218	ILE
1	R	318	LEU
1	R	458	LEU
1	R	509	CYS
1	S	92	ILE
1	S	153	ASN
1	S	218	ILE
1	S	318	LEU
1	S	458	LEU
1	S	509	CYS
1	T	92	ILE

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Mol	Chain	Res	Type
1	T	153	ASN
1	T	218	ILE
1	T	318	LEU
1	T	458	LEU
1	T	509	CYS
1	U	92	ILE
1	U	153	ASN
1	U	256	ASN
1	U	318	LEU
1	U	458	LEU
1	U	509	CYS
1	V	92	ILE
1	V	153	ASN
1	V	256	ASN
1	V	318	LEU
1	V	458	LEU
1	W	92	ILE
1	W	153	ASN
1	W	256	ASN
1	W	318	LEU
1	W	458	LEU
1	W	509	CYS
1	X	92	ILE
1	X	153	ASN
1	X	256	ASN
1	X	318	LEU
1	X	458	LEU
1	X	509	CYS
1	P	92	ILE
1	P	153	ASN
1	P	218	ILE
1	P	256	ASN
1	P	318	LEU
1	P	458	LEU
1	H	92	ILE
1	H	153	ASN
1	H	256	ASN
1	H	318	LEU
1	H	458	LEU
1	I	92	ILE
1	I	153	ASN
1	I	256	ASN

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Mol	Chain	Res	Type
1	I	318	LEU
1	I	458	LEU
1	I	509	CYS
1	J	92	ILE
1	J	153	ASN
1	J	256	ASN
1	J	318	LEU
1	J	458	LEU
1	K	92	ILE
1	K	153	ASN
1	K	256	ASN
1	K	318	LEU
1	K	458	LEU
1	K	509	CYS
1	G	92	ILE
1	G	153	ASN
1	G	185	THR
1	G	218	ILE
1	G	256	ASN
1	G	318	LEU
1	G	458	LEU
2	A	149	ASN
2	A	375	VAL
2	A	404	LEU
2	A	497	THR
2	A	510	ILE
2	A	528	ILE
2	A	535	VAL
2	A	658	ASN
2	A	841	LEU
2	A	873	ILE
2	A	1000	LEU
2	A	1068	VAL
2	A	1361	VAL
6	F	92	LEU
6	F	489	CYS
7	B	128	ILE
7	B	494	VAL
7	B	511	LEU
7	B	623	CYS
7	B	673	LEU
7	B	713	LEU

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Mol	Chain	Res	Type
7	B	714	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (262) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	53	ASN
1	L	82	ASN
1	L	99	ASN
1	L	140	ASN
1	L	157	ASN
1	L	161	ASN
1	L	281	HIS
1	L	465	ASN
1	L	482	ASN
1	L	494	ASN
1	M	53	ASN
1	M	82	ASN
1	M	99	ASN
1	M	140	ASN
1	M	157	ASN
1	M	161	ASN
1	M	281	HIS
1	M	380	ASN
1	M	465	ASN
1	M	482	ASN
1	M	494	ASN
1	N	53	ASN
1	N	82	ASN
1	N	99	ASN
1	N	140	ASN
1	N	157	ASN
1	N	161	ASN
1	N	281	HIS
1	N	324	HIS
1	N	465	ASN
1	N	482	ASN
1	N	494	ASN
1	O	53	ASN
1	O	82	ASN
1	O	99	ASN
1	O	140	ASN
1	O	157	ASN

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Mol	Chain	Res	Type
1	O	161	ASN
1	O	281	HIS
1	O	465	ASN
1	O	482	ASN
1	O	494	ASN
1	Q	53	ASN
1	Q	82	ASN
1	Q	99	ASN
1	Q	140	ASN
1	Q	157	ASN
1	Q	161	ASN
1	Q	281	HIS
1	Q	363	HIS
1	Q	380	ASN
1	Q	399	ASN
1	Q	465	ASN
1	Q	482	ASN
1	Q	494	ASN
1	R	53	ASN
1	R	82	ASN
1	R	99	ASN
1	R	140	ASN
1	R	157	ASN
1	R	161	ASN
1	R	465	ASN
1	R	482	ASN
1	R	494	ASN
1	S	53	ASN
1	S	82	ASN
1	S	99	ASN
1	S	102	ASN
1	S	140	ASN
1	S	157	ASN
1	S	161	ASN
1	S	399	ASN
1	S	465	ASN
1	S	482	ASN
1	S	494	ASN
1	T	53	ASN
1	T	82	ASN
1	T	99	ASN
1	T	102	ASN

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Mol	Chain	Res	Type
1	T	140	ASN
1	T	157	ASN
1	T	161	ASN
1	T	167	ASN
1	T	281	HIS
1	T	465	ASN
1	T	482	ASN
1	T	494	ASN
1	U	53	ASN
1	U	82	ASN
1	U	99	ASN
1	U	102	ASN
1	U	140	ASN
1	U	157	ASN
1	U	161	ASN
1	U	167	ASN
1	U	199	GLN
1	U	281	HIS
1	U	465	ASN
1	U	482	ASN
1	U	494	ASN
1	V	53	ASN
1	V	82	ASN
1	V	99	ASN
1	V	102	ASN
1	V	140	ASN
1	V	157	ASN
1	V	161	ASN
1	V	167	ASN
1	V	199	GLN
1	V	281	HIS
1	V	465	ASN
1	V	482	ASN
1	V	494	ASN
1	W	53	ASN
1	W	82	ASN
1	W	99	ASN
1	W	102	ASN
1	W	140	ASN
1	W	157	ASN
1	W	161	ASN
1	W	167	ASN

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Mol	Chain	Res	Type
1	W	281	HIS
1	W	324	HIS
1	W	465	ASN
1	W	482	ASN
1	W	494	ASN
1	X	39	GLN
1	X	53	ASN
1	X	82	ASN
1	X	85	GLN
1	X	99	ASN
1	X	102	ASN
1	X	140	ASN
1	X	157	ASN
1	X	161	ASN
1	X	167	ASN
1	X	213	ASN
1	X	324	HIS
1	X	465	ASN
1	X	467	HIS
1	X	482	ASN
1	X	494	ASN
1	P	53	ASN
1	P	82	ASN
1	P	99	ASN
1	P	140	ASN
1	P	157	ASN
1	P	161	ASN
1	P	199	GLN
1	P	465	ASN
1	P	467	HIS
1	P	482	ASN
1	P	494	ASN
1	H	53	ASN
1	H	82	ASN
1	H	99	ASN
1	H	140	ASN
1	H	157	ASN
1	H	161	ASN
1	H	167	ASN
1	H	281	HIS
1	H	465	ASN
1	H	482	ASN

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Mol	Chain	Res	Type
1	H	494	ASN
1	I	53	ASN
1	I	82	ASN
1	I	99	ASN
1	I	140	ASN
1	I	157	ASN
1	I	161	ASN
1	I	281	HIS
1	I	465	ASN
1	I	482	ASN
1	I	494	ASN
1	J	53	ASN
1	J	82	ASN
1	J	99	ASN
1	J	140	ASN
1	J	157	ASN
1	J	161	ASN
1	J	281	HIS
1	J	324	HIS
1	J	465	ASN
1	J	482	ASN
1	J	494	ASN
1	K	53	ASN
1	K	82	ASN
1	K	99	ASN
1	K	140	ASN
1	K	157	ASN
1	K	161	ASN
1	K	281	HIS
1	K	363	HIS
1	K	465	ASN
1	K	482	ASN
1	K	494	ASN
1	G	39	GLN
1	G	53	ASN
1	G	82	ASN
1	G	102	ASN
1	G	140	ASN
1	G	157	ASN
1	G	161	ASN
1	G	281	HIS
1	G	324	HIS

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Mol	Chain	Res	Type
1	G	399	ASN
1	G	465	ASN
1	G	467	HIS
1	G	472	ASN
1	G	482	ASN
1	G	494	ASN
2	A	149	ASN
2	A	236	ASN
2	A	257	ASN
2	A	294	ASN
2	A	320	ASN
2	A	374	GLN
2	A	658	ASN
2	A	785	GLN
2	A	1002	HIS
2	A	1029	ASN
2	A	1061	ASN
2	A	1090	ASN
2	A	1112	GLN
2	A	1204	GLN
2	A	1268	ASN
2	A	1278	GLN
2	A	1288	GLN
2	A	1319	HIS
3	C	126	ASN
3	C	249	HIS
3	C	260	HIS
3	C	405	ASN
3	C	450	HIS
3	C	457	ASN
4	D	157	ASN
4	D	266	ASN
4	D	282	HIS
4	D	643	HIS
5	E	21	ASN
5	E	46	GLN
5	E	81	GLN
5	E	104	HIS
5	E	175	HIS
6	F	71	GLN
6	F	120	GLN
6	F	135	GLN

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Mol	Chain	Res	Type
6	F	241	GLN
6	F	250	ASN
6	F	270	HIS
6	F	286	GLN
6	F	305	ASN
6	F	435	HIS
6	F	550	GLN
6	F	552	GLN
7	B	26	HIS
7	B	44	GLN
7	B	57	GLN
7	B	263	HIS
7	B	304	GLN
7	B	333	HIS
7	B	364	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 ⓘ

38 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	$\# Z > 2$
8	NAG	Y	1	8,1	14,14,15	0.57	0	17,19,21	0.91	1 (5%)
8	NAG	Y	2	8	14,14,15	0.59	0	17,19,21	0.53	0
8	NAG	Z	1	8,1	14,14,15	0.56	0	17,19,21	0.92	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	NAG	Z	2	8	14,14,15	0.59	1 (7%)	17,19,21	0.54	0
8	NAG	a	1	8,1	14,14,15	0.54	0	17,19,21	0.91	1 (5%)
8	NAG	a	2	8	14,14,15	0.60	1 (7%)	17,19,21	0.55	0
8	NAG	b	1	8,1	14,14,15	0.64	0	17,19,21	0.96	1 (5%)
8	NAG	b	2	8	14,14,15	0.60	1 (7%)	17,19,21	0.54	0
8	NAG	c	1	8,1	14,14,15	0.63	0	17,19,21	0.98	1 (5%)
8	NAG	c	2	8	14,14,15	0.58	0	17,19,21	0.54	0
8	NAG	d	1	8,1	14,14,15	0.64	0	17,19,21	0.96	1 (5%)
8	NAG	d	2	8	14,14,15	0.57	0	17,19,21	0.55	0
8	NAG	e	1	8,1	14,14,15	0.64	0	17,19,21	0.95	1 (5%)
8	NAG	e	2	8	14,14,15	0.60	1 (7%)	17,19,21	0.55	0
8	NAG	f	1	8,1	14,14,15	0.59	0	17,19,21	0.92	1 (5%)
8	NAG	f	2	8	14,14,15	0.59	0	17,19,21	0.55	0
8	NAG	g	1	8,1	14,14,15	0.58	0	17,19,21	0.91	1 (5%)
8	NAG	g	2	8	14,14,15	0.58	0	17,19,21	0.55	0
8	NAG	h	1	8,1	14,14,15	0.58	0	17,19,21	0.92	1 (5%)
8	NAG	h	2	8	14,14,15	0.57	0	17,19,21	0.55	0
8	NAG	i	1	8,1	14,14,15	0.57	0	17,19,21	0.91	1 (5%)
8	NAG	i	2	8	14,14,15	0.58	0	17,19,21	0.54	0
8	NAG	j	1	8,1	14,14,15	0.56	0	17,19,21	0.90	1 (5%)
8	NAG	j	2	8	14,14,15	0.55	0	17,19,21	0.55	0
8	NAG	k	1	8,1	14,14,15	0.58	0	17,19,21	0.93	1 (5%)
8	NAG	k	2	8	14,14,15	0.59	0	17,19,21	0.54	0
8	NAG	l	1	8,1	14,14,15	0.58	0	17,19,21	0.90	1 (5%)
8	NAG	l	2	8	14,14,15	0.60	1 (7%)	17,19,21	0.54	0
8	NAG	m	1	8,1	14,14,15	0.56	0	17,19,21	0.91	1 (5%)
8	NAG	m	2	8	14,14,15	0.60	1 (7%)	17,19,21	0.54	0
8	NAG	n	1	8,1	14,14,15	0.55	0	17,19,21	0.91	1 (5%)
8	NAG	n	2	8	14,14,15	0.59	0	17,19,21	0.54	0
8	NAG	o	1	8,1	14,14,15	0.56	0	17,19,21	0.91	1 (5%)
8	NAG	o	2	8	14,14,15	0.58	0	17,19,21	0.56	0
8	NAG	p	1	8,1	14,14,15	0.78	1 (7%)	17,19,21	1.06	1 (5%)
8	NAG	p	2	8	14,14,15	0.64	1 (7%)	17,19,21	0.53	0
8	NAG	q	1	8,3	14,14,15	0.55	0	17,19,21	1.41	2 (11%)
8	NAG	q	2	8	14,14,15	0.29	0	17,19,21	0.37	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
8	NAG	Y	1	8,1	-	4/6/23/26	0/1/1/1
8	NAG	Y	2	8	-	2/6/23/26	0/1/1/1
8	NAG	Z	1	8,1	-	4/6/23/26	0/1/1/1
8	NAG	Z	2	8	-	2/6/23/26	0/1/1/1
8	NAG	a	1	8,1	-	4/6/23/26	0/1/1/1
8	NAG	a	2	8	-	2/6/23/26	0/1/1/1
8	NAG	b	1	8,1	-	4/6/23/26	0/1/1/1
8	NAG	b	2	8	-	2/6/23/26	0/1/1/1
8	NAG	c	1	8,1	-	4/6/23/26	0/1/1/1
8	NAG	c	2	8	-	2/6/23/26	0/1/1/1
8	NAG	d	1	8,1	-	4/6/23/26	0/1/1/1
8	NAG	d	2	8	-	2/6/23/26	0/1/1/1
8	NAG	e	1	8,1	-	4/6/23/26	0/1/1/1
8	NAG	e	2	8	-	2/6/23/26	0/1/1/1
8	NAG	f	1	8,1	-	4/6/23/26	0/1/1/1
8	NAG	f	2	8	-	2/6/23/26	0/1/1/1
8	NAG	g	1	8,1	-	4/6/23/26	0/1/1/1
8	NAG	g	2	8	-	2/6/23/26	0/1/1/1
8	NAG	h	1	8,1	-	4/6/23/26	0/1/1/1
8	NAG	h	2	8	-	2/6/23/26	0/1/1/1
8	NAG	i	1	8,1	-	4/6/23/26	0/1/1/1
8	NAG	i	2	8	-	2/6/23/26	0/1/1/1
8	NAG	j	1	8,1	-	4/6/23/26	0/1/1/1
8	NAG	j	2	8	-	2/6/23/26	0/1/1/1
8	NAG	k	1	8,1	-	4/6/23/26	0/1/1/1
8	NAG	k	2	8	-	2/6/23/26	0/1/1/1
8	NAG	l	1	8,1	-	4/6/23/26	0/1/1/1
8	NAG	l	2	8	-	2/6/23/26	0/1/1/1
8	NAG	m	1	8,1	-	4/6/23/26	0/1/1/1
8	NAG	m	2	8	-	2/6/23/26	0/1/1/1
8	NAG	n	1	8,1	-	4/6/23/26	0/1/1/1
8	NAG	n	2	8	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	NAG	o	1	8,1	-	4/6/23/26	0/1/1/1
8	NAG	o	2	8	-	2/6/23/26	0/1/1/1
8	NAG	p	1	8,1	-	4/6/23/26	0/1/1/1
8	NAG	p	2	8	-	2/6/23/26	0/1/1/1
8	NAG	q	1	8,3	-	6/6/23/26	0/1/1/1
8	NAG	q	2	8	-	2/6/23/26	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	p	1	NAG	C1-C2	2.21	1.55	1.52
8	p	2	NAG	C1-C2	2.18	1.55	1.52
8	e	2	NAG	C1-C2	2.04	1.55	1.52
8	m	2	NAG	C1-C2	2.04	1.55	1.52
8	b	2	NAG	C1-C2	2.03	1.55	1.52
8	a	2	NAG	C1-C2	2.03	1.55	1.52
8	Z	2	NAG	C1-C2	2.03	1.55	1.52
8	l	2	NAG	C1-C2	2.01	1.55	1.52

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	q	1	NAG	C2-N2-C7	4.62	129.09	122.90
8	p	1	NAG	C1-O5-C5	3.49	116.86	112.19
8	c	1	NAG	C1-O5-C5	3.10	116.34	112.19
8	d	1	NAG	C1-O5-C5	3.05	116.27	112.19
8	b	1	NAG	C1-O5-C5	3.04	116.26	112.19
8	e	1	NAG	C1-O5-C5	3.00	116.21	112.19
8	k	1	NAG	C1-O5-C5	2.95	116.14	112.19
8	h	1	NAG	C1-O5-C5	2.92	116.09	112.19
8	f	1	NAG	C1-O5-C5	2.91	116.08	112.19
8	Z	1	NAG	C1-O5-C5	2.89	116.06	112.19
8	a	1	NAG	C1-O5-C5	2.87	116.03	112.19
8	g	1	NAG	C1-O5-C5	2.87	116.03	112.19
8	n	1	NAG	C1-O5-C5	2.84	116.00	112.19
8	i	1	NAG	C1-O5-C5	2.84	115.99	112.19
8	m	1	NAG	C1-O5-C5	2.83	115.98	112.19
8	o	1	NAG	C1-O5-C5	2.83	115.98	112.19
8	Y	1	NAG	C1-O5-C5	2.83	115.98	112.19
8	j	1	NAG	C1-O5-C5	2.81	115.95	112.19
8	l	1	NAG	C1-O5-C5	2.80	115.94	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	q	1	NAG	C1-C2-N2	2.37	114.17	110.43

There are no chirality outliers.

All (116) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	p	2	NAG	O5-C5-C6-O6
8	q	2	NAG	O5-C5-C6-O6
8	h	1	NAG	O5-C5-C6-O6
8	p	1	NAG	O5-C5-C6-O6
8	e	1	NAG	O5-C5-C6-O6
8	g	1	NAG	O5-C5-C6-O6
8	k	1	NAG	O5-C5-C6-O6
8	c	1	NAG	O5-C5-C6-O6
8	f	1	NAG	O5-C5-C6-O6
8	i	1	NAG	O5-C5-C6-O6
8	l	1	NAG	O5-C5-C6-O6
8	q	2	NAG	C4-C5-C6-O6
8	b	1	NAG	O5-C5-C6-O6
8	d	1	NAG	O5-C5-C6-O6
8	p	2	NAG	C4-C5-C6-O6
8	c	2	NAG	O5-C5-C6-O6
8	e	2	NAG	O5-C5-C6-O6
8	m	2	NAG	O5-C5-C6-O6
8	Y	2	NAG	O5-C5-C6-O6
8	b	2	NAG	O5-C5-C6-O6
8	j	2	NAG	O5-C5-C6-O6
8	n	2	NAG	O5-C5-C6-O6
8	o	2	NAG	O5-C5-C6-O6
8	h	2	NAG	O5-C5-C6-O6
8	o	1	NAG	O5-C5-C6-O6
8	q	1	NAG	C8-C7-N2-C2
8	q	1	NAG	O7-C7-N2-C2
8	Z	2	NAG	O5-C5-C6-O6
8	d	2	NAG	O5-C5-C6-O6
8	g	2	NAG	O5-C5-C6-O6
8	i	2	NAG	O5-C5-C6-O6
8	j	1	NAG	O5-C5-C6-O6
8	k	2	NAG	O5-C5-C6-O6
8	l	2	NAG	O5-C5-C6-O6
8	m	1	NAG	O5-C5-C6-O6
8	n	1	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
8	a	2	NAG	O5-C5-C6-O6
8	f	2	NAG	O5-C5-C6-O6
8	Y	1	NAG	O5-C5-C6-O6
8	a	1	NAG	O5-C5-C6-O6
8	n	2	NAG	C4-C5-C6-O6
8	Z	1	NAG	O5-C5-C6-O6
8	b	2	NAG	C4-C5-C6-O6
8	o	2	NAG	C4-C5-C6-O6
8	Y	2	NAG	C4-C5-C6-O6
8	c	2	NAG	C4-C5-C6-O6
8	e	2	NAG	C4-C5-C6-O6
8	j	2	NAG	C4-C5-C6-O6
8	m	2	NAG	C4-C5-C6-O6
8	q	1	NAG	O5-C5-C6-O6
8	d	2	NAG	C4-C5-C6-O6
8	h	2	NAG	C4-C5-C6-O6
8	g	2	NAG	C4-C5-C6-O6
8	i	2	NAG	C4-C5-C6-O6
8	Z	2	NAG	C4-C5-C6-O6
8	a	2	NAG	C4-C5-C6-O6
8	f	2	NAG	C4-C5-C6-O6
8	k	2	NAG	C4-C5-C6-O6
8	p	1	NAG	C4-C5-C6-O6
8	h	1	NAG	C4-C5-C6-O6
8	l	2	NAG	C4-C5-C6-O6
8	e	1	NAG	C4-C5-C6-O6
8	k	1	NAG	C4-C5-C6-O6
8	g	1	NAG	C4-C5-C6-O6
8	b	1	NAG	C4-C5-C6-O6
8	d	1	NAG	C4-C5-C6-O6
8	f	1	NAG	C4-C5-C6-O6
8	i	1	NAG	C4-C5-C6-O6
8	c	1	NAG	C4-C5-C6-O6
8	l	1	NAG	C4-C5-C6-O6
8	o	1	NAG	C4-C5-C6-O6
8	n	1	NAG	C4-C5-C6-O6
8	m	1	NAG	C4-C5-C6-O6
8	j	1	NAG	C4-C5-C6-O6
8	Y	1	NAG	C4-C5-C6-O6
8	a	1	NAG	C4-C5-C6-O6
8	Z	1	NAG	C4-C5-C6-O6
8	Y	1	NAG	C3-C2-N2-C7

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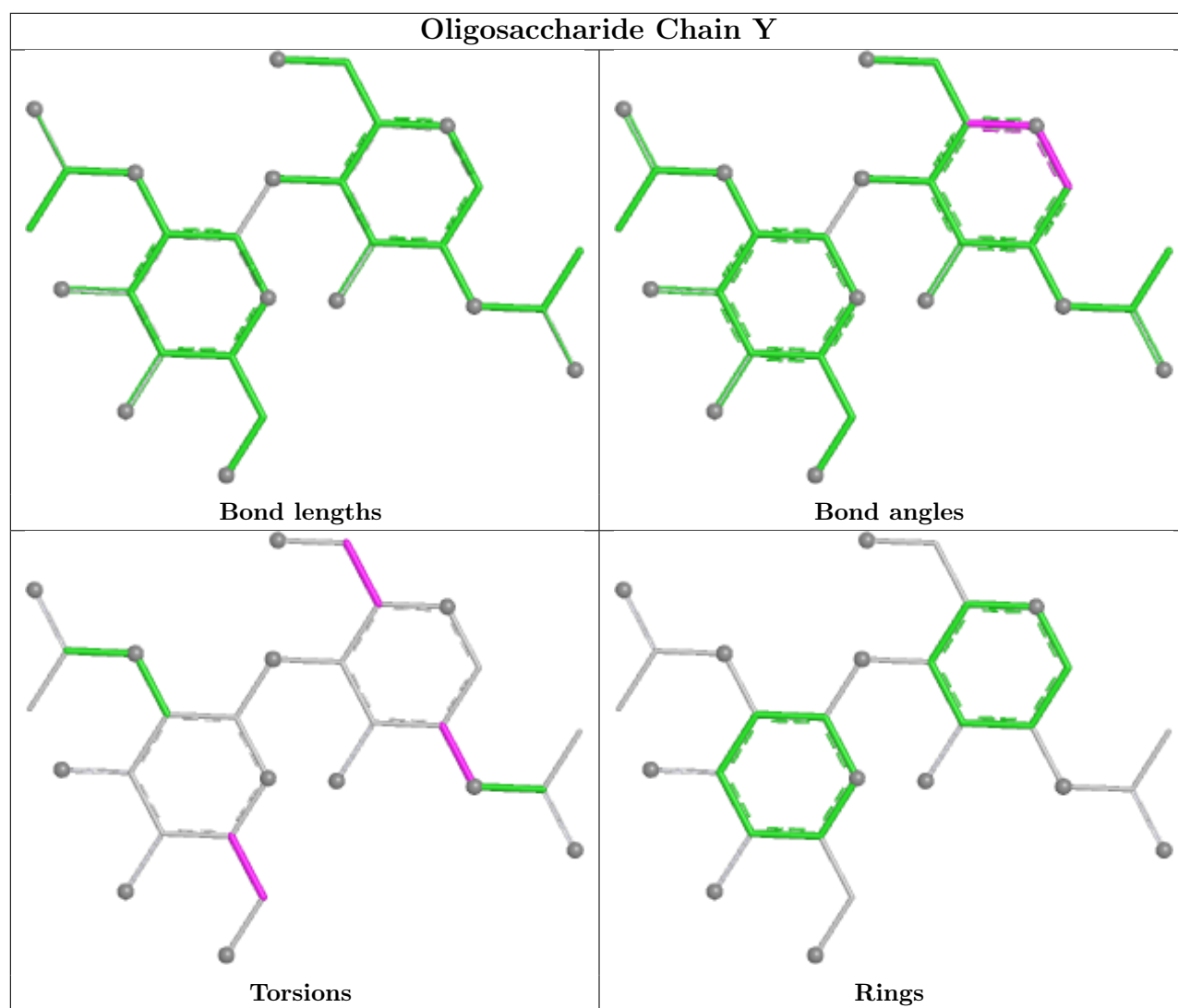
Mol	Chain	Res	Type	Atoms
8	Z	1	NAG	C3-C2-N2-C7
8	a	1	NAG	C3-C2-N2-C7
8	b	1	NAG	C3-C2-N2-C7
8	c	1	NAG	C3-C2-N2-C7
8	d	1	NAG	C3-C2-N2-C7
8	e	1	NAG	C3-C2-N2-C7
8	f	1	NAG	C3-C2-N2-C7
8	g	1	NAG	C3-C2-N2-C7
8	h	1	NAG	C3-C2-N2-C7
8	i	1	NAG	C3-C2-N2-C7
8	j	1	NAG	C3-C2-N2-C7
8	k	1	NAG	C3-C2-N2-C7
8	l	1	NAG	C3-C2-N2-C7
8	m	1	NAG	C3-C2-N2-C7
8	n	1	NAG	C3-C2-N2-C7
8	o	1	NAG	C3-C2-N2-C7
8	p	1	NAG	C3-C2-N2-C7
8	Y	1	NAG	C1-C2-N2-C7
8	Z	1	NAG	C1-C2-N2-C7
8	a	1	NAG	C1-C2-N2-C7
8	b	1	NAG	C1-C2-N2-C7
8	c	1	NAG	C1-C2-N2-C7
8	d	1	NAG	C1-C2-N2-C7
8	e	1	NAG	C1-C2-N2-C7
8	f	1	NAG	C1-C2-N2-C7
8	g	1	NAG	C1-C2-N2-C7
8	h	1	NAG	C1-C2-N2-C7
8	i	1	NAG	C1-C2-N2-C7
8	j	1	NAG	C1-C2-N2-C7
8	k	1	NAG	C1-C2-N2-C7
8	l	1	NAG	C1-C2-N2-C7
8	m	1	NAG	C1-C2-N2-C7
8	n	1	NAG	C1-C2-N2-C7
8	o	1	NAG	C1-C2-N2-C7
8	p	1	NAG	C1-C2-N2-C7
8	q	1	NAG	C1-C2-N2-C7
8	q	1	NAG	C3-C2-N2-C7
8	q	1	NAG	C4-C5-C6-O6

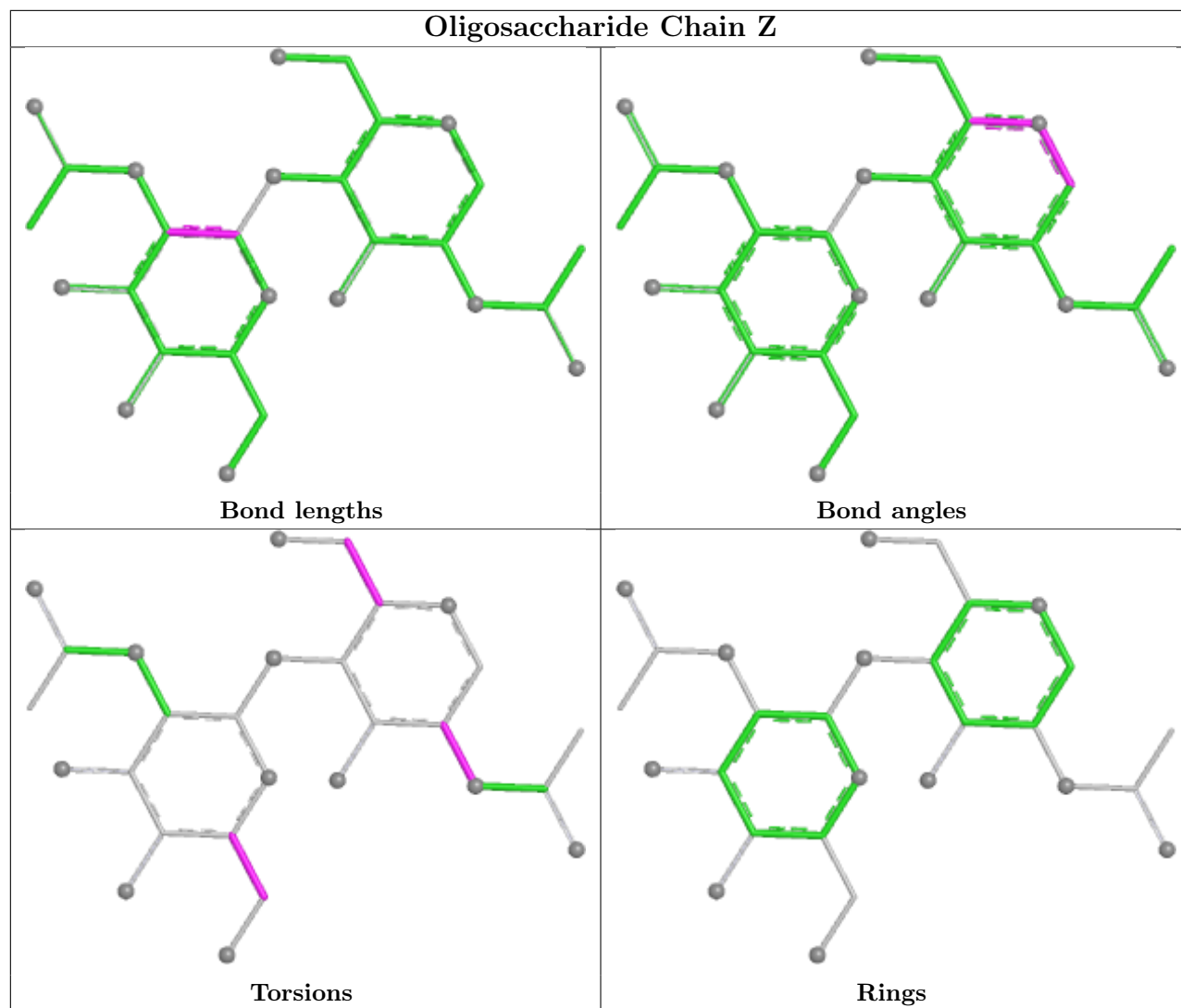
There are no ring outliers.

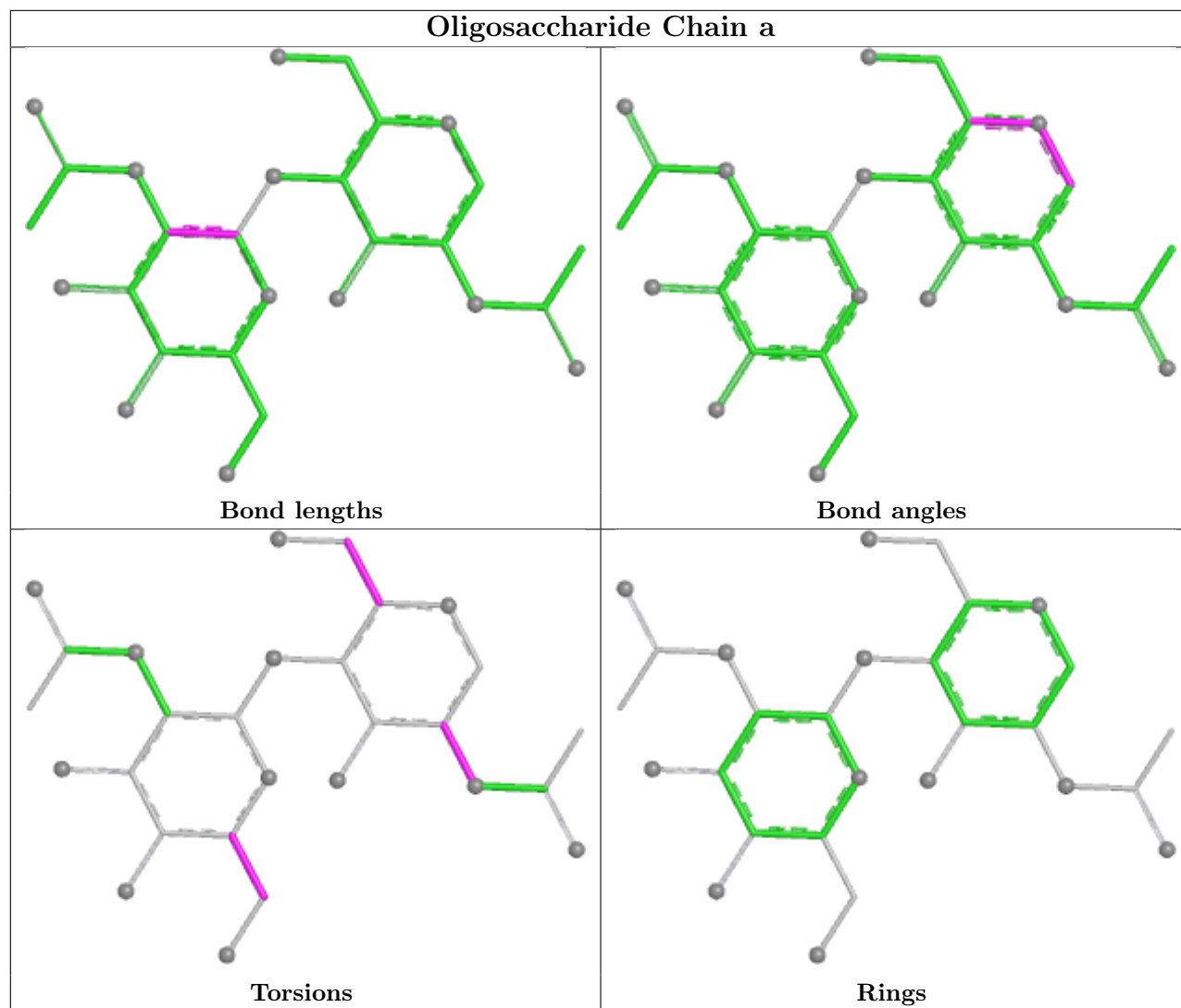
36 monomers are involved in 40 short contacts:

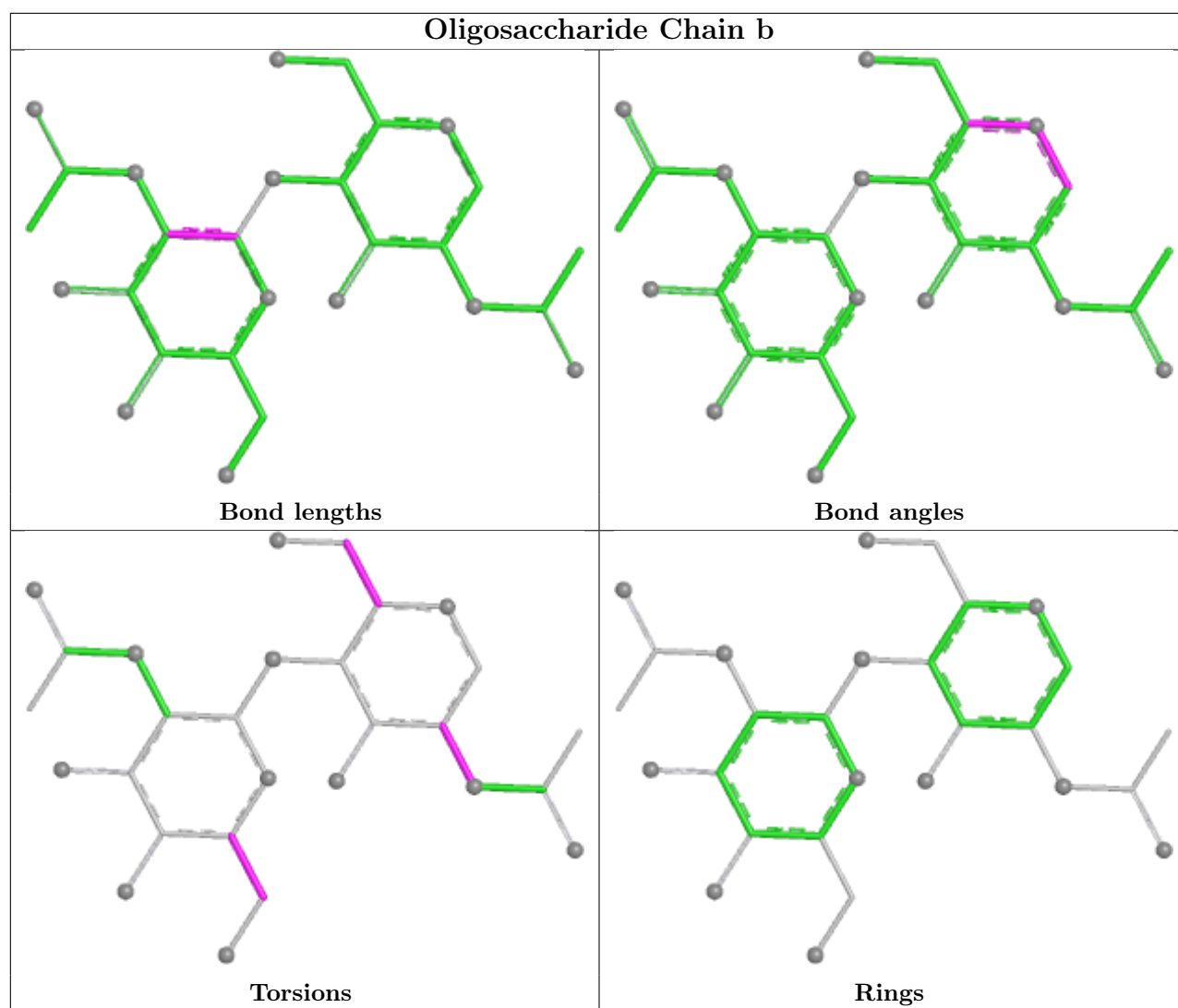
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	Z	1	NAG	2	0
8	j	1	NAG	1	0
8	a	1	NAG	2	0
8	h	1	NAG	2	0
8	k	1	NAG	1	0
8	g	1	NAG	2	0
8	e	1	NAG	3	0
8	d	1	NAG	3	0
8	n	1	NAG	2	0
8	p	2	NAG	1	0
8	m	1	NAG	2	0
8	l	1	NAG	2	0
8	i	1	NAG	2	0
8	h	2	NAG	1	0
8	Z	2	NAG	1	0
8	d	2	NAG	1	0
8	n	2	NAG	1	0
8	m	2	NAG	1	0
8	a	2	NAG	1	0
8	f	1	NAG	2	0
8	p	1	NAG	3	0
8	c	2	NAG	1	0
8	o	2	NAG	1	0
8	g	2	NAG	1	0
8	j	2	NAG	1	0
8	Y	1	NAG	2	0
8	b	2	NAG	1	0
8	o	1	NAG	2	0
8	f	2	NAG	1	0
8	q	1	NAG	1	0
8	Y	2	NAG	1	0
8	c	1	NAG	3	0
8	e	2	NAG	1	0
8	b	1	NAG	3	0
8	i	2	NAG	1	0
8	l	2	NAG	1	0

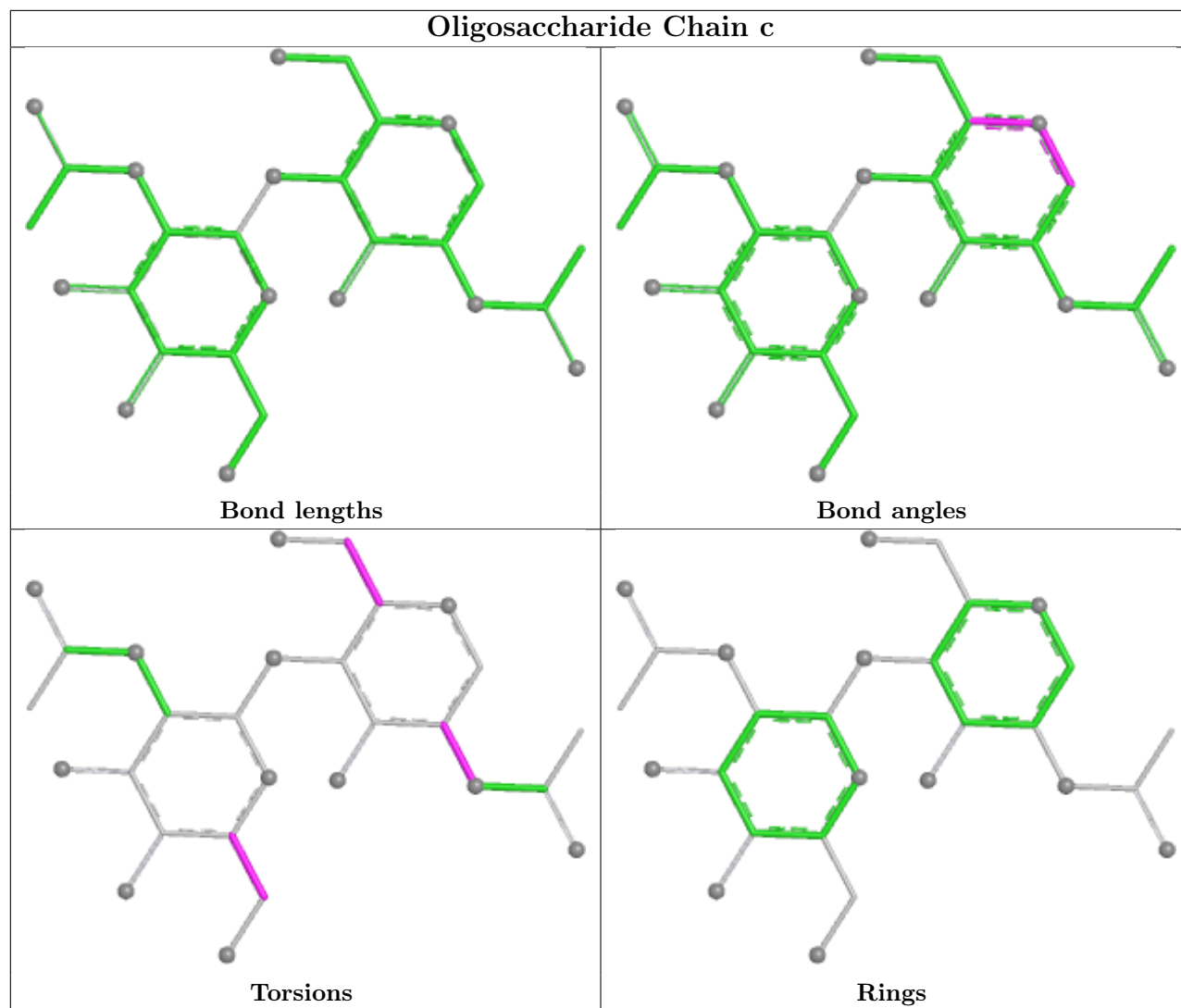
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

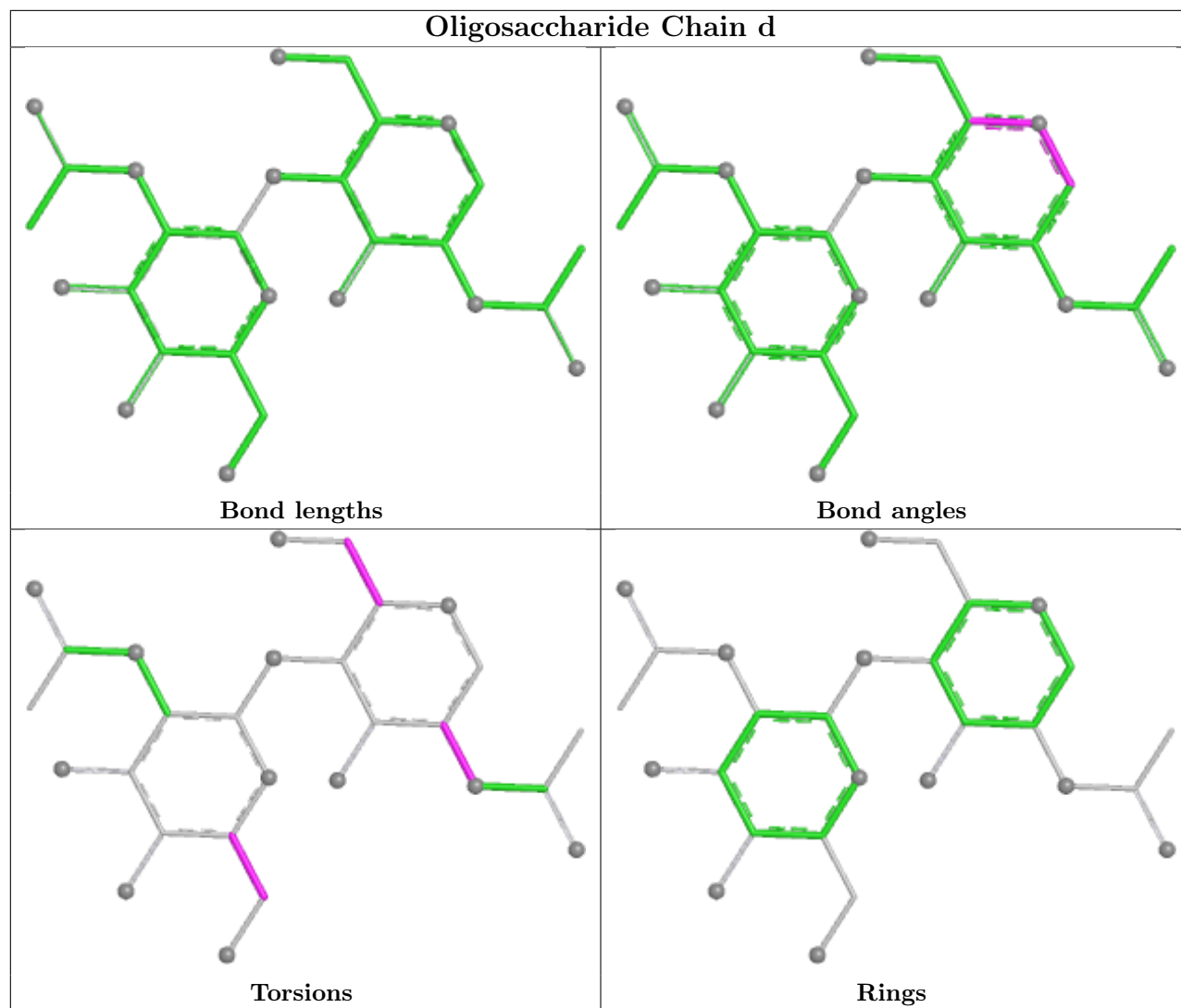


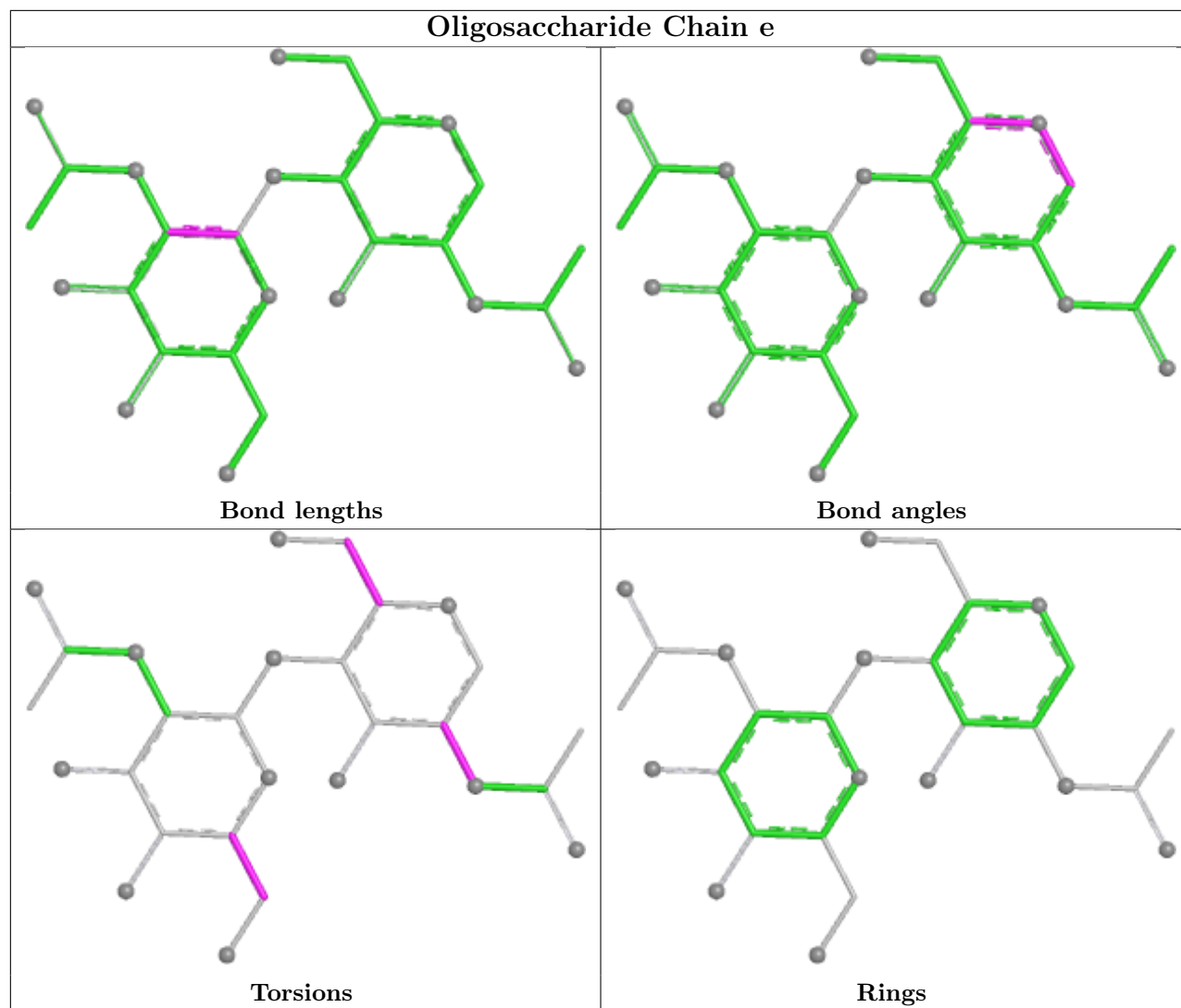


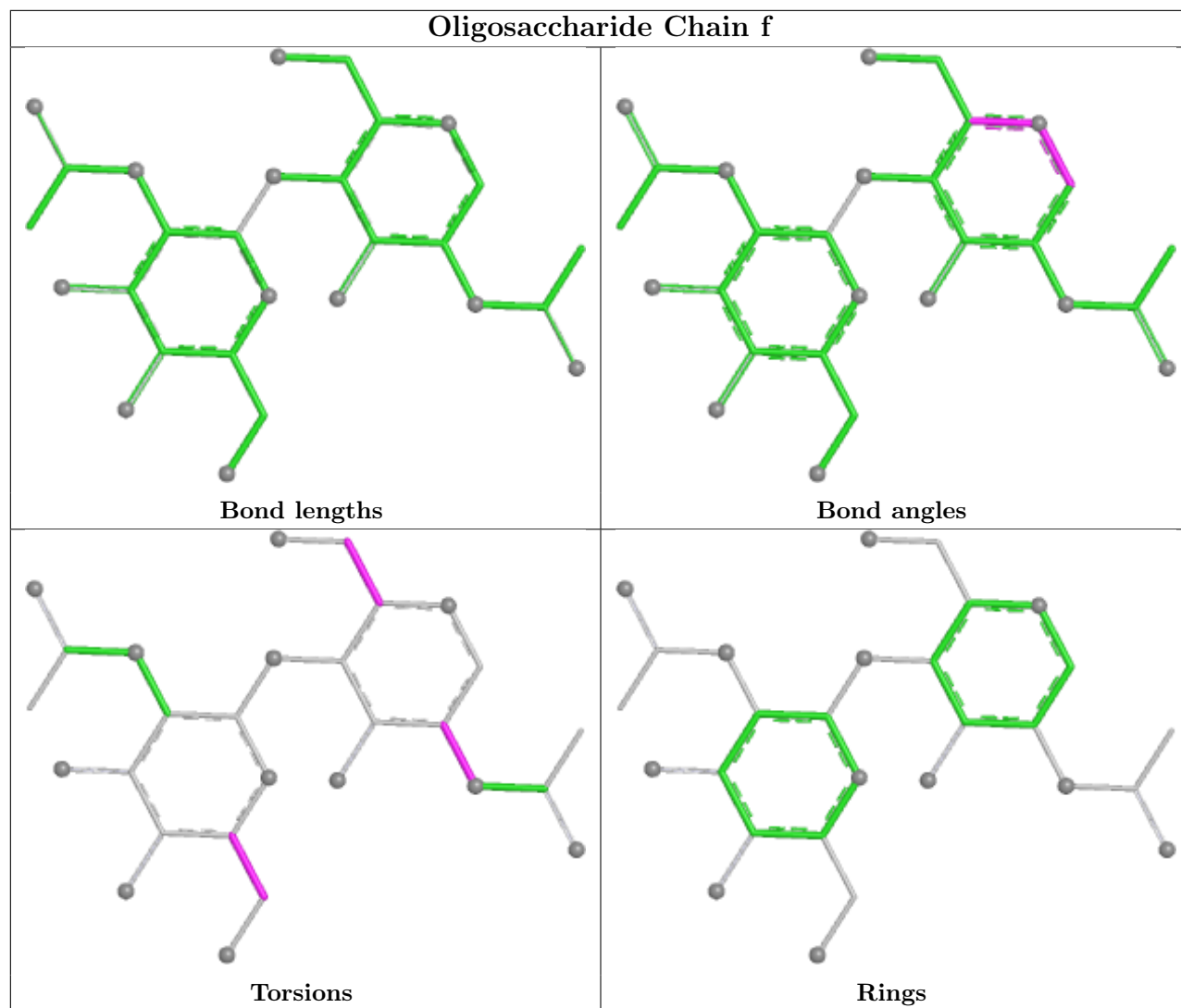


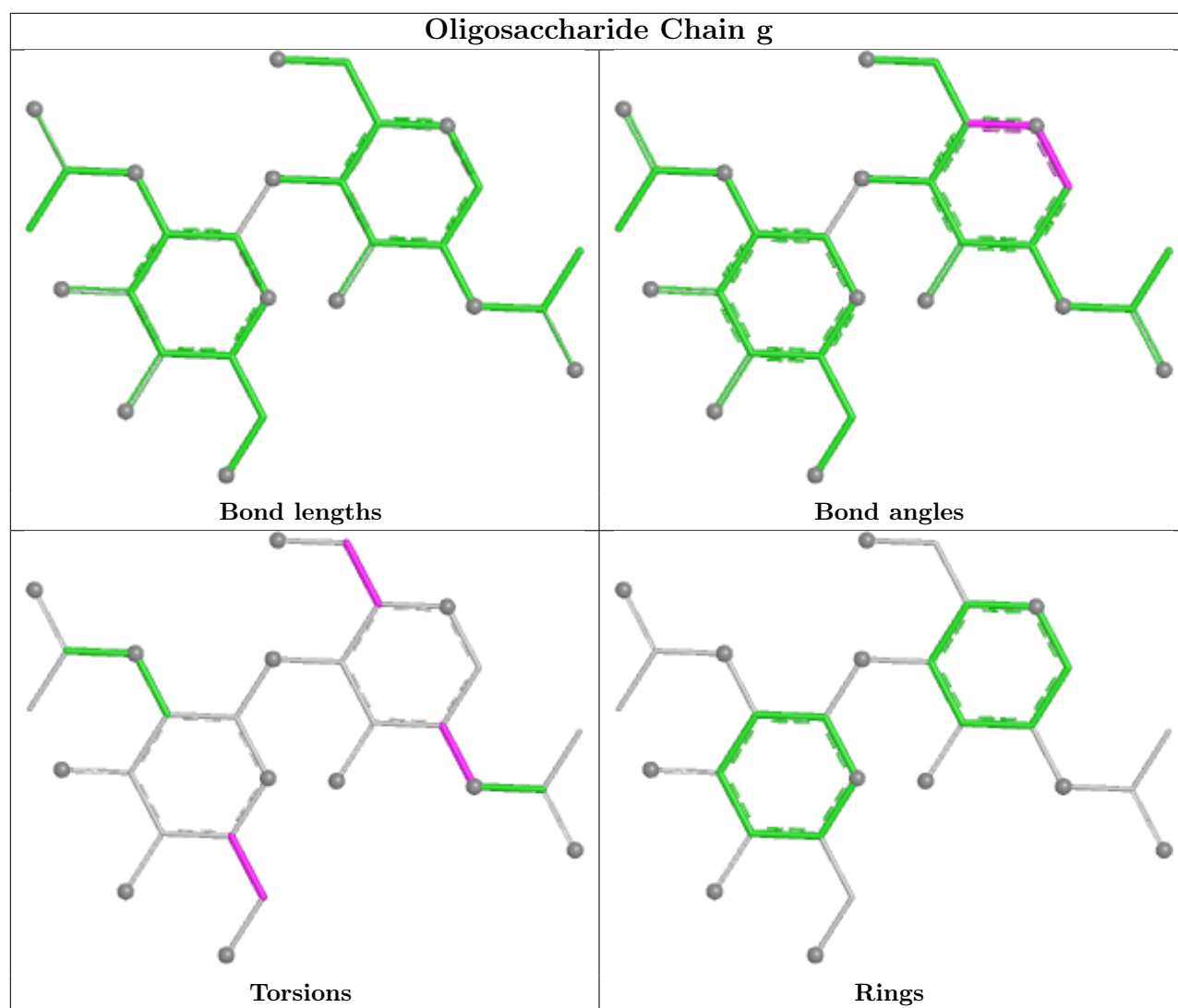


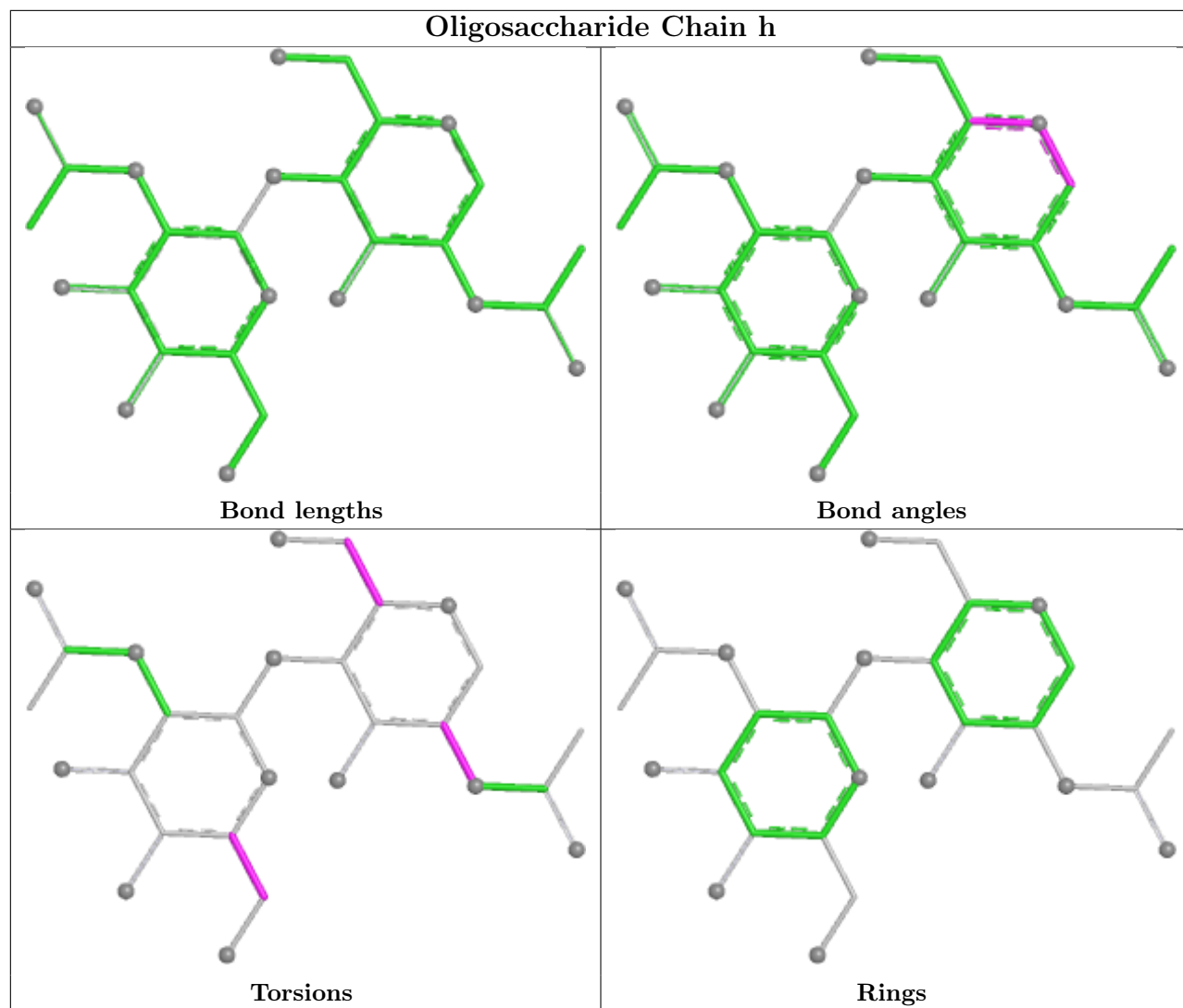


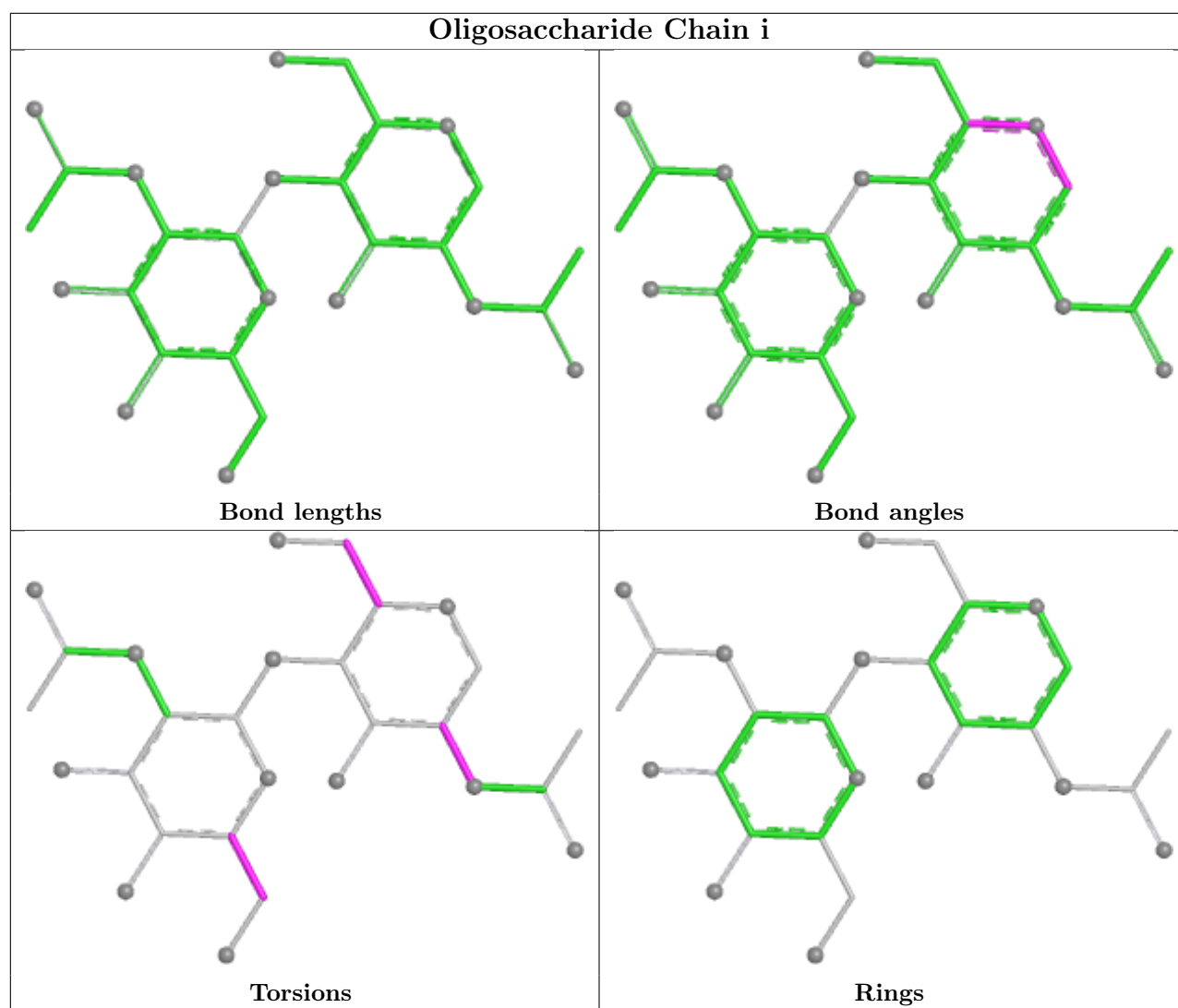


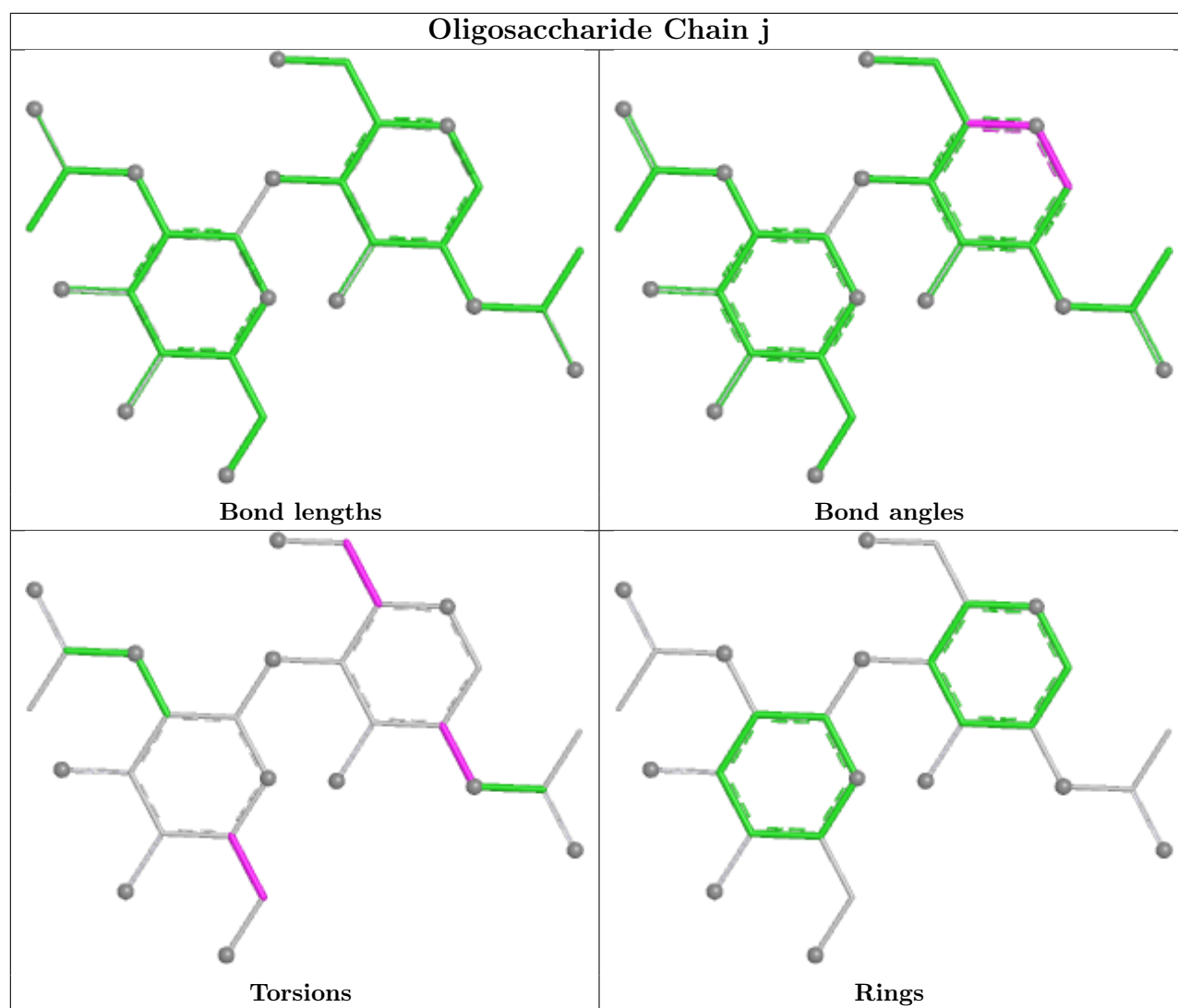


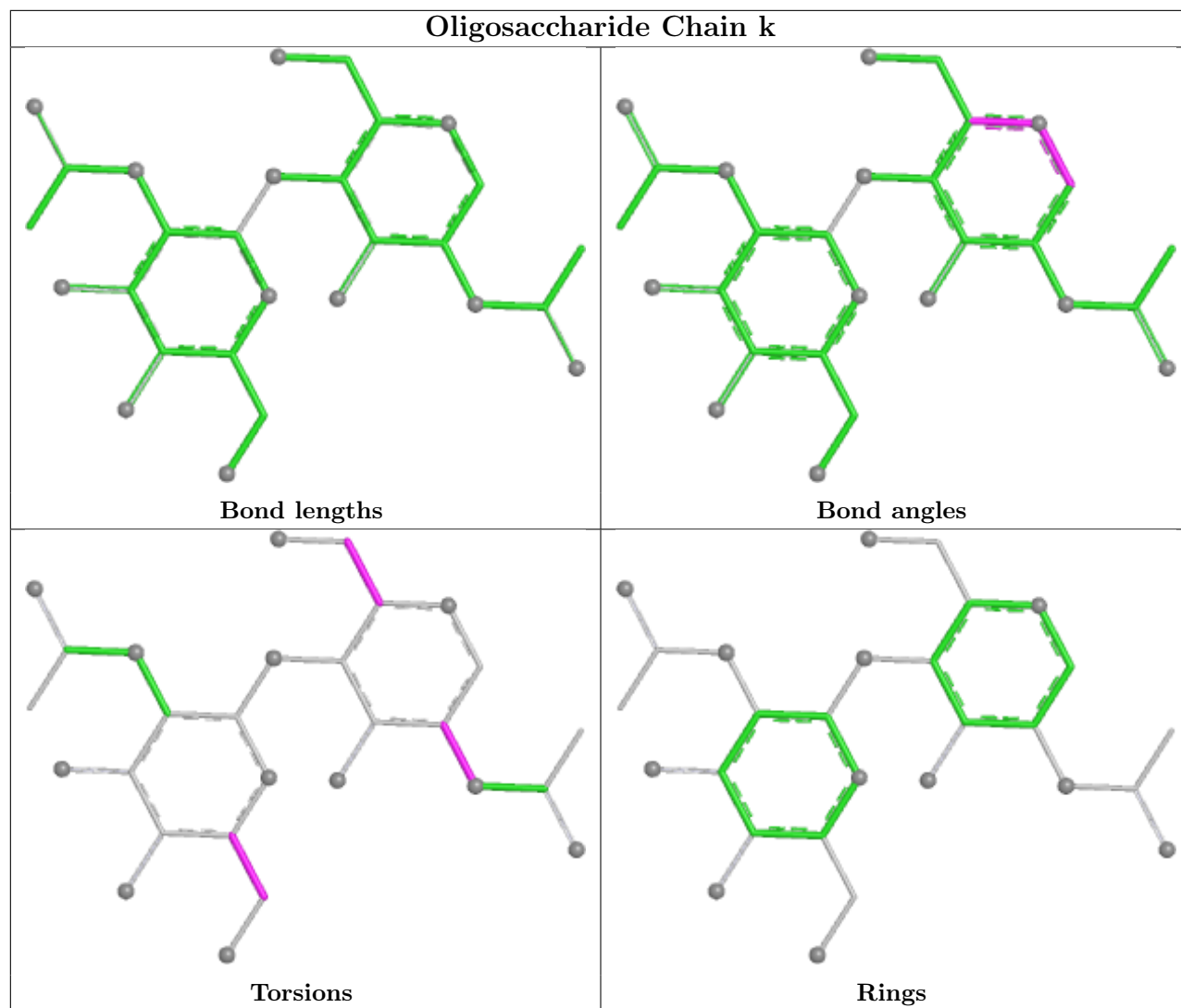


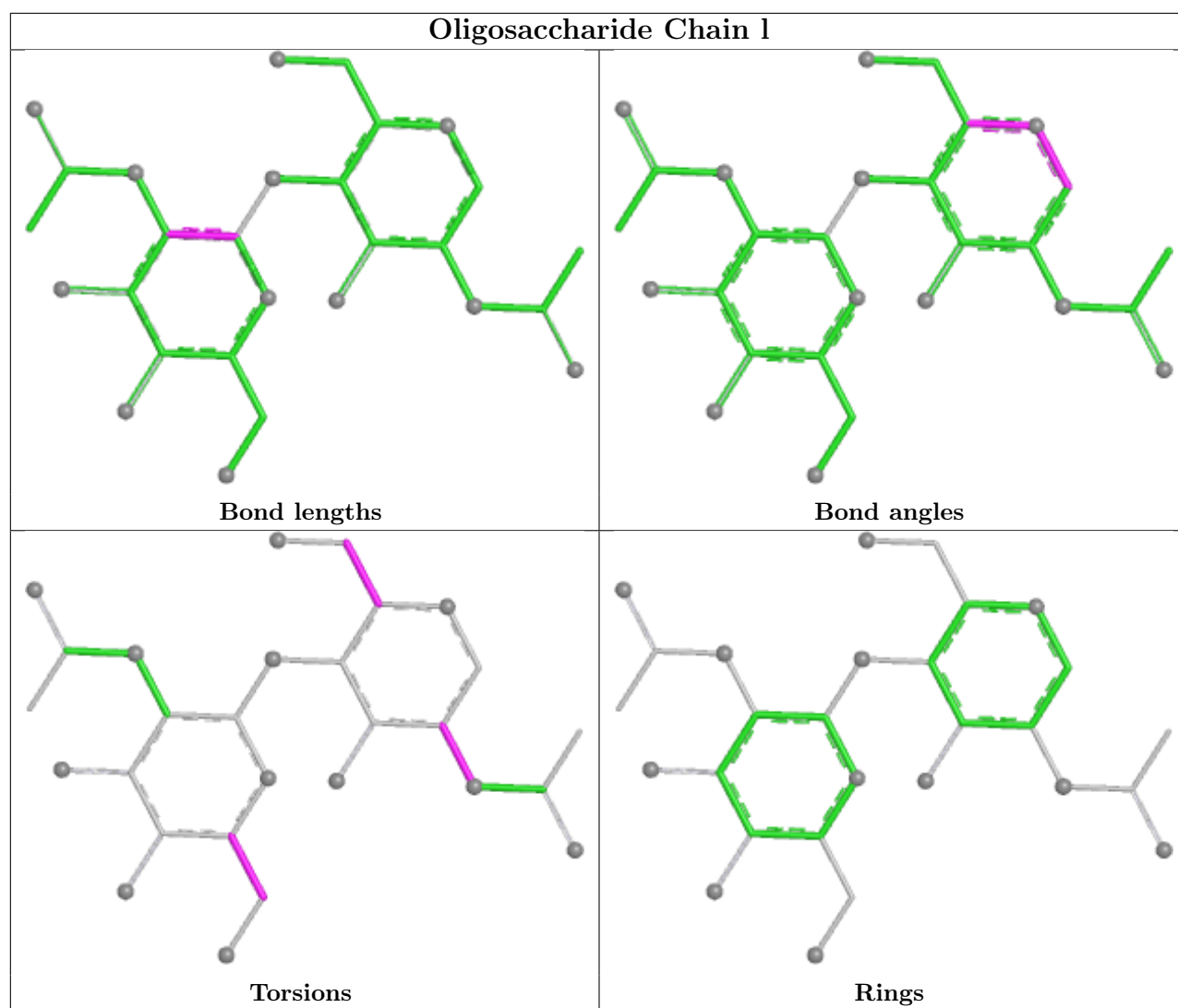


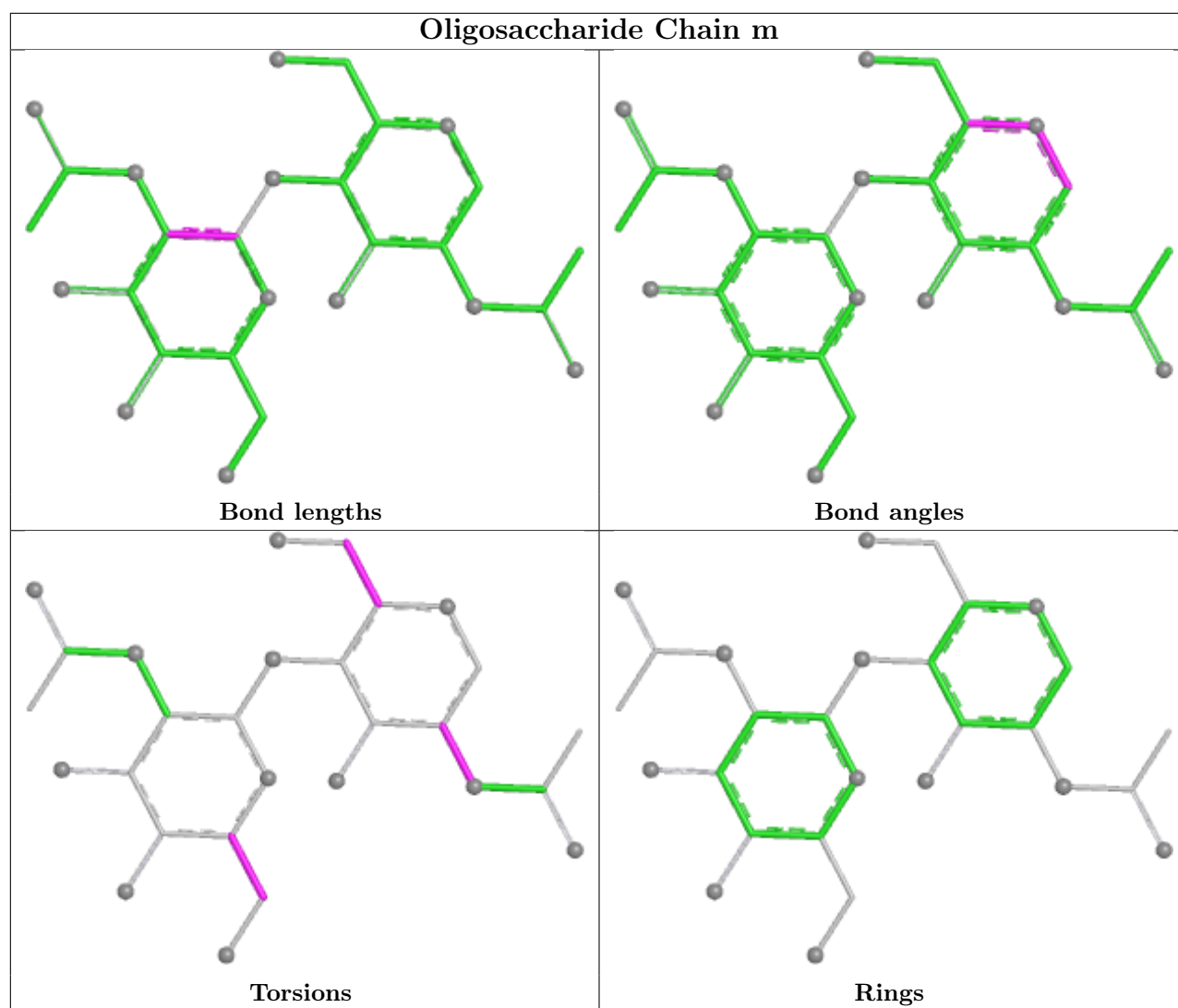


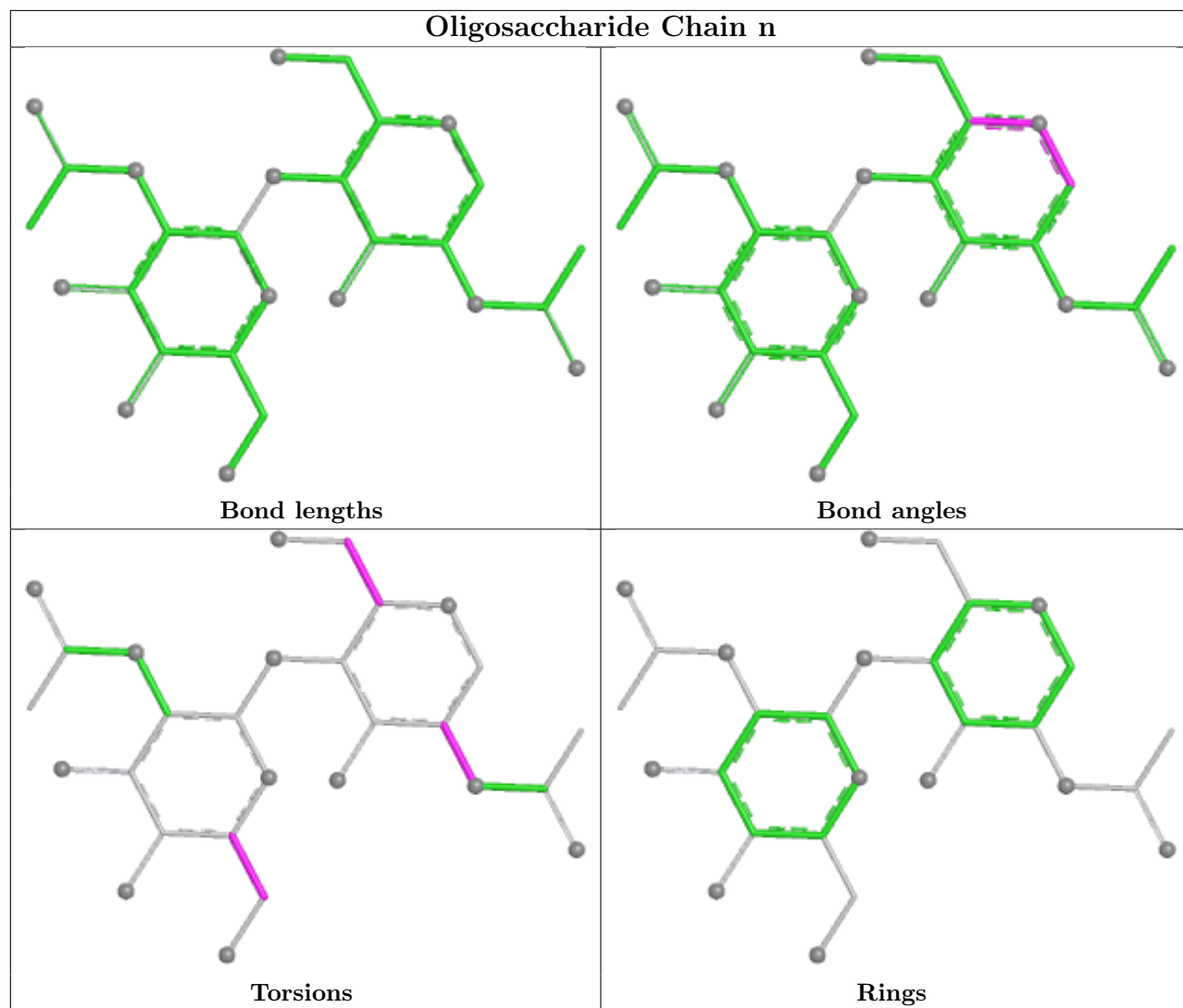


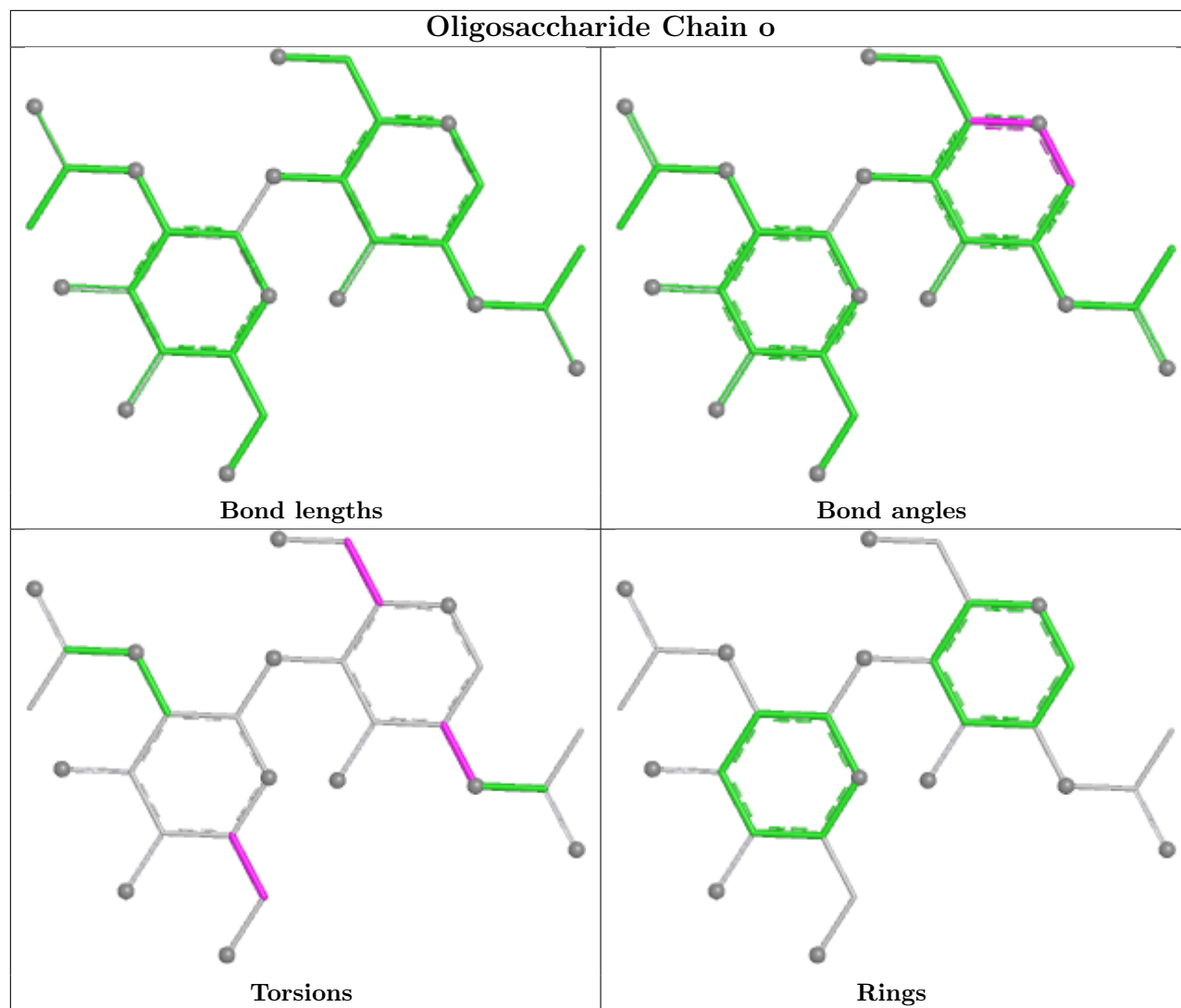


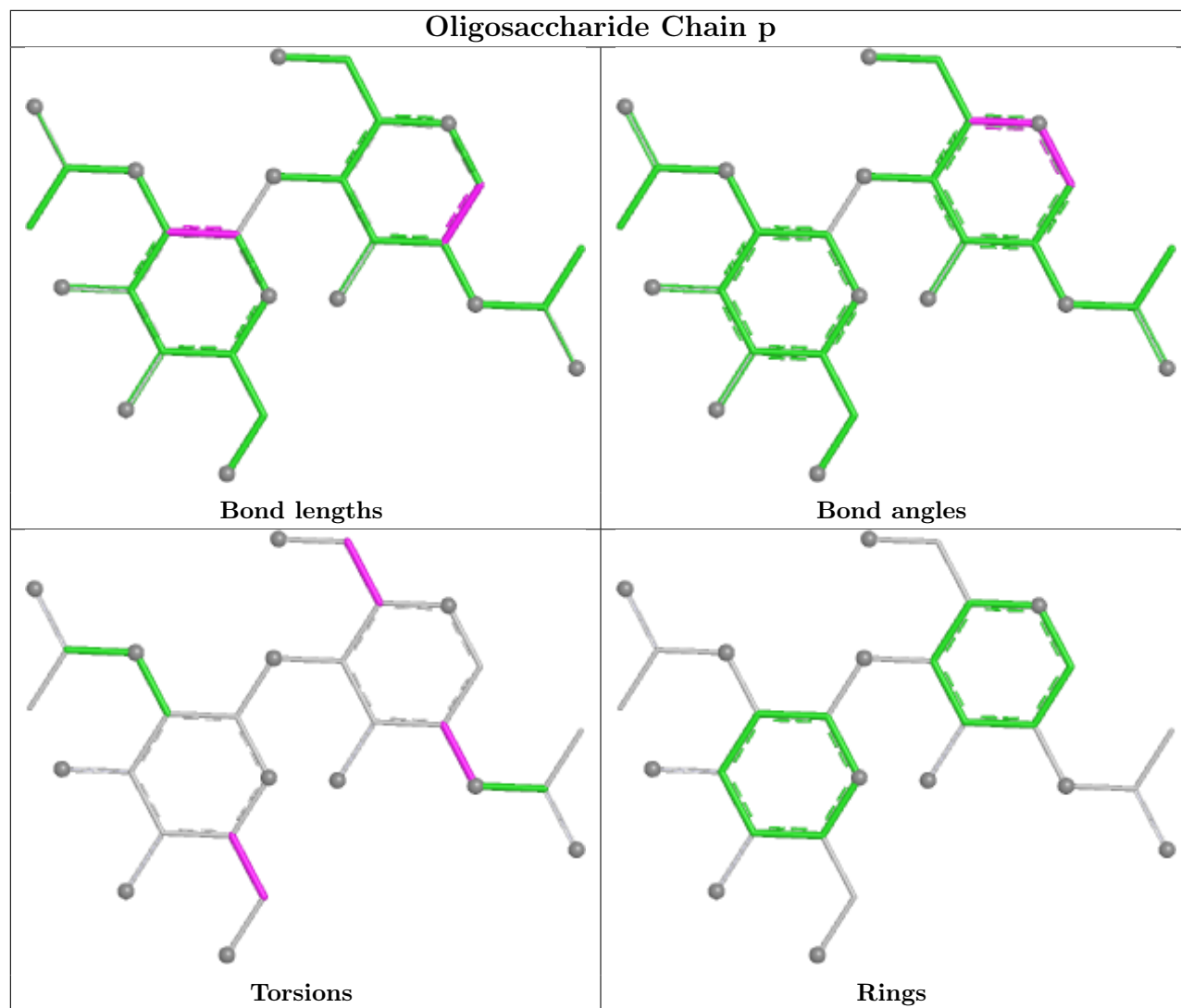


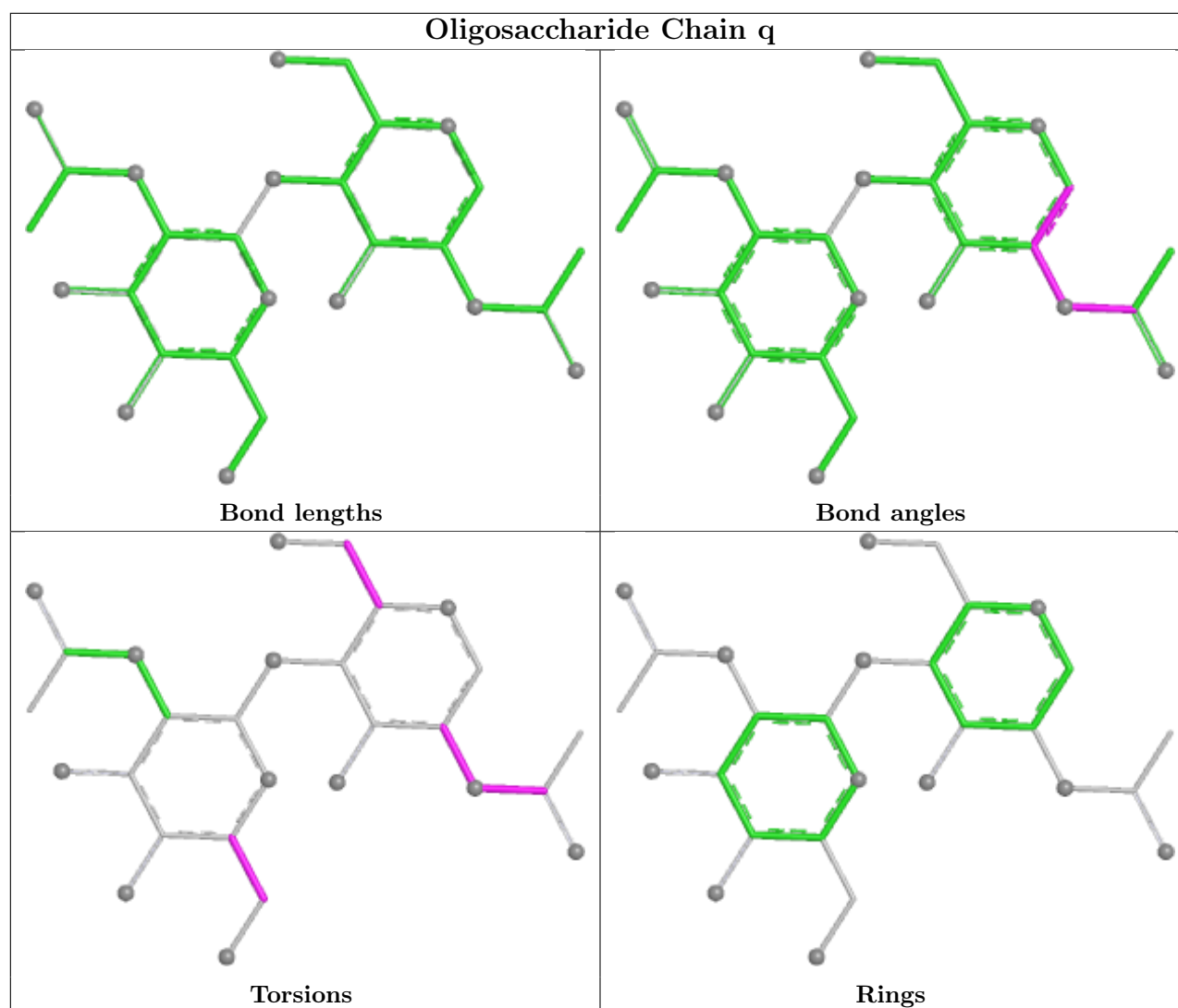












5.6 Ligand geometry [i](#)

38 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	$\# Z > 2$
9	NAG	K	604	1	14,14,15	0.56	0	17,19,21	1.35	2 (11%)
9	NAG	R	604	1	14,14,15	0.61	1 (7%)	17,19,21	1.34	2 (11%)
9	NAG	Q	604	1	14,14,15	0.62	1 (7%)	17,19,21	1.35	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	NAG	W	603	1	14,14,15	0.27	0	17,19,21	0.43	0
9	NAG	Q	603	1	14,14,15	0.22	0	17,19,21	0.44	0
9	NAG	M	604	1	14,14,15	0.60	0	17,19,21	1.35	2 (11%)
9	NAG	N	604	1	14,14,15	0.69	1 (7%)	17,19,21	1.37	2 (11%)
9	NAG	S	604	1	14,14,15	0.59	0	17,19,21	1.35	2 (11%)
9	NAG	V	603	1	14,14,15	0.27	0	17,19,21	0.47	0
9	NAG	G	603	1	14,14,15	0.53	0	17,19,21	0.66	0
9	NAG	G	604	1	14,14,15	0.58	0	17,19,21	1.36	2 (11%)
9	NAG	P	604	1	14,14,15	0.55	0	17,19,21	1.30	1 (5%)
9	NAG	J	603	1	14,14,15	0.56	0	17,19,21	0.43	0
9	NAG	M	603	1	14,14,15	0.28	0	17,19,21	0.46	0
9	NAG	L	603	1	14,14,15	0.32	0	17,19,21	0.49	0
9	NAG	T	604	1	14,14,15	0.55	0	17,19,21	1.30	2 (11%)
9	NAG	U	603	1	14,14,15	0.60	0	17,19,21	0.43	0
9	NAG	H	604	1	14,14,15	0.55	0	17,19,21	1.33	2 (11%)
9	NAG	D	901	4	14,14,15	0.37	0	17,19,21	0.48	0
9	NAG	O	604	1	14,14,15	0.60	0	17,19,21	1.35	2 (11%)
9	NAG	I	604	1	14,14,15	0.53	0	17,19,21	1.32	2 (11%)
9	NAG	R	603	1	14,14,15	0.20	0	17,19,21	0.43	0
9	NAG	O	603	1	14,14,15	0.30	0	17,19,21	0.48	0
9	NAG	X	603	1	14,14,15	0.70	0	17,19,21	0.45	0
9	NAG	X	604	1	14,14,15	0.57	0	17,19,21	1.33	2 (11%)
9	NAG	L	604	1	14,14,15	0.57	0	17,19,21	1.35	2 (11%)
9	NAG	U	604	1	14,14,15	0.57	0	17,19,21	1.31	2 (11%)
9	NAG	K	603	1	14,14,15	0.29	0	17,19,21	0.44	0
9	NAG	V	604	1	14,14,15	0.54	0	17,19,21	1.31	2 (11%)
9	NAG	N	603	1	14,14,15	0.26	0	17,19,21	0.38	0
9	NAG	P	603	1	14,14,15	0.39	0	17,19,21	0.46	0
9	NAG	I	603	1	14,14,15	0.32	0	17,19,21	0.46	0
9	NAG	S	603	1	14,14,15	0.23	0	17,19,21	0.39	0
9	NAG	H	603	1	14,14,15	0.33	0	17,19,21	0.46	0
9	NAG	T	603	1	14,14,15	0.25	0	17,19,21	0.37	0
9	NAG	J	604	1	14,14,15	0.57	0	17,19,21	1.30	2 (11%)
9	NAG	W	604	1	14,14,15	0.54	0	17,19,21	1.31	2 (11%)
9	NAG	B	1001	7	14,14,15	0.53	0	17,19,21	1.34	2 (11%)

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
9	NAG	K	604	1	-	6/6/23/26	0/1/1/1
9	NAG	R	604	1	-	4/6/23/26	0/1/1/1
9	NAG	Q	604	1	-	4/6/23/26	0/1/1/1
9	NAG	W	603	1	-	0/6/23/26	0/1/1/1
9	NAG	Q	603	1	-	2/6/23/26	0/1/1/1
9	NAG	M	604	1	-	6/6/23/26	0/1/1/1
9	NAG	N	604	1	-	4/6/23/26	0/1/1/1
9	NAG	S	604	1	-	4/6/23/26	0/1/1/1
9	NAG	V	603	1	-	0/6/23/26	0/1/1/1
9	NAG	G	603	1	-	0/6/23/26	0/1/1/1
9	NAG	G	604	1	-	4/6/23/26	0/1/1/1
9	NAG	P	604	1	-	6/6/23/26	0/1/1/1
9	NAG	J	603	1	-	2/6/23/26	0/1/1/1
9	NAG	M	603	1	-	0/6/23/26	0/1/1/1
9	NAG	L	603	1	-	1/6/23/26	0/1/1/1
9	NAG	T	604	1	-	5/6/23/26	0/1/1/1
9	NAG	U	603	1	-	2/6/23/26	0/1/1/1
9	NAG	H	604	1	-	6/6/23/26	0/1/1/1
9	NAG	D	901	4	-	4/6/23/26	0/1/1/1
9	NAG	O	604	1	-	4/6/23/26	0/1/1/1
9	NAG	I	604	1	-	6/6/23/26	0/1/1/1
9	NAG	R	603	1	-	2/6/23/26	0/1/1/1
9	NAG	O	603	1	-	0/6/23/26	0/1/1/1
9	NAG	X	603	1	-	3/6/23/26	0/1/1/1
9	NAG	X	604	1	-	6/6/23/26	0/1/1/1
9	NAG	L	604	1	-	6/6/23/26	0/1/1/1
9	NAG	U	604	1	-	6/6/23/26	0/1/1/1
9	NAG	K	603	1	-	1/6/23/26	0/1/1/1
9	NAG	V	604	1	-	6/6/23/26	0/1/1/1
9	NAG	N	603	1	-	2/6/23/26	0/1/1/1
9	NAG	P	603	1	-	0/6/23/26	0/1/1/1
9	NAG	I	603	1	-	0/6/23/26	0/1/1/1
9	NAG	S	603	1	-	2/6/23/26	0/1/1/1
9	NAG	H	603	1	-	1/6/23/26	0/1/1/1
9	NAG	T	603	1	-	2/6/23/26	0/1/1/1
9	NAG	J	604	1	-	6/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	NAG	W	604	1	-	6/6/23/26	0/1/1/1
9	NAG	B	1001	7	-	5/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	N	604	NAG	C1-C2	2.31	1.55	1.52
9	Q	604	NAG	C1-C2	2.06	1.55	1.52
9	R	604	NAG	C1-C2	2.00	1.55	1.52

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	I	604	NAG	C2-N2-C7	4.59	129.05	122.90
9	U	604	NAG	C2-N2-C7	4.58	129.04	122.90
9	H	604	NAG	C2-N2-C7	4.57	129.03	122.90
9	W	604	NAG	C2-N2-C7	4.56	129.01	122.90
9	P	604	NAG	C2-N2-C7	4.55	129.00	122.90
9	V	604	NAG	C2-N2-C7	4.55	129.00	122.90
9	B	1001	NAG	C2-N2-C7	4.55	129.00	122.90
9	X	604	NAG	C2-N2-C7	4.54	128.99	122.90
9	J	604	NAG	C2-N2-C7	4.54	128.99	122.90
9	G	604	NAG	C2-N2-C7	4.53	128.98	122.90
9	T	604	NAG	C2-N2-C7	4.53	128.97	122.90
9	L	604	NAG	C2-N2-C7	4.53	128.97	122.90
9	S	604	NAG	C2-N2-C7	4.53	128.97	122.90
9	Q	604	NAG	C2-N2-C7	4.49	128.92	122.90
9	K	604	NAG	C2-N2-C7	4.49	128.92	122.90
9	M	604	NAG	C2-N2-C7	4.49	128.91	122.90
9	O	604	NAG	C2-N2-C7	4.47	128.88	122.90
9	R	604	NAG	C2-N2-C7	4.45	128.87	122.90
9	N	604	NAG	C2-N2-C7	4.43	128.84	122.90
9	B	1001	NAG	C1-C2-N2	2.16	113.83	110.43
9	N	604	NAG	C1-O5-C5	2.15	115.07	112.19
9	X	604	NAG	C1-C2-N2	2.08	113.71	110.43
9	H	604	NAG	C1-C2-N2	2.06	113.69	110.43
9	O	604	NAG	C1-C2-N2	2.05	113.67	110.43
9	K	604	NAG	C1-C2-N2	2.05	113.67	110.43
9	J	604	NAG	C1-C2-N2	2.04	113.64	110.43
9	T	604	NAG	C1-C2-N2	2.04	113.64	110.43
9	M	604	NAG	C1-C2-N2	2.04	113.64	110.43
9	W	604	NAG	C1-C2-N2	2.03	113.63	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	G	604	NAG	C1-C2-N2	2.03	113.63	110.43
9	L	604	NAG	C1-C2-N2	2.02	113.62	110.43
9	I	604	NAG	C1-C2-N2	2.02	113.62	110.43
9	R	604	NAG	C1-C2-N2	2.01	113.59	110.43
9	V	604	NAG	C1-C2-N2	2.01	113.59	110.43
9	S	604	NAG	C1-C2-N2	2.00	113.59	110.43
9	U	604	NAG	C1-C2-N2	2.00	113.59	110.43

There are no chirality outliers.

All (124) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	S	603	NAG	C4-C5-C6-O6
9	N	603	NAG	C4-C5-C6-O6
9	Q	603	NAG	C4-C5-C6-O6
9	T	603	NAG	C4-C5-C6-O6
9	R	603	NAG	C4-C5-C6-O6
9	S	603	NAG	O5-C5-C6-O6
9	U	603	NAG	C4-C5-C6-O6
9	J	603	NAG	C4-C5-C6-O6
9	N	603	NAG	O5-C5-C6-O6
9	X	603	NAG	C4-C5-C6-O6
9	W	604	NAG	O5-C5-C6-O6
9	H	604	NAG	O5-C5-C6-O6
9	J	604	NAG	O5-C5-C6-O6
9	Q	603	NAG	O5-C5-C6-O6
9	V	604	NAG	O5-C5-C6-O6
9	X	604	NAG	O5-C5-C6-O6
9	I	604	NAG	O5-C5-C6-O6
9	D	901	NAG	O5-C5-C6-O6
9	R	603	NAG	O5-C5-C6-O6
9	T	603	NAG	O5-C5-C6-O6
9	U	604	NAG	O5-C5-C6-O6
9	U	603	NAG	O5-C5-C6-O6
9	X	603	NAG	O5-C5-C6-O6
9	J	603	NAG	O5-C5-C6-O6
9	L	604	NAG	C8-C7-N2-C2
9	L	604	NAG	O7-C7-N2-C2
9	M	604	NAG	C8-C7-N2-C2
9	M	604	NAG	O7-C7-N2-C2
9	N	604	NAG	C8-C7-N2-C2
9	N	604	NAG	O7-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
9	O	604	NAG	C8-C7-N2-C2
9	O	604	NAG	O7-C7-N2-C2
9	Q	604	NAG	C8-C7-N2-C2
9	Q	604	NAG	O7-C7-N2-C2
9	R	604	NAG	C8-C7-N2-C2
9	R	604	NAG	O7-C7-N2-C2
9	S	604	NAG	C8-C7-N2-C2
9	S	604	NAG	O7-C7-N2-C2
9	T	604	NAG	C8-C7-N2-C2
9	T	604	NAG	O7-C7-N2-C2
9	U	604	NAG	C8-C7-N2-C2
9	U	604	NAG	O7-C7-N2-C2
9	V	604	NAG	C8-C7-N2-C2
9	V	604	NAG	O7-C7-N2-C2
9	W	604	NAG	C8-C7-N2-C2
9	W	604	NAG	O7-C7-N2-C2
9	X	604	NAG	C8-C7-N2-C2
9	X	604	NAG	O7-C7-N2-C2
9	P	604	NAG	C8-C7-N2-C2
9	P	604	NAG	O7-C7-N2-C2
9	H	604	NAG	C8-C7-N2-C2
9	H	604	NAG	O7-C7-N2-C2
9	I	604	NAG	C8-C7-N2-C2
9	I	604	NAG	O7-C7-N2-C2
9	J	604	NAG	C8-C7-N2-C2
9	J	604	NAG	O7-C7-N2-C2
9	K	604	NAG	C8-C7-N2-C2
9	K	604	NAG	O7-C7-N2-C2
9	G	604	NAG	C8-C7-N2-C2
9	G	604	NAG	O7-C7-N2-C2
9	D	901	NAG	C8-C7-N2-C2
9	D	901	NAG	O7-C7-N2-C2
9	B	1001	NAG	C8-C7-N2-C2
9	B	1001	NAG	O7-C7-N2-C2
9	P	604	NAG	O5-C5-C6-O6
9	T	604	NAG	O5-C5-C6-O6
9	H	604	NAG	C4-C5-C6-O6
9	W	604	NAG	C4-C5-C6-O6
9	J	604	NAG	C4-C5-C6-O6
9	U	604	NAG	C4-C5-C6-O6
9	X	604	NAG	C4-C5-C6-O6
9	I	604	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
9	V	604	NAG	C4-C5-C6-O6
9	B	1001	NAG	O5-C5-C6-O6
9	D	901	NAG	C4-C5-C6-O6
9	L	604	NAG	C4-C5-C6-O6
9	K	604	NAG	C4-C5-C6-O6
9	L	604	NAG	O5-C5-C6-O6
9	K	604	NAG	O5-C5-C6-O6
9	M	604	NAG	C4-C5-C6-O6
9	H	603	NAG	C4-C5-C6-O6
9	M	604	NAG	O5-C5-C6-O6
9	L	604	NAG	C1-C2-N2-C7
9	M	604	NAG	C1-C2-N2-C7
9	N	604	NAG	C1-C2-N2-C7
9	O	604	NAG	C1-C2-N2-C7
9	Q	604	NAG	C1-C2-N2-C7
9	R	604	NAG	C1-C2-N2-C7
9	S	604	NAG	C1-C2-N2-C7
9	T	604	NAG	C1-C2-N2-C7
9	U	604	NAG	C1-C2-N2-C7
9	V	604	NAG	C1-C2-N2-C7
9	W	604	NAG	C1-C2-N2-C7
9	X	603	NAG	C1-C2-N2-C7
9	X	604	NAG	C1-C2-N2-C7
9	P	604	NAG	C1-C2-N2-C7
9	H	604	NAG	C1-C2-N2-C7
9	I	604	NAG	C1-C2-N2-C7
9	J	604	NAG	C1-C2-N2-C7
9	K	604	NAG	C1-C2-N2-C7
9	G	604	NAG	C1-C2-N2-C7
9	B	1001	NAG	C1-C2-N2-C7
9	L	604	NAG	C3-C2-N2-C7
9	M	604	NAG	C3-C2-N2-C7
9	N	604	NAG	C3-C2-N2-C7
9	O	604	NAG	C3-C2-N2-C7
9	Q	604	NAG	C3-C2-N2-C7
9	R	604	NAG	C3-C2-N2-C7
9	S	604	NAG	C3-C2-N2-C7
9	T	604	NAG	C3-C2-N2-C7
9	U	604	NAG	C3-C2-N2-C7
9	V	604	NAG	C3-C2-N2-C7
9	W	604	NAG	C3-C2-N2-C7
9	X	604	NAG	C3-C2-N2-C7

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Mol	Chain	Res	Type	Atoms
9	P	604	NAG	C3-C2-N2-C7
9	H	604	NAG	C3-C2-N2-C7
9	I	604	NAG	C3-C2-N2-C7
9	J	604	NAG	C3-C2-N2-C7
9	K	604	NAG	C3-C2-N2-C7
9	G	604	NAG	C3-C2-N2-C7
9	B	1001	NAG	C3-C2-N2-C7
9	L	603	NAG	C4-C5-C6-O6
9	P	604	NAG	C4-C5-C6-O6
9	K	603	NAG	C4-C5-C6-O6

There are no ring outliers.

34 monomers are involved in 40 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	K	604	NAG	1	0
9	R	604	NAG	1	0
9	Q	604	NAG	1	0
9	W	603	NAG	1	0
9	Q	603	NAG	1	0
9	M	604	NAG	1	0
9	N	604	NAG	1	0
9	S	604	NAG	1	0
9	V	603	NAG	1	0
9	G	604	NAG	2	0
9	P	604	NAG	1	0
9	J	603	NAG	1	0
9	M	603	NAG	1	0
9	L	603	NAG	1	0
9	T	604	NAG	2	0
9	U	603	NAG	2	0
9	H	604	NAG	1	0
9	D	901	NAG	1	0
9	O	604	NAG	1	0
9	I	604	NAG	1	0
9	R	603	NAG	1	0
9	X	603	NAG	3	0
9	X	604	NAG	1	0
9	L	604	NAG	1	0
9	U	604	NAG	1	0
9	K	603	NAG	1	0
9	V	604	NAG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	N	603	NAG	1	0
9	I	603	NAG	2	0
9	H	603	NAG	1	0
9	T	603	NAG	1	0
9	J	604	NAG	1	0
9	W	604	NAG	1	0
9	B	1001	NAG	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
4	D	3
6	F	3
1	G	2
1	X	2
1	W	2
1	T	2
1	U	2
1	V	2
1	P	2
1	H	2
1	M	2
1	Q	2
1	O	2
1	R	2
1	N	2
1	S	2
1	J	2
1	K	2
1	L	2
7	B	2
1	I	2
3	C	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	G	370:PHE	C	371:SER	N	7.60
1	X	370:PHE	C	371:SER	N	7.54
1	W	370:PHE	C	371:SER	N	7.35
1	T	370:PHE	C	371:SER	N	7.33
1	U	370:PHE	C	371:SER	N	7.32
1	V	370:PHE	C	371:SER	N	7.30
1	P	370:PHE	C	371:SER	N	7.30
1	D	629:ILE	C	630:ALA	N	7.29
1	H	370:PHE	C	371:SER	N	7.26
1	M	370:PHE	C	371:SER	N	7.24
1	Q	370:PHE	C	371:SER	N	7.18
1	O	370:PHE	C	371:SER	N	7.16
1	R	370:PHE	C	371:SER	N	7.16
1	N	370:PHE	C	371:SER	N	7.15
1	S	370:PHE	C	371:SER	N	7.15
1	J	370:PHE	C	371:SER	N	7.15
1	K	370:PHE	C	371:SER	N	7.15
1	L	370:PHE	C	371:SER	N	7.13
1	B	409:LEU	C	410:PHE	N	7.08
1	I	370:PHE	C	371:SER	N	7.07
1	D	224:PHE	C	225:PHE	N	6.21
1	D	344:PHE	C	345:VAL	N	5.97
1	B	284:PHE	C	285:TYR	N	5.74
1	C	336:GLU	C	337:GLU	N	5.16
1	F	357:LYS	C	358:ILE	N	4.87
1	C	388:GLU	C	389:LEU	N	3.92
1	L	523:GLN	C	524:LYS	N	3.45
1	N	523:GLN	C	524:LYS	N	3.45
1	M	523:GLN	C	524:LYS	N	3.44
1	O	523:GLN	C	524:LYS	N	3.44
1	I	523:GLN	C	524:LYS	N	3.44
1	Q	523:GLN	C	524:LYS	N	3.43
1	S	523:GLN	C	524:LYS	N	3.43
1	W	523:GLN	C	524:LYS	N	3.43
1	P	523:GLN	C	524:LYS	N	3.43
1	H	523:GLN	C	524:LYS	N	3.43
1	J	523:GLN	C	524:LYS	N	3.43
1	K	523:GLN	C	524:LYS	N	3.43
1	R	523:GLN	C	524:LYS	N	3.42
1	U	523:GLN	C	524:LYS	N	3.42
1	V	523:GLN	C	524:LYS	N	3.42
1	G	523:GLN	C	524:LYS	N	3.42
1	T	523:GLN	C	524:LYS	N	3.41

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	X	523:GLN	C	524:LYS	N	3.39
1	F	228:GLY	C	229:SER	N	3.17
1	F	179:PRO	C	180:TYR	N	3.15

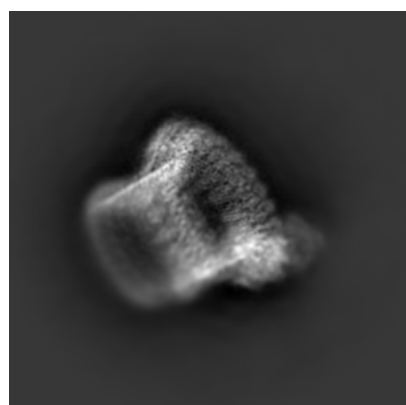
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-0107. These allow visual inspection of the internal detail of the map and identification of artifacts.

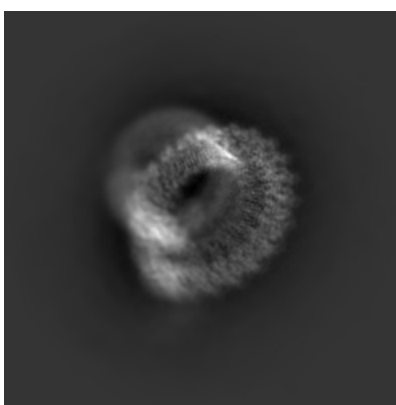
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

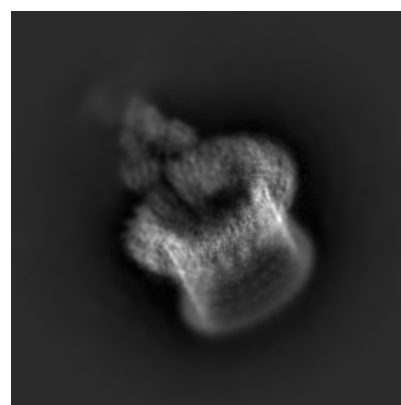
6.1.1 Primary map



X



Y



Z

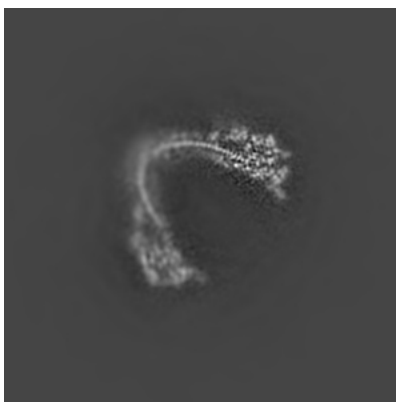
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

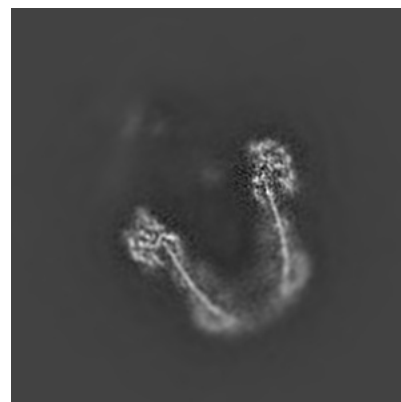
6.2.1 Primary map



X Index: 180



Y Index: 180

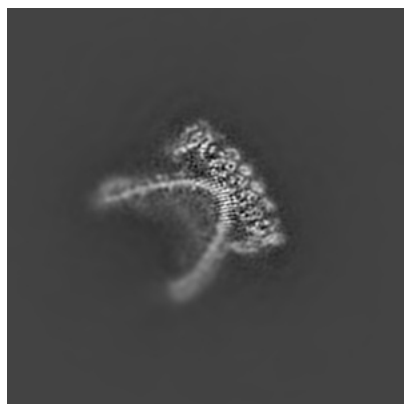


Z Index: 180

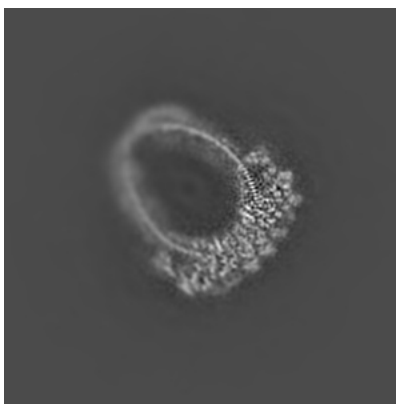
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

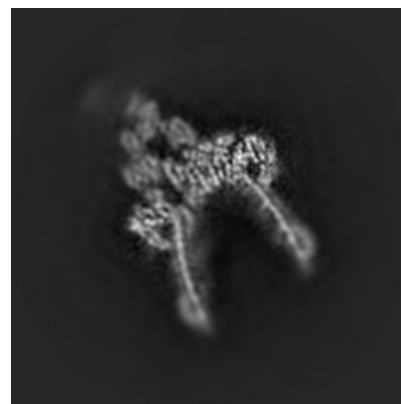
6.3.1 Primary map



X Index: 230



Y Index: 150

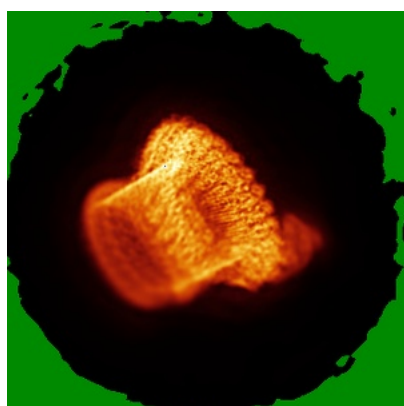


Z Index: 145

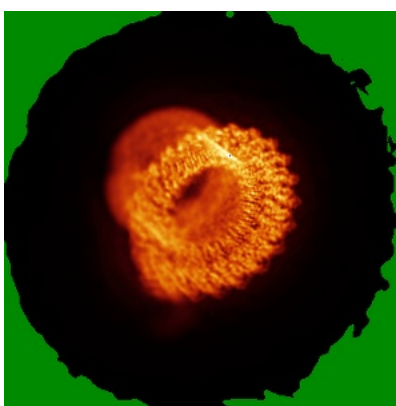
The images above show the largest variance slices of the map in three orthogonal directions.

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

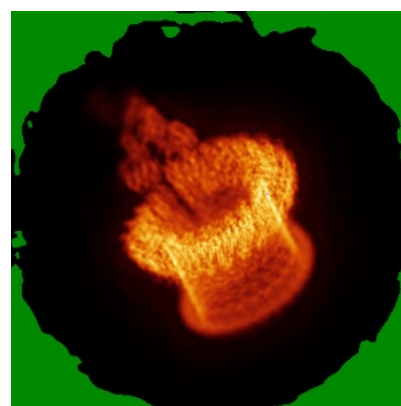
6.4.1 Primary map



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.

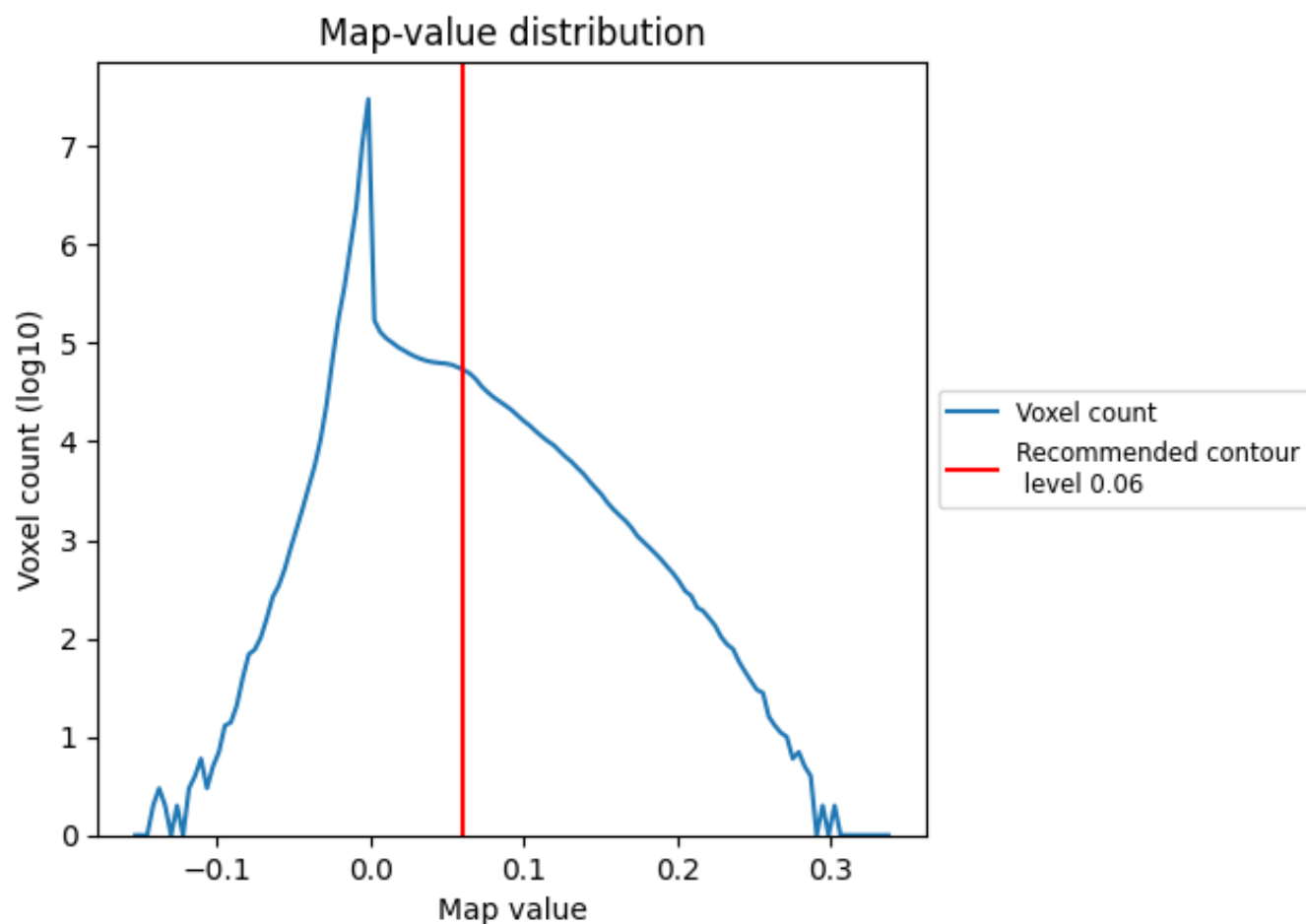
6.6 Mask visualisation

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

7 Map analysis [i](#)

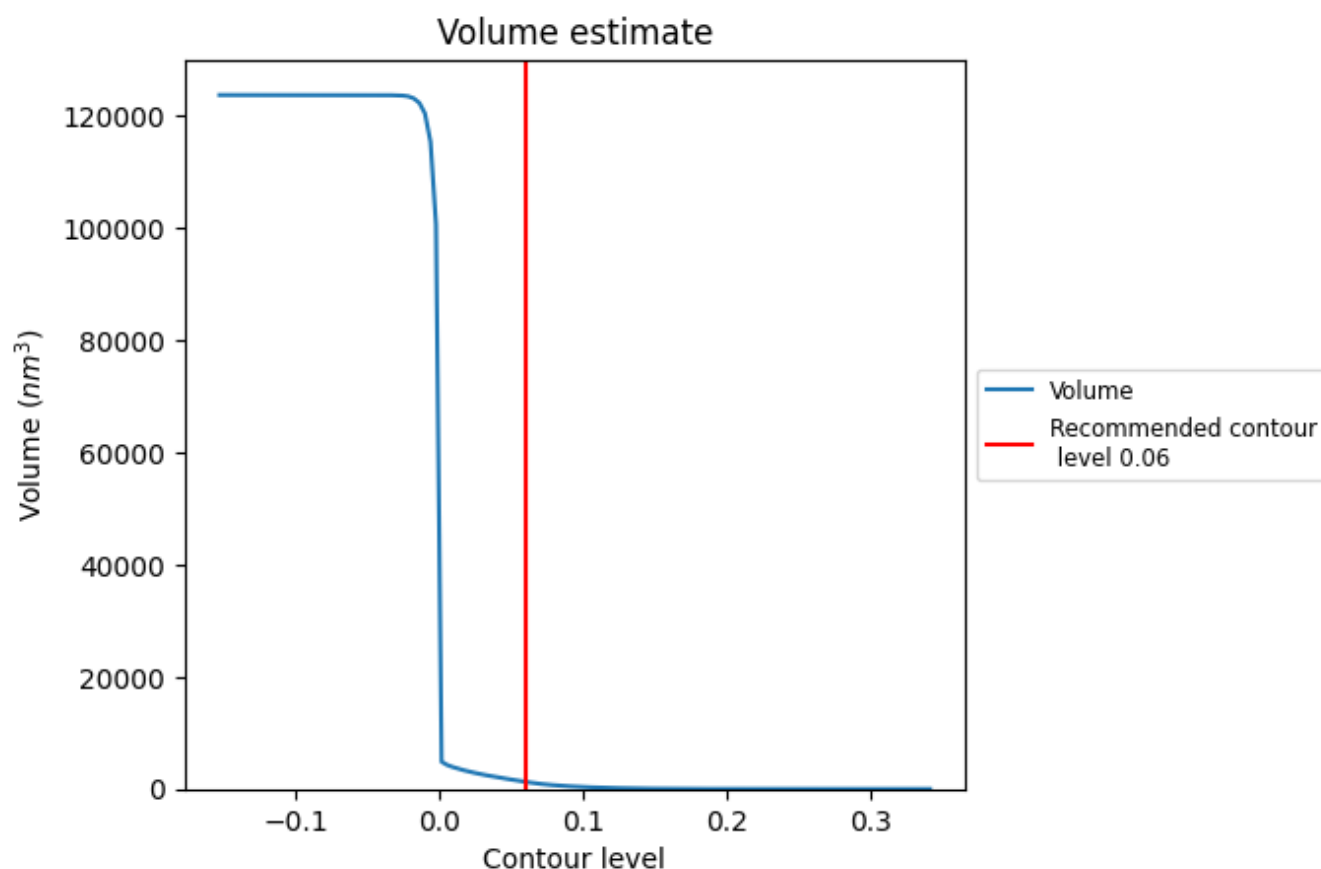
This section contains the results of statistical analysis of the map.

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.

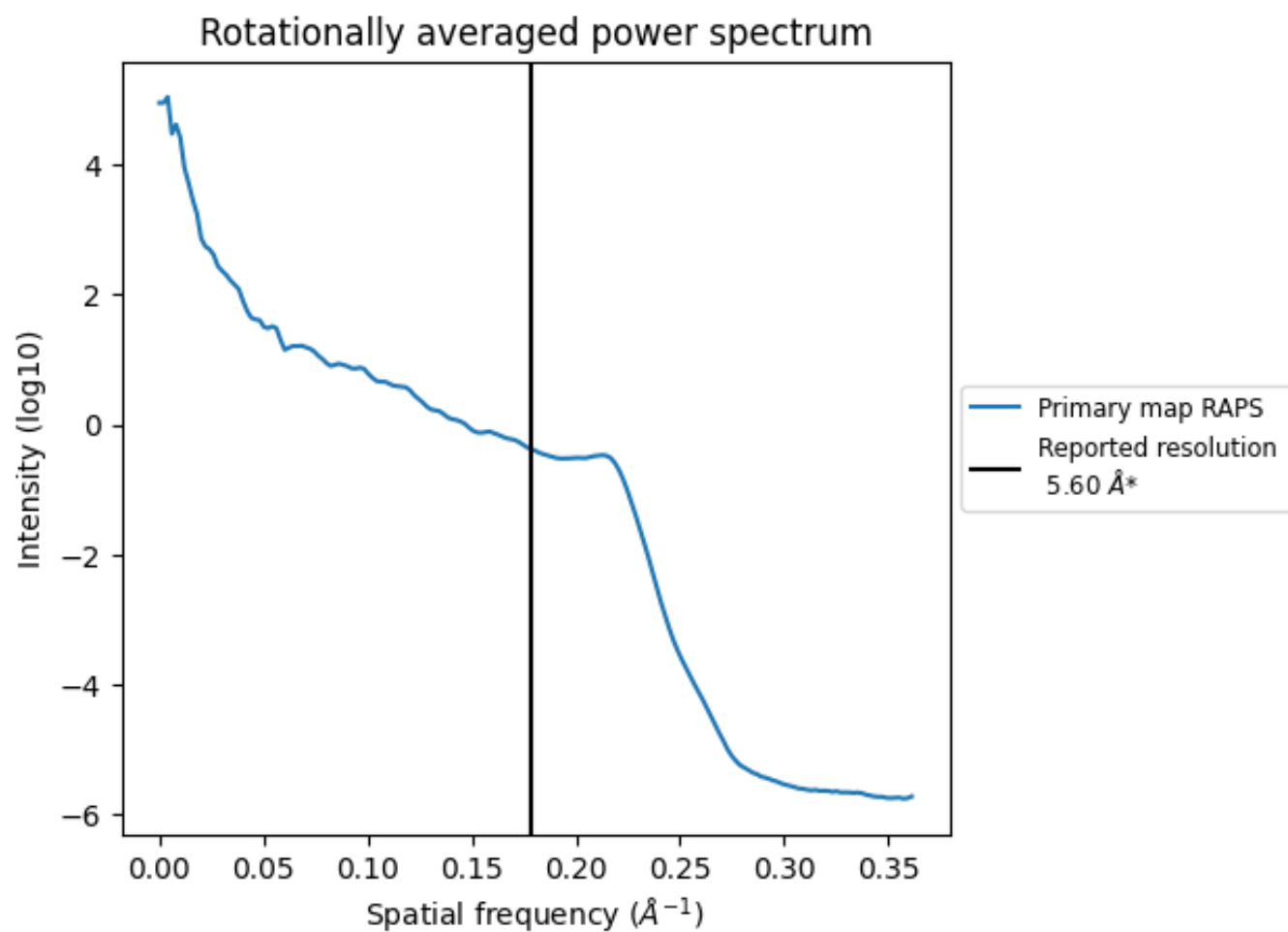
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1262 nm³; this corresponds to an approximate mass of 1140 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 [i](#)



*Reported resolution corresponds to spatial frequency of 0.179 Å⁻¹

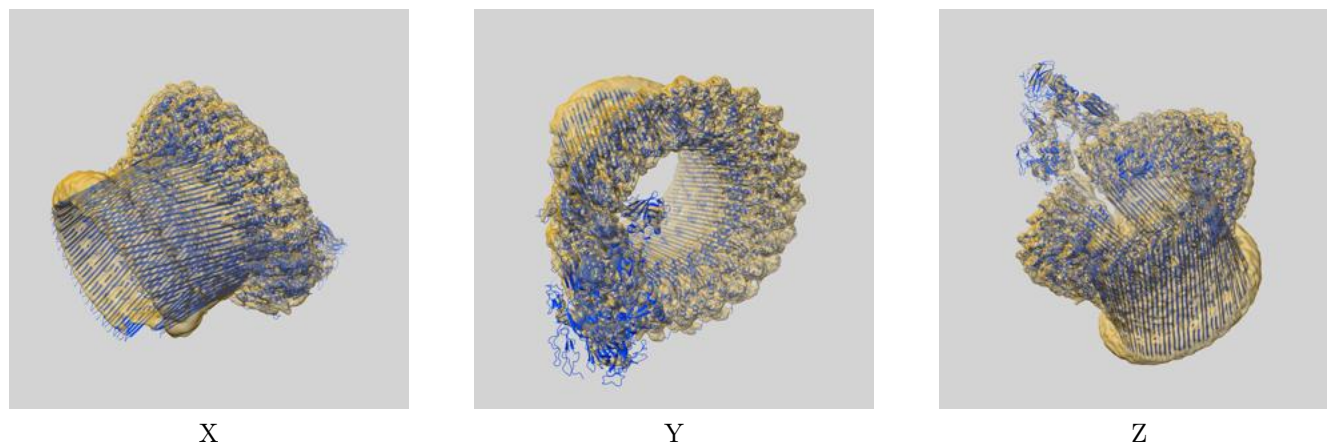
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

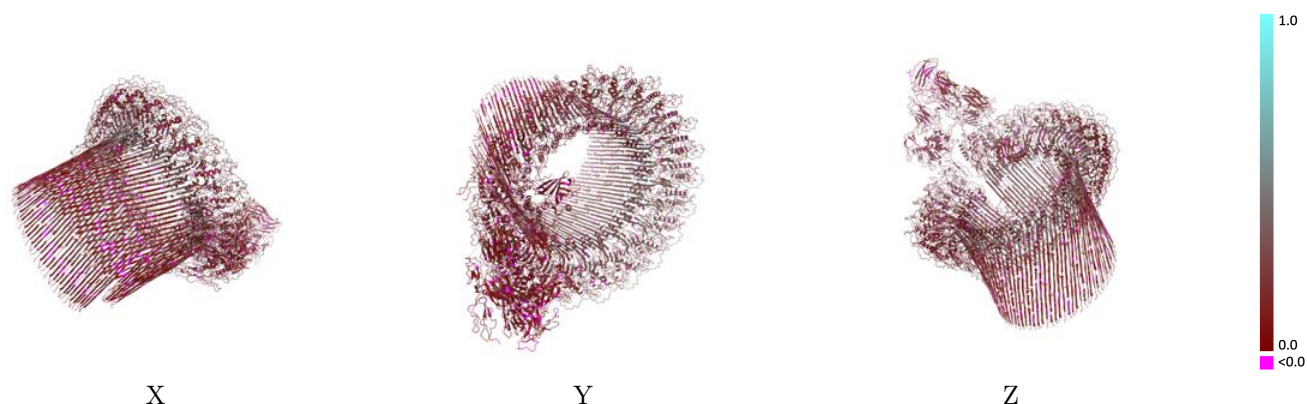
This section contains information regarding the fit between EMDB map EMD-0107 and PDB model 6H04. Per-residue inclusion information can be found in [section 3](#) on [page 11](#).

9.1 Map-model overlay [i](#)



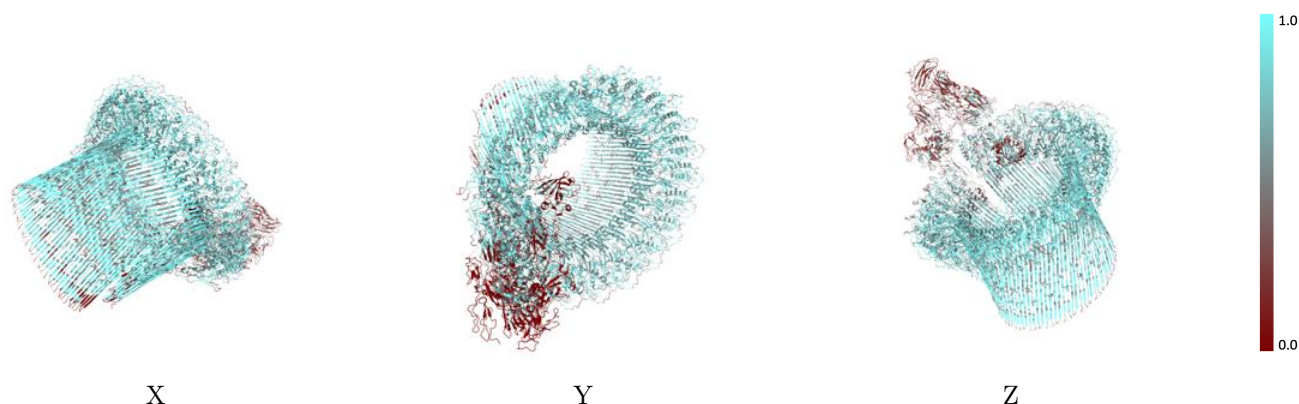
The images above show the 3D surface view of the map at the recommended contour level 0.06 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



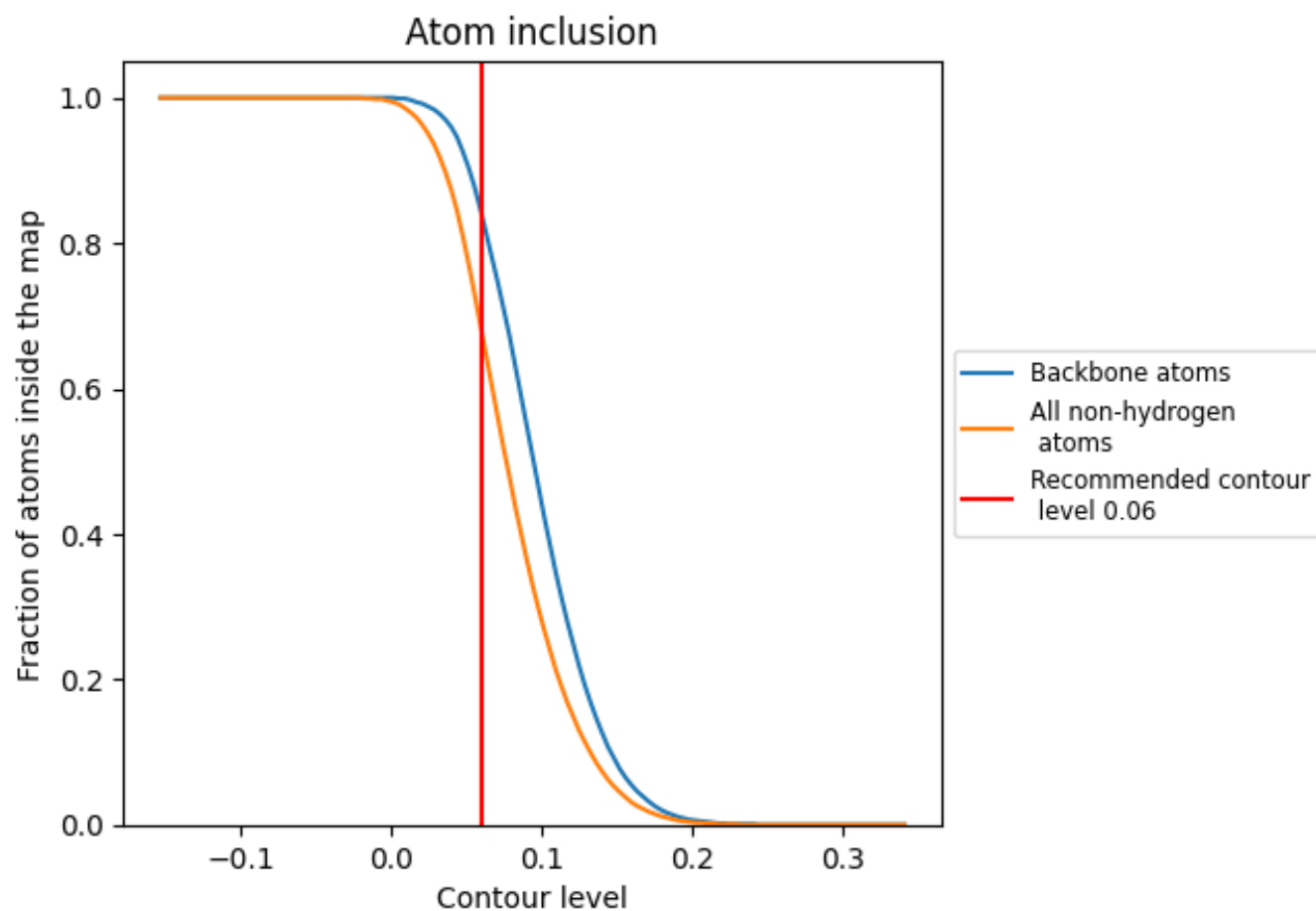
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.06).

9.4 Atom inclusion [i](#)



At the recommended contour level, 84% of all backbone atoms, 68% 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 (0.06) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6820	 0.1790
A	 0.2710	 0.1130
B	 0.5610	 0.1380
C	 0.7160	 0.1580
D	 0.5950	 0.1530
E	 0.1680	 0.1100
F	 0.7440	 0.1520
G	 0.7370	 0.1560
H	 0.7850	 0.2120
I	 0.7800	 0.2110
J	 0.7840	 0.2210
K	 0.7810	 0.2180
L	 0.7900	 0.2300
M	 0.7900	 0.2270
N	 0.7930	 0.2280
O	 0.7860	 0.2230
P	 0.7740	 0.1990
Q	 0.7860	 0.2160
R	 0.7790	 0.2030
S	 0.7710	 0.1950
T	 0.7570	 0.1770
U	 0.7460	 0.1670
V	 0.7420	 0.1650
W	 0.7040	 0.1530
X	 0.5960	 0.1360
Y	 0.6070	 0.2400
Z	 0.5710	 0.1570
a	 0.5710	 0.1930
b	 0.4640	 0.2000
c	 0.3570	 0.1650
d	 0.3930	 0.2230
e	 0.3570	 0.1810
f	 0.2140	 0.1620
g	 0.2500	 0.1420
h	 0.2140	 0.0800



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Chain	Atom inclusion	Q-score
i	 0.3210	 0.0700
j	 0.3210	 0.1070
k	 0.4640	 0.1910
l	 0.3930	 0.2410
m	 0.5360	 0.2910
n	 0.4290	 0.2080
o	 0.3570	 0.1580
p	 0.4290	 0.2220
q	 0.2860	 0.1200