



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:00 PM UTC

PDB ID : 1Z8L / pdb_00001z8l
Title : Crystal structure of prostate-specific membrane antigen, a tumor marker and peptidase
Authors : Davis, M.I.; Bennett, M.J.; Thomas, L.M.; Bjorkman, P.J.
Deposited on : 2005-03-30
Resolution : 3.50 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

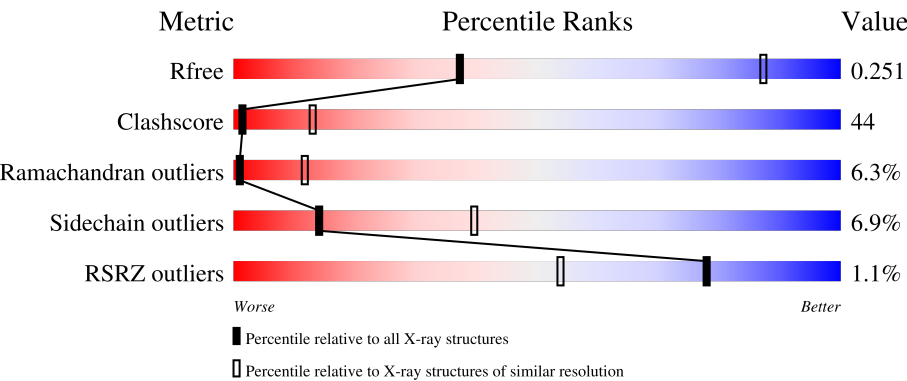
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.50 Å.

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



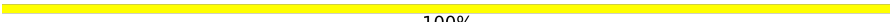
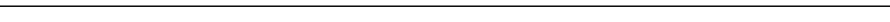
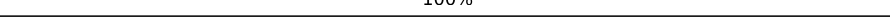
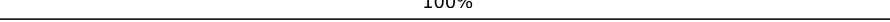
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	1085 (3.54-3.46)
Clashscore	190562	1140 (3.54-3.46)
Ramachandran outliers	187476	1113 (3.54-3.46)
Sidechain outliers	187428	1114 (3.54-3.46)
RSRZ outliers	180081	1084 (3.54-3.46)

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

Mol	Chain	Length	Quality of chain
1	A	695	% 36%50%12%.
1	B	695	36%51%12%.
1	C	695	36%51%12%.
1	D	695	3% 36%51%12%.
2	E	2	100%

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Mol	Chain	Length	Quality of chain
2	G	2	 100%
2	J	2	 100%
2	L	2	 100%
2	O	2	 100%
2	Q	2	 100%
2	T	2	 100%
2	V	2	 100%
3	F	2	 100%
3	H	2	 50% 50%
3	I	2	 100%
3	K	2	 100%
3	M	2	 100%
3	N	2	 100%
3	P	2	 100%
3	R	2	 50% 50%
3	S	2	 100%
3	U	2	 100%
3	W	2	 50% 50%
3	X	2	 100%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	G	1	X	-	-	-
2	NAG	L	1	X	-	-	-
2	NAG	Q	1	X	-	-	-
2	NAG	V	1	X	-	-	-

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 22836 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Glutamate carboxypeptidase II.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	695	Total	C	N	O	S	0	0	0
			5536	3559	929	1031	17			
1	B	695	Total	C	N	O	S	0	0	0
			5536	3559	929	1031	17			
1	C	695	Total	C	N	O	S	0	0	0
			5536	3559	929	1031	17			
1	D	695	Total	C	N	O	S	0	0	0
			5536	3559	929	1031	17			

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



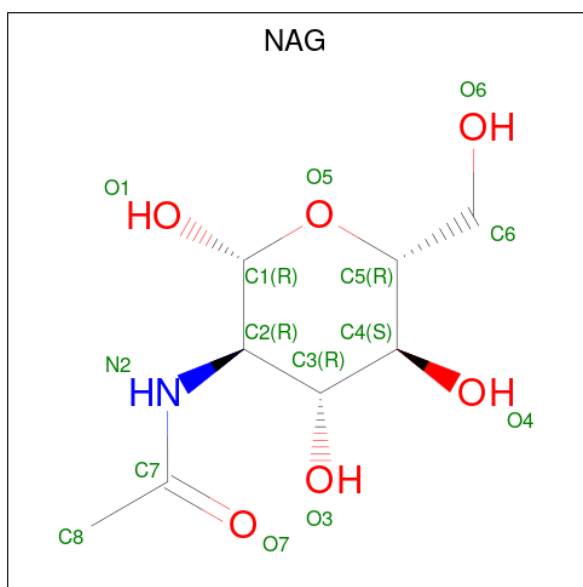
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	G	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	J	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	L	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	O	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	Q	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	T	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	V	2	Total	C	N	O	0	0	0
			28	16	2	10			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	F	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	H	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	I	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	K	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	M	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	N	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	P	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	R	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	S	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	U	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	W	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	X	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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

- Molecule 5 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	2	Total	Zn	0	0
			2	2		
5	B	2	Total	Zn	0	0
			2	2		
5	C	2	Total	Zn	0	0
			2	2		
5	D	2	Total	Zn	0	0
			2	2		

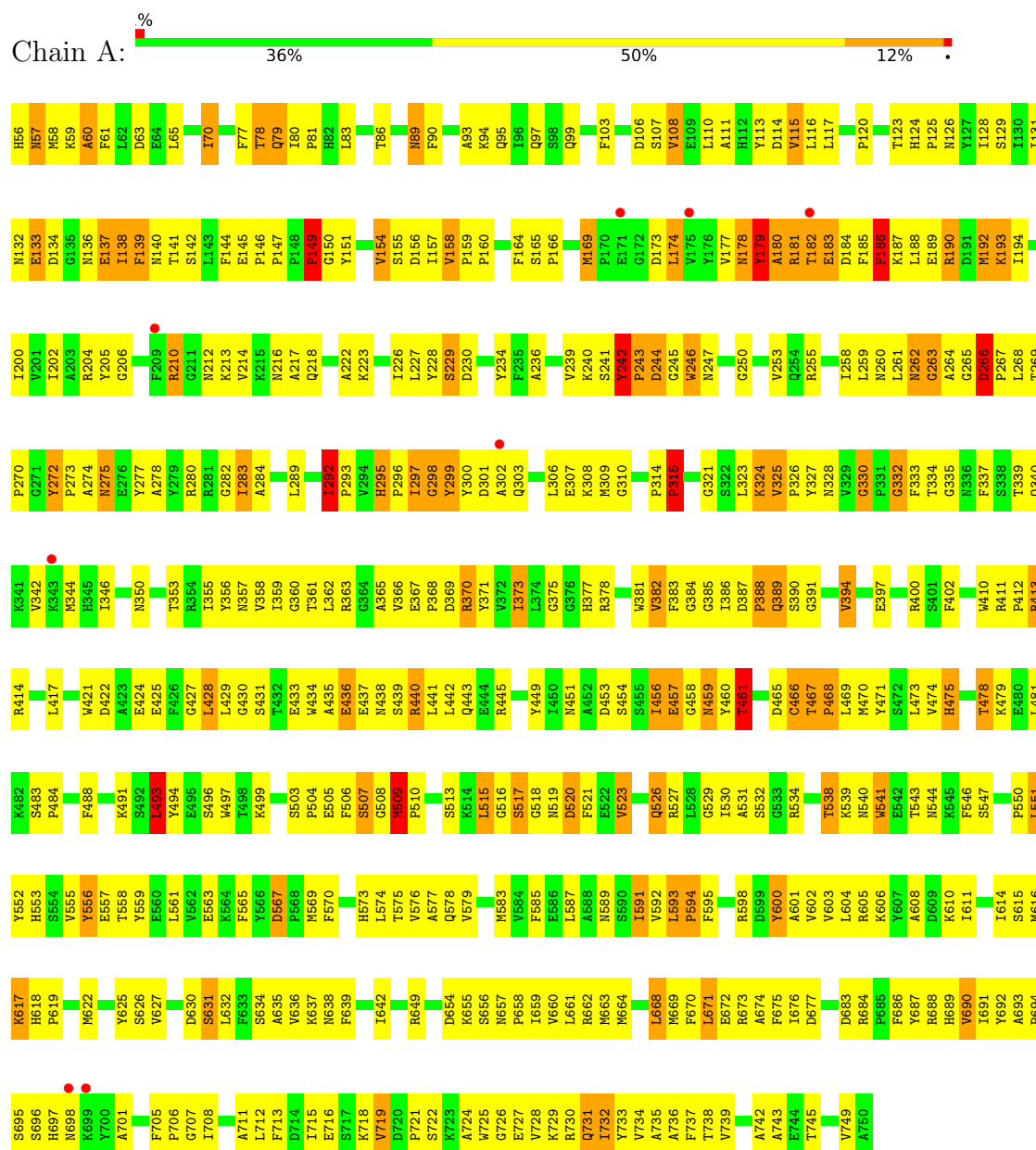
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	3	Total 3	O 3	0	0
6	B	3	Total 3	O 3	0	0
6	C	4	Total 4	O 4	0	0
6	D	2	Total 2	O 2	0	0

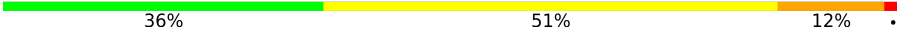
3 Residue-property plots

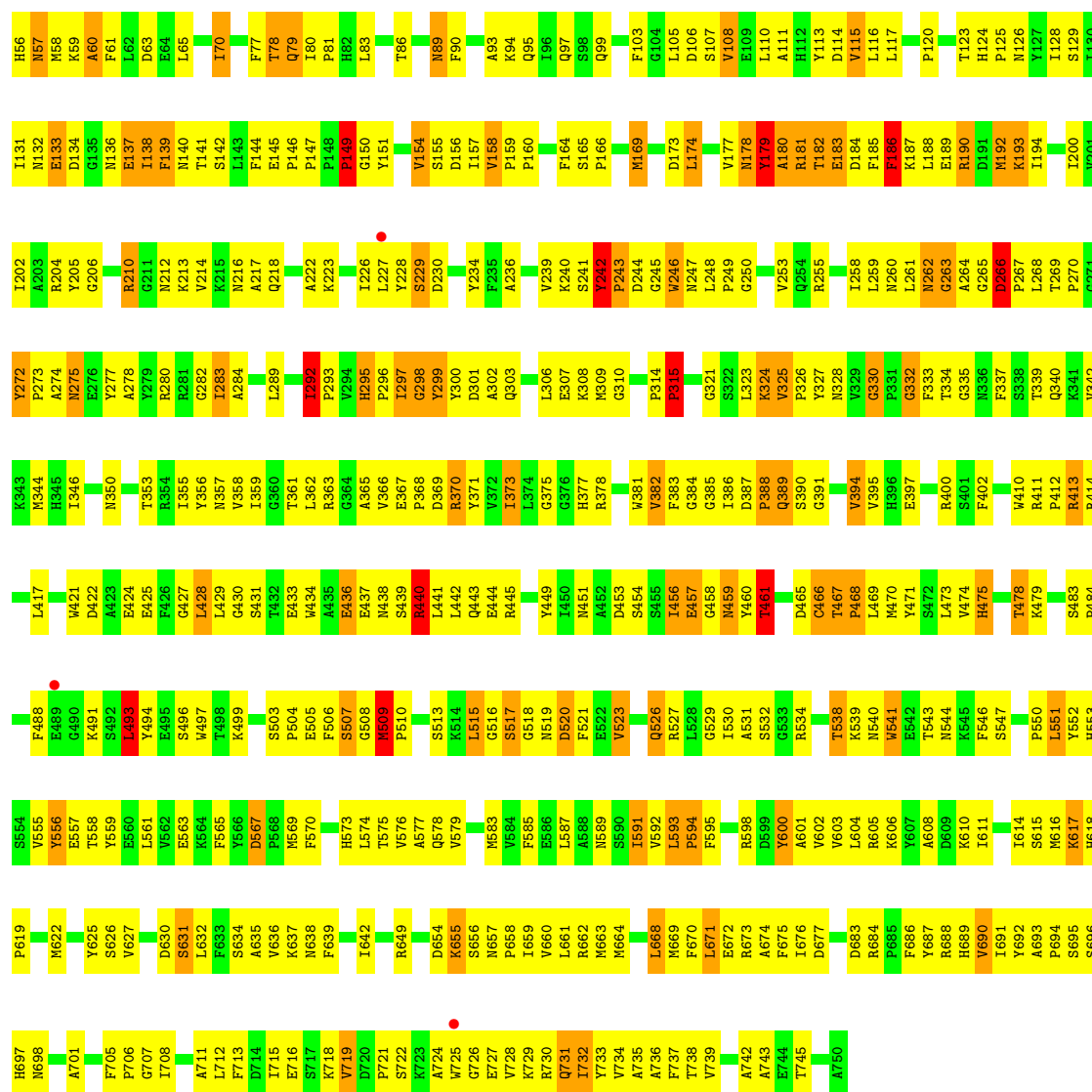
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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 dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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: Glutamate carboxypeptidase II

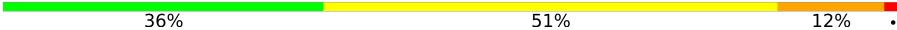


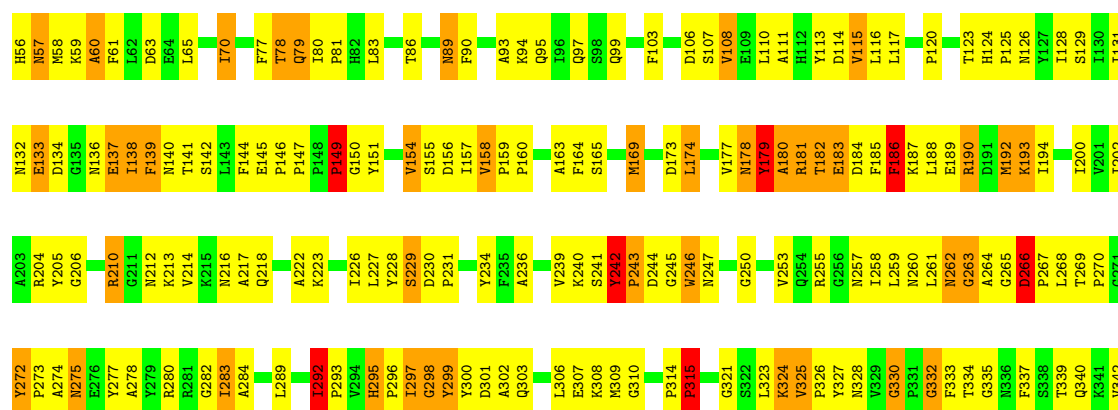
• Molecule 1: Glutamate carboxypeptidase II

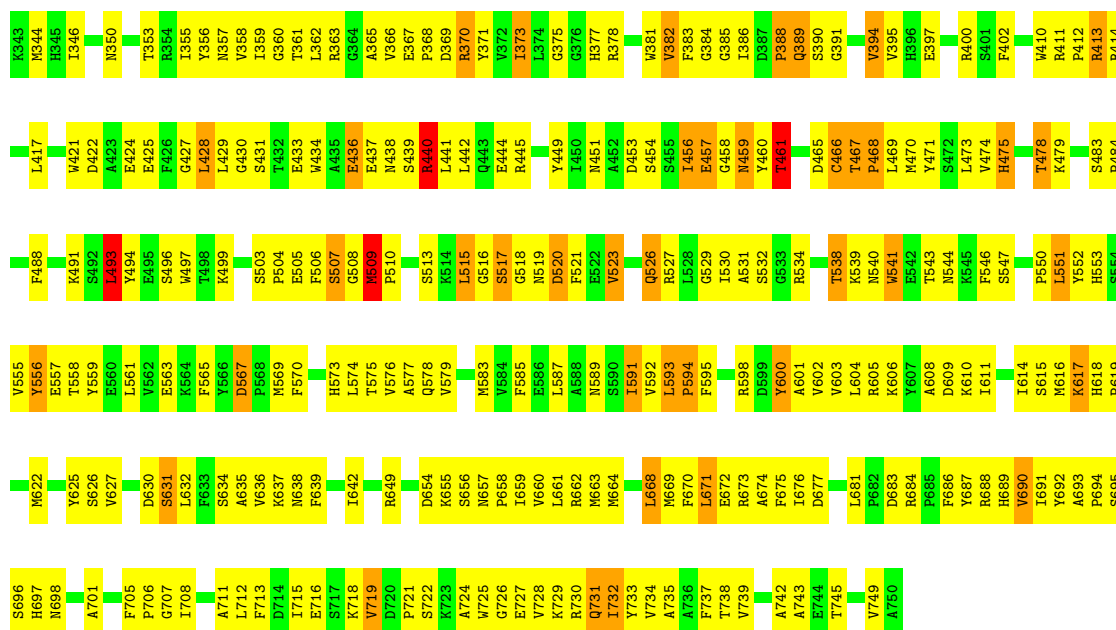
Chain B:  36% 51% 12% .



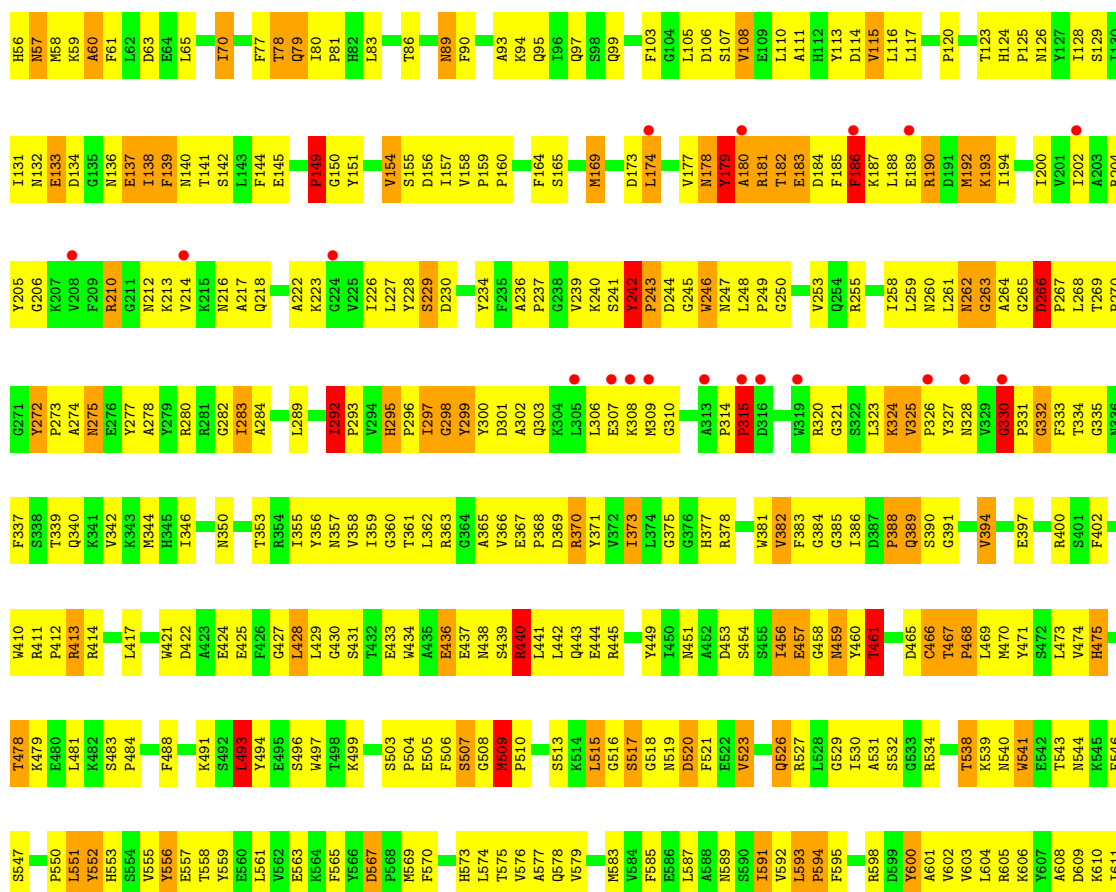
• Molecule 1: Glutamate carboxypeptidase II

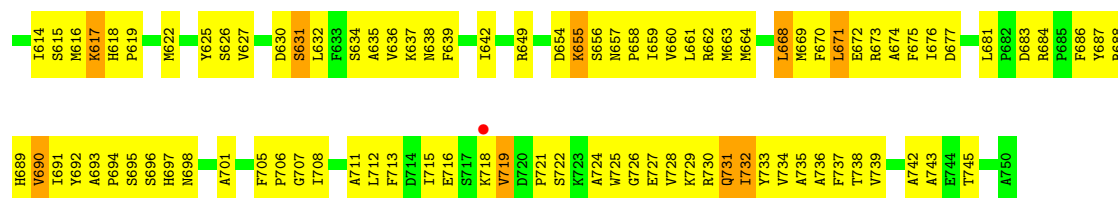
Chain C:  36% 51% 12% .





• Molecule 1: Glutamate carboxypeptidase II





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

Chain E:  100%

MAG1
NDG2

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

Chain G:  100%

MAG1
NDG2

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

Chain J:  100%

MAG1
NDG2

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

Chain L:  100%

MAG1
NDG2

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

Chain O:  100%

MAG1
NDG2

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

Chain Q:  100%

MAG1
NDG2

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

Chain T:  100%MAG1
NDG2

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

Chain V:  100%MAG1
NDG2

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

Chain F:  100%MAG1
MAG2

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

Chain H:  50% 50%MAG1
MAG2

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

Chain I:  100%MAG1
MAG2

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

Chain K:  100%MAG1
MAG2

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

Chain M:  100%

MAG1
MAG2

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

Chain N:  100%

MAG1
MAG2

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

Chain P:  100%

MAG1
MAG2

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

Chain R:  50% 50%

MAG1
MAG2

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

Chain S:  100%

MAG1
MAG2

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

Chain U:  100%

MAG1
MAG2

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

Chain W:  50% 50%

MAG1
MAG2

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

Chain X:

100%

MAG1
MAG2

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	74.86Å 157.76Å 133.84Å 90.00° 93.24° 90.00°	Depositor
Resolution (Å)	30.00 – 3.50 30.00 – 3.50	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-3.50) 98.9 (30.00-3.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.81 (at 3.39Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.252 , 0.284 0.258 , 0.251	Depositor DCC
R_{free} test set	3798 reflections (4.74%)	wwPDB-VP
Wilson B-factor (Å ²)	77.0	Xtriage
Anisotropy	0.291	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 89.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	22836	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.34% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.50	0/5693	1.13	57/7720 (0.7%)
1	B	0.50	0/5693	1.13	57/7720 (0.7%)
1	C	0.50	0/5693	1.13	57/7720 (0.7%)
1	D	0.50	0/5693	1.13	57/7720 (0.7%)
All	All	0.50	0/22772	1.13	228/30880 (0.7%)

There are no bond length outliers.

All (228) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	182	THR	N-CA-C	-12.05	98.81	113.15
1	B	182	THR	N-CA-C	-12.03	98.83	113.15
1	D	182	THR	N-CA-C	-12.02	98.84	113.15
1	C	182	THR	N-CA-C	-12.02	98.85	113.15
1	C	266	ASP	N-CA-C	-9.50	97.76	109.83
1	D	266	ASP	N-CA-C	-9.50	97.77	109.83
1	A	266	ASP	N-CA-C	-9.48	97.79	109.83
1	B	266	ASP	N-CA-C	-9.48	97.79	109.83
1	A	272	TYR	CA-C-N	8.99	129.04	119.78
1	A	272	TYR	C-N-CA	8.99	129.04	119.78
1	C	272	TYR	CA-C-N	8.99	129.04	119.78
1	C	272	TYR	C-N-CA	8.99	129.04	119.78
1	B	272	TYR	CA-C-N	8.97	129.02	119.78
1	B	272	TYR	C-N-CA	8.97	129.02	119.78
1	D	272	TYR	CA-C-N	8.96	129.01	119.78
1	D	272	TYR	C-N-CA	8.96	129.01	119.78
1	D	244	ASP	N-CA-C	-8.16	101.43	112.94
1	A	244	ASP	N-CA-C	-8.15	101.44	112.94
1	B	244	ASP	N-CA-C	-8.14	101.46	112.94
1	C	244	ASP	N-CA-C	-8.13	101.48	112.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	509	MET	CA-C-N	8.04	128.09	119.89
1	D	509	MET	C-N-CA	8.04	128.09	119.89
1	D	593	LEU	CA-C-N	8.03	129.88	119.84
1	D	593	LEU	C-N-CA	8.03	129.88	119.84
1	C	509	MET	CA-C-N	8.03	128.07	119.89
1	C	509	MET	C-N-CA	8.03	128.07	119.89
1	A	593	LEU	CA-C-N	8.02	129.87	119.84
1	A	593	LEU	C-N-CA	8.02	129.87	119.84
1	B	509	MET	CA-C-N	8.02	128.06	119.89
1	B	509	MET	C-N-CA	8.02	128.06	119.89
1	B	593	LEU	CA-C-N	7.99	129.83	119.84
1	B	593	LEU	C-N-CA	7.99	129.83	119.84
1	C	593	LEU	CA-C-N	7.98	129.82	119.84
1	C	593	LEU	C-N-CA	7.98	129.82	119.84
1	A	509	MET	CA-C-N	7.97	128.02	119.89
1	A	509	MET	C-N-CA	7.97	128.02	119.89
1	D	373	ILE	N-CA-C	7.61	118.83	108.17
1	B	373	ILE	N-CA-C	7.59	118.80	108.17
1	C	373	ILE	N-CA-C	7.59	118.80	108.17
1	A	373	ILE	N-CA-C	7.59	118.79	108.17
1	B	158	VAL	N-CA-C	7.42	115.25	107.76
1	A	158	VAL	N-CA-C	7.42	115.25	107.76
1	D	158	VAL	N-CA-C	7.40	115.24	107.76
1	C	158	VAL	N-CA-C	7.37	115.20	107.76
1	C	124	HIS	CA-C-N	7.13	127.16	119.89
1	C	124	HIS	C-N-CA	7.13	127.16	119.89
1	D	124	HIS	CA-C-N	7.12	127.15	119.89
1	D	124	HIS	C-N-CA	7.12	127.15	119.89
1	B	124	HIS	CA-C-N	7.09	127.12	119.89
1	B	124	HIS	C-N-CA	7.09	127.12	119.89
1	A	124	HIS	CA-C-N	7.08	127.11	119.89
1	A	124	HIS	C-N-CA	7.08	127.11	119.89
1	D	190	ARG	N-CA-C	-6.95	104.95	113.50
1	A	190	ARG	N-CA-C	-6.95	104.95	113.50
1	B	190	ARG	N-CA-C	-6.93	104.97	113.50
1	C	190	ARG	N-CA-C	-6.92	104.99	113.50
1	C	436	GLU	N-CA-C	-6.86	103.02	111.33
1	D	436	GLU	N-CA-C	-6.85	103.04	111.33
1	A	567	ASP	CA-C-N	6.84	126.36	119.24
1	A	567	ASP	C-N-CA	6.84	126.36	119.24
1	B	436	GLU	N-CA-C	-6.82	103.08	111.33
1	B	567	ASP	CA-C-N	6.81	126.32	119.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	567	ASP	C-N-CA	6.81	126.32	119.24
1	D	567	ASP	CA-C-N	6.80	126.32	119.24
1	D	567	ASP	C-N-CA	6.80	126.32	119.24
1	C	567	ASP	CA-C-N	6.80	126.31	119.24
1	C	567	ASP	C-N-CA	6.80	126.31	119.24
1	A	436	GLU	N-CA-C	-6.79	103.11	111.33
1	C	299	TYR	N-CA-C	6.66	119.54	111.82
1	A	299	TYR	N-CA-C	6.66	119.54	111.82
1	B	299	TYR	N-CA-C	6.65	119.53	111.82
1	C	459	ASN	N-CA-C	-6.63	104.78	114.39
1	D	299	TYR	N-CA-C	6.62	119.50	111.82
1	B	459	ASN	N-CA-C	-6.60	104.82	114.39
1	D	459	ASN	N-CA-C	-6.59	104.83	114.39
1	A	459	ASN	N-CA-C	-6.59	104.83	114.39
1	C	300	TYR	N-CA-C	-6.57	104.16	111.71
1	B	300	TYR	N-CA-C	-6.56	104.16	111.71
1	D	300	TYR	N-CA-C	-6.55	104.18	111.71
1	C	295	HIS	CA-C-N	6.54	127.06	119.99
1	C	295	HIS	C-N-CA	6.54	127.06	119.99
1	A	300	TYR	N-CA-C	-6.54	104.19	111.71
1	D	295	HIS	CA-C-N	6.48	126.98	119.99
1	D	295	HIS	C-N-CA	6.48	126.98	119.99
1	B	295	HIS	CA-C-N	6.44	126.95	119.99
1	B	295	HIS	C-N-CA	6.44	126.95	119.99
1	A	295	HIS	CA-C-N	6.43	126.93	119.99
1	A	295	HIS	C-N-CA	6.43	126.93	119.99
1	D	726	GLY	N-CA-C	-6.37	105.11	112.50
1	A	726	GLY	N-CA-C	-6.35	105.13	112.50
1	B	726	GLY	N-CA-C	-6.35	105.14	112.50
1	C	371	TYR	N-CA-C	6.33	119.55	109.24
1	C	726	GLY	N-CA-C	-6.32	105.17	112.50
1	D	371	TYR	N-CA-C	6.30	119.52	109.24
1	B	371	TYR	N-CA-C	6.29	119.48	109.24
1	A	371	TYR	N-CA-C	6.27	119.46	109.24
1	C	242	TYR	N-CA-C	6.26	123.65	109.81
1	D	242	TYR	N-CA-C	6.26	123.64	109.81
1	B	242	TYR	N-CA-C	6.24	123.61	109.81
1	A	242	TYR	N-CA-C	6.24	123.60	109.81
1	B	93	ALA	N-CA-C	-6.14	104.50	111.07
1	A	93	ALA	N-CA-C	-6.14	104.50	111.07
1	C	677	ASP	CA-C-N	6.13	127.50	119.84
1	C	677	ASP	C-N-CA	6.13	127.50	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	93	ALA	N-CA-C	-6.12	104.52	111.07
1	D	677	ASP	CA-C-N	6.11	127.48	119.84
1	D	677	ASP	C-N-CA	6.11	127.48	119.84
1	B	677	ASP	CA-C-N	6.10	127.47	119.84
1	B	677	ASP	C-N-CA	6.10	127.47	119.84
1	D	93	ALA	N-CA-C	-6.10	104.54	111.07
1	A	677	ASP	CA-C-N	6.08	127.45	119.84
1	A	677	ASP	C-N-CA	6.08	127.45	119.84
1	C	339	THR	N-CA-C	-6.08	105.83	113.18
1	D	719	VAL	N-CA-C	6.07	116.74	110.36
1	A	719	VAL	N-CA-C	6.07	116.73	110.36
1	B	719	VAL	N-CA-C	6.06	116.72	110.36
1	C	719	VAL	N-CA-C	6.05	116.72	110.36
1	A	339	THR	N-CA-C	-6.04	105.87	113.18
1	B	339	THR	N-CA-C	-6.03	105.89	113.18
1	D	339	THR	N-CA-C	-6.00	105.92	113.18
1	A	732	ILE	N-CA-C	-6.00	104.50	110.62
1	B	732	ILE	N-CA-C	-5.99	104.51	110.62
1	D	394	VAL	N-CA-C	-5.99	104.67	110.42
1	C	394	VAL	N-CA-C	-5.97	104.69	110.42
1	A	394	VAL	N-CA-C	-5.96	104.69	110.42
1	B	394	VAL	N-CA-C	-5.96	104.70	110.42
1	C	732	ILE	N-CA-C	-5.94	104.56	110.62
1	D	732	ILE	N-CA-C	-5.93	104.58	110.62
1	A	509	MET	N-CA-C	5.92	115.11	108.25
1	B	509	MET	N-CA-C	5.91	115.10	108.25
1	B	330	GLY	CA-C-N	5.90	127.22	119.84
1	B	330	GLY	C-N-CA	5.90	127.22	119.84
1	C	79	GLN	N-CA-C	5.90	119.57	112.38
1	C	509	MET	N-CA-C	5.89	115.09	108.25
1	C	330	GLY	CA-C-N	5.88	127.19	119.84
1	C	330	GLY	C-N-CA	5.88	127.19	119.84
1	D	79	GLN	N-CA-C	5.87	119.54	112.38
1	D	509	MET	N-CA-C	5.86	115.05	108.25
1	D	330	GLY	CA-C-N	5.86	127.17	119.84
1	D	330	GLY	C-N-CA	5.86	127.17	119.84
1	A	79	GLN	N-CA-C	5.86	119.52	112.38
1	A	330	GLY	CA-C-N	5.85	127.15	119.84
1	A	330	GLY	C-N-CA	5.85	127.15	119.84
1	B	79	GLN	N-CA-C	5.85	119.52	112.38
1	B	89	ASN	N-CA-C	-5.84	105.05	111.82
1	C	89	ASN	N-CA-C	-5.83	105.06	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	89	ASN	N-CA-C	-5.82	105.07	111.82
1	C	78	THR	N-CA-C	5.82	120.52	112.90
1	D	493	LEU	N-CA-C	-5.81	104.95	111.28
1	D	89	ASN	N-CA-C	-5.81	105.08	111.82
1	D	78	THR	N-CA-C	5.80	120.50	112.90
1	D	298	GLY	N-CA-C	-5.80	103.80	113.02
1	B	298	GLY	N-CA-C	-5.79	103.82	113.02
1	B	78	THR	N-CA-C	5.78	120.48	112.90
1	C	493	LEU	N-CA-C	-5.78	104.98	111.28
1	C	298	GLY	N-CA-C	-5.78	103.83	113.02
1	A	298	GLY	N-CA-C	-5.77	103.84	113.02
1	D	413	ARG	N-CA-C	-5.77	104.68	110.97
1	B	493	LEU	N-CA-C	-5.76	105.00	111.28
1	A	493	LEU	N-CA-C	-5.76	105.00	111.28
1	A	78	THR	N-CA-C	5.75	120.44	112.90
1	A	413	ARG	N-CA-C	-5.75	104.70	110.97
1	B	413	ARG	N-CA-C	-5.74	104.71	110.97
1	C	413	ARG	N-CA-C	-5.74	104.71	110.97
1	A	461	THR	N-CA-C	5.68	122.91	110.80
1	C	461	THR	N-CA-C	5.68	122.90	110.80
1	B	461	THR	N-CA-C	5.67	122.88	110.80
1	D	461	THR	N-CA-C	5.67	122.87	110.80
1	A	523	VAL	CB-CA-C	-5.66	104.74	111.81
1	A	617	LYS	N-CA-C	-5.66	106.42	113.15
1	C	617	LYS	N-CA-C	-5.65	106.43	113.15
1	D	617	LYS	N-CA-C	-5.65	106.43	113.15
1	D	523	VAL	CB-CA-C	-5.64	104.75	111.81
1	B	617	LYS	N-CA-C	-5.64	106.44	113.15
1	B	523	VAL	CB-CA-C	-5.63	104.77	111.81
1	C	523	VAL	CB-CA-C	-5.61	104.80	111.81
1	D	546	PHE	N-CA-C	5.60	117.14	110.19
1	C	546	PHE	N-CA-C	5.58	117.11	110.19
1	B	546	PHE	N-CA-C	5.57	117.09	110.19
1	A	546	PHE	N-CA-C	5.55	117.07	110.19
1	A	223	LYS	N-CA-C	-5.50	106.93	113.97
1	B	223	LYS	N-CA-C	-5.48	106.96	113.97
1	C	223	LYS	N-CA-C	-5.47	106.97	113.97
1	D	466	CYS	N-CA-C	5.46	116.75	108.07
1	D	223	LYS	N-CA-C	-5.46	106.99	113.97
1	B	466	CYS	N-CA-C	5.45	116.74	108.07
1	C	466	CYS	N-CA-C	5.43	116.71	108.07
1	A	466	CYS	N-CA-C	5.42	116.69	108.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	158	VAL	CA-C-N	5.38	125.92	120.38
1	D	158	VAL	C-N-CA	5.38	125.92	120.38
1	B	158	VAL	CA-C-N	5.37	125.91	120.38
1	B	158	VAL	C-N-CA	5.37	125.91	120.38
1	C	158	VAL	CA-C-N	5.37	125.91	120.38
1	C	158	VAL	C-N-CA	5.37	125.91	120.38
1	A	158	VAL	CA-C-N	5.32	125.86	120.38
1	A	158	VAL	C-N-CA	5.32	125.86	120.38
1	B	169	MET	CA-C-N	5.28	125.70	119.99
1	B	169	MET	C-N-CA	5.28	125.70	119.99
1	D	169	MET	CA-C-N	5.28	125.70	119.99
1	D	169	MET	C-N-CA	5.28	125.70	119.99
1	A	169	MET	CA-C-N	5.28	125.69	119.99
1	A	169	MET	C-N-CA	5.28	125.69	119.99
1	C	169	MET	CA-C-N	5.28	125.69	119.99
1	C	169	MET	C-N-CA	5.28	125.69	119.99
1	C	115	VAL	N-CA-C	5.21	116.81	108.89
1	B	115	VAL	N-CA-C	5.20	116.79	108.89
1	D	115	VAL	N-CA-C	5.19	116.78	108.89
1	A	115	VAL	N-CA-C	5.19	116.78	108.89
1	B	186	PHE	N-CA-C	-5.16	106.83	113.23
1	D	186	PHE	N-CA-C	-5.16	106.83	113.23
1	C	186	PHE	N-CA-C	-5.15	106.84	113.23
1	A	186	PHE	N-CA-C	-5.15	106.85	113.23
1	C	378	ARG	N-CA-C	-5.13	107.67	114.04
1	D	378	ARG	N-CA-C	-5.12	107.69	114.04
1	B	378	ARG	N-CA-C	-5.10	107.71	114.04
1	A	378	ARG	N-CA-C	-5.09	107.73	114.04
1	C	593	LEU	N-CA-C	5.09	116.10	109.64
1	A	593	LEU	N-CA-C	5.09	116.10	109.64
1	B	593	LEU	N-CA-C	5.07	116.08	109.64
1	D	593	LEU	N-CA-C	5.06	116.07	109.64
1	B	292	ILE	CA-C-N	5.04	125.03	119.89
1	B	292	ILE	C-N-CA	5.04	125.03	119.89
1	D	292	ILE	CA-C-N	5.04	125.03	119.89
1	D	292	ILE	C-N-CA	5.04	125.03	119.89
1	C	292	ILE	CA-C-N	5.03	125.02	119.89
1	C	292	ILE	C-N-CA	5.03	125.02	119.89
1	A	292	ILE	CA-C-N	5.02	125.01	119.89
1	A	292	ILE	C-N-CA	5.02	125.01	119.89

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5536	0	5373	492	11
1	B	5536	0	5373	500	9
1	C	5536	0	5373	496	14
1	D	5536	0	5373	499	16
2	E	28	0	24	2	0
2	G	28	0	24	1	1
2	J	28	0	24	2	0
2	L	28	0	24	1	0
2	O	28	0	24	1	0
2	Q	28	0	24	1	0
2	T	28	0	24	1	0
2	V	28	0	24	1	0
3	F	28	0	25	1	0
3	H	28	0	25	5	0
3	I	28	0	25	0	0
3	K	28	0	25	1	0
3	M	28	0	25	5	1
3	N	28	0	25	0	0
3	P	28	0	25	1	0
3	R	28	0	25	5	0
3	S	28	0	25	0	0
3	U	28	0	25	1	0
3	W	28	0	25	5	0
3	X	28	0	25	0	0
4	A	28	0	26	5	0
4	B	28	0	26	6	0
4	C	28	0	26	5	0
4	D	28	0	26	5	0
5	A	2	0	0	0	0
5	B	2	0	0	0	0
5	C	2	0	0	0	0
5	D	2	0	0	0	0
6	A	3	0	0	0	0
6	B	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	C	4	0	0	0	0
6	D	2	0	0	0	0
All	All	22836	0	22088	1966	26

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 44.

All (1966) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:140:ASN:HB2	4:A:1760:NAG:H62	1.33	1.10
1:C:140:ASN:HB2	4:C:3760:NAG:H62	1.33	1.10
1:D:128:ILE:HD13	1:D:226:ILE:HD12	1.33	1.08
1:C:128:ILE:HD13	1:C:226:ILE:HD12	1.33	1.07
1:A:128:ILE:HD13	1:A:226:ILE:HD12	1.33	1.07
1:B:128:ILE:HD13	1:B:226:ILE:HD12	1.33	1.07
1:D:140:ASN:HB2	4:D:4760:NAG:H62	1.33	1.07
1:B:655:LYS:O	1:D:656:SER:HA	1.54	1.06
1:A:181:ARG:HB2	1:A:186:PHE:HD1	1.21	1.05
1:B:140:ASN:HB2	4:B:2760:NAG:H62	1.33	1.05
1:B:181:ARG:HB2	1:B:186:PHE:HD1	1.21	1.04
1:B:307:GLU:HA	1:B:325:VAL:HG21	1.40	1.03
1:D:307:GLU:HA	1:D:325:VAL:HG21	1.40	1.03
1:A:307:GLU:HA	1:A:325:VAL:HG21	1.40	1.02
1:C:192:MET:HE1	1:C:315:PRO:HG3	1.42	1.01
1:C:307:GLU:HA	1:C:325:VAL:HG21	1.40	1.01
1:D:181:ARG:HB2	1:D:186:PHE:HD1	1.21	1.01
1:B:192:MET:HE1	1:B:315:PRO:HG3	1.42	1.01
1:C:181:ARG:HB2	1:C:186:PHE:HD1	1.21	1.00
1:A:325:VAL:HG22	1:A:326:PRO:HD2	1.45	0.99
1:A:663:MET:HG2	1:B:369:ASP:CG	1.86	0.99
1:A:192:MET:HE1	1:A:315:PRO:HG3	1.42	0.98
1:B:382:VAL:HG23	1:B:383:PHE:H	1.28	0.98
1:C:325:VAL:HG22	1:C:326:PRO:HD2	1.45	0.97
1:B:325:VAL:HG22	1:B:326:PRO:HD2	1.45	0.97
1:A:181:ARG:C	1:A:183:GLU:H	1.71	0.97
1:D:325:VAL:HG22	1:D:326:PRO:HD2	1.45	0.97
1:A:382:VAL:HG23	1:A:383:PHE:H	1.28	0.96
1:D:192:MET:HE1	1:D:315:PRO:HG3	1.42	0.96
1:D:181:ARG:HB2	1:D:186:PHE:CD1	2.00	0.96
1:A:181:ARG:HB2	1:A:186:PHE:CD1	2.00	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:382:VAL:HG23	1:C:383:PHE:H	1.28	0.96
1:D:382:VAL:HG23	1:D:383:PHE:H	1.28	0.96
1:C:181:ARG:HB2	1:C:186:PHE:CD1	2.00	0.96
1:D:181:ARG:C	1:D:183:GLU:H	1.71	0.95
1:B:181:ARG:HB2	1:B:186:PHE:CD1	2.00	0.95
1:C:181:ARG:C	1:C:183:GLU:H	1.71	0.95
1:B:181:ARG:C	1:B:183:GLU:H	1.71	0.90
1:D:240:LYS:HB2	1:D:245:GLY:HA2	1.53	0.90
1:A:181:ARG:HB3	1:A:216:ASN:HB3	1.53	0.90
1:A:240:LYS:HB2	1:A:245:GLY:HA2	1.53	0.90
1:B:240:LYS:HB2	1:B:245:GLY:HA2	1.53	0.90
1:B:115:VAL:HG11	1:B:429:LEU:HD13	1.55	0.89
1:B:116:LEU:HD11	1:B:350:ASN:HB3	1.54	0.89
1:A:116:LEU:HD11	1:A:350:ASN:HB3	1.54	0.89
1:B:654:ASP:HB2	1:D:591:ILE:HD11	1.53	0.89
1:D:181:ARG:HB3	1:D:216:ASN:HB3	1.53	0.89
1:D:116:LEU:HD11	1:D:350:ASN:HB3	1.54	0.88
1:C:663:MET:HG2	1:D:369:ASP:CG	1.98	0.88
1:C:181:ARG:HB3	1:C:216:ASN:HB3	1.52	0.88
1:D:115:VAL:HG11	1:D:429:LEU:HD13	1.55	0.88
1:C:240:LYS:HB2	1:C:245:GLY:HA2	1.53	0.88
1:A:173:ASP:HB3	1:A:332:GLY:H	1.39	0.88
1:B:173:ASP:HB3	1:B:332:GLY:H	1.39	0.87
1:B:181:ARG:HB3	1:B:216:ASN:HB3	1.53	0.87
1:D:173:ASP:HB3	1:D:332:GLY:H	1.39	0.87
1:A:81:PRO:HA	1:A:382:VAL:O	1.75	0.87
1:B:246:TRP:HZ2	3:M:1:NAG:H82	1.39	0.86
1:C:115:VAL:HG11	1:C:429:LEU:HD13	1.55	0.86
1:D:246:TRP:HZ2	3:W:1:NAG:H82	1.39	0.86
1:D:81:PRO:HA	1:D:382:VAL:O	1.75	0.86
1:C:116:LEU:HD11	1:C:350:ASN:HB3	1.54	0.86
1:A:246:TRP:HZ2	3:H:1:NAG:H82	1.39	0.86
1:C:81:PRO:HA	1:C:382:VAL:O	1.75	0.85
1:B:81:PRO:HA	1:B:382:VAL:O	1.75	0.85
1:C:246:TRP:HZ2	3:R:1:NAG:H82	1.40	0.85
1:D:70:ILE:CD1	1:D:573:HIS:HB3	2.07	0.85
1:D:478:THR:HG23	1:D:494:TYR:HB2	1.58	0.85
1:B:70:ILE:CD1	1:B:573:HIS:HB3	2.07	0.85
1:A:115:VAL:HG11	1:A:429:LEU:HD13	1.55	0.85
1:A:70:ILE:CD1	1:A:573:HIS:HB3	2.07	0.85
1:A:478:THR:HG23	1:A:494:TYR:HB2	1.59	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:70:ILE:CD1	1:C:573:HIS:HB3	2.07	0.84
1:B:478:THR:HG23	1:B:494:TYR:HB2	1.59	0.84
1:C:173:ASP:HB3	1:C:332:GLY:H	1.39	0.84
1:C:478:THR:HG23	1:C:494:TYR:HB2	1.59	0.84
1:A:749:VAL:HG12	1:B:445:ARG:CZ	2.08	0.83
1:C:366:VAL:C	1:C:368:PRO:HD3	2.03	0.83
1:A:366:VAL:C	1:A:368:PRO:HD3	2.03	0.83
1:B:366:VAL:C	1:B:368:PRO:HD3	2.03	0.83
1:D:366:VAL:C	1:D:368:PRO:HD3	2.03	0.82
1:A:255:ARG:HD2	1:A:553:HIS:O	1.80	0.82
1:C:255:ARG:HD2	1:C:553:HIS:O	1.79	0.81
1:B:255:ARG:HD2	1:B:553:HIS:O	1.79	0.81
1:D:468:PRO:HA	1:D:471:TYR:CE1	2.16	0.81
1:A:468:PRO:HA	1:A:471:TYR:CE1	2.16	0.80
1:D:255:ARG:HD2	1:D:553:HIS:O	1.79	0.80
1:D:690:VAL:HG21	1:D:738:THR:HG21	1.63	0.80
1:D:157:ILE:HD11	1:D:383:PHE:CZ	2.17	0.80
1:C:690:VAL:HG21	1:C:738:THR:HG21	1.63	0.80
1:B:468:PRO:HA	1:B:471:TYR:CE1	2.16	0.80
1:C:468:PRO:HA	1:C:471:TYR:CE1	2.16	0.80
1:D:241:SER:O	1:D:243:PRO:HD2	1.82	0.80
1:B:157:ILE:HD11	1:B:383:PHE:CZ	2.17	0.80
1:A:157:ILE:HD11	1:A:383:PHE:CZ	2.17	0.80
1:B:690:VAL:HG21	1:B:738:THR:HG21	1.63	0.79
1:C:241:SER:O	1:C:243:PRO:HD2	1.82	0.79
1:C:157:ILE:HD11	1:C:383:PHE:CZ	2.17	0.79
1:C:382:VAL:HG23	1:C:383:PHE:N	1.97	0.79
1:C:77:PHE:HB3	1:C:389:GLN:HG3	1.65	0.79
1:B:241:SER:O	1:B:243:PRO:HD2	1.82	0.79
1:D:719:VAL:O	1:D:721:PRO:HD3	1.84	0.78
1:A:241:SER:O	1:A:243:PRO:HD2	1.82	0.78
1:B:382:VAL:HG23	1:B:383:PHE:N	1.96	0.78
1:A:551:LEU:HD22	1:A:556:TYR:HB2	1.66	0.78
1:D:228:TYR:HB2	1:D:297:ILE:HG22	1.66	0.78
1:B:719:VAL:O	1:B:721:PRO:HD3	1.84	0.78
1:C:228:TYR:HB2	1:C:297:ILE:HG22	1.66	0.78
1:D:382:VAL:HG23	1:D:383:PHE:N	1.96	0.78
1:B:551:LEU:HD22	1:B:556:TYR:HB2	1.66	0.78
1:A:690:VAL:HG21	1:A:738:THR:HG21	1.64	0.77
1:A:719:VAL:O	1:A:721:PRO:HD3	1.84	0.77
1:C:719:VAL:O	1:C:721:PRO:HD3	1.84	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:174:LEU:HD11	1:B:342:VAL:HG13	1.66	0.77
1:A:228:TYR:HB2	1:A:297:ILE:HG22	1.66	0.77
1:B:228:TYR:HB2	1:B:297:ILE:HG22	1.66	0.77
1:C:174:LEU:HD11	1:C:342:VAL:HG13	1.66	0.77
1:D:77:PHE:HB3	1:D:389:GLN:HG3	1.65	0.77
1:D:551:LEU:HD22	1:D:556:TYR:HB2	1.66	0.77
1:A:77:PHE:HB3	1:A:389:GLN:HG3	1.65	0.77
1:D:174:LEU:HD11	1:D:342:VAL:HG13	1.66	0.77
1:C:240:LYS:H	1:C:240:LYS:HD2	1.50	0.77
1:C:551:LEU:HD22	1:C:556:TYR:HB2	1.66	0.77
1:B:240:LYS:H	1:B:240:LYS:HD2	1.50	0.77
1:C:70:ILE:HD13	1:C:573:HIS:HB3	1.67	0.77
1:A:382:VAL:HG23	1:A:383:PHE:N	1.96	0.76
1:C:732:ILE:HD12	1:C:733:TYR:N	2.01	0.76
1:D:240:LYS:H	1:D:240:LYS:HD2	1.50	0.76
1:A:174:LEU:HD11	1:A:342:VAL:HG13	1.66	0.76
1:A:145:GLU:CD	1:A:555:VAL:HG23	2.11	0.76
1:B:70:ILE:HD13	1:B:573:HIS:HB3	1.67	0.76
1:B:732:ILE:HD12	1:B:733:TYR:N	2.01	0.76
1:B:77:PHE:HB3	1:B:389:GLN:HG3	1.65	0.76
1:C:145:GLU:CD	1:C:555:VAL:HG23	2.11	0.76
1:A:674:ALA:O	1:B:440:ARG:NH1	2.19	0.75
1:B:145:GLU:CD	1:B:555:VAL:HG23	2.11	0.75
1:D:70:ILE:HD13	1:D:573:HIS:HB3	1.67	0.75
1:A:70:ILE:HD13	1:A:573:HIS:HB3	1.67	0.75
1:A:421:TRP:CE3	1:A:431:SER:HA	2.21	0.75
1:B:192:MET:HE1	1:B:315:PRO:CG	2.17	0.75
1:A:192:MET:HE1	1:A:315:PRO:CG	2.17	0.75
1:B:421:TRP:CE3	1:B:431:SER:HA	2.21	0.75
1:D:503:SER:HB2	1:D:510:PRO:O	1.87	0.75
1:D:632:LEU:O	1:D:636:VAL:HG23	1.87	0.75
1:A:515:LEU:HD21	1:A:534:ARG:HG2	1.68	0.75
1:B:515:LEU:HD21	1:B:534:ARG:HG2	1.68	0.75
1:A:732:ILE:HD12	1:A:733:TYR:N	2.01	0.74
1:C:515:LEU:HD21	1:C:534:ARG:HG2	1.68	0.74
1:D:421:TRP:CE3	1:D:431:SER:HA	2.21	0.74
1:C:421:TRP:CE3	1:C:431:SER:HA	2.21	0.74
1:A:698:ASN:HD22	1:A:701:ALA:HB3	1.53	0.74
1:C:503:SER:HB2	1:C:510:PRO:O	1.87	0.74
1:A:632:LEU:O	1:A:636:VAL:HG23	1.87	0.74
1:D:192:MET:HE1	1:D:315:PRO:CG	2.17	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:145:GLU:CD	1:D:555:VAL:HG23	2.11	0.74
1:A:240:LYS:H	1:A:240:LYS:HD2	1.50	0.74
1:B:503:SER:HB2	1:B:510:PRO:O	1.87	0.73
1:B:632:LEU:O	1:B:636:VAL:HG23	1.87	0.73
1:D:698:ASN:HD22	1:D:701:ALA:HB3	1.53	0.73
1:D:732:ILE:HD12	1:D:733:TYR:N	2.01	0.73
1:B:654:ASP:CB	1:D:591:ILE:HD11	2.17	0.73
1:D:515:LEU:HD21	1:D:534:ARG:HG2	1.68	0.73
1:B:465:ASP:OD1	1:B:513:SER:HB2	1.88	0.73
1:B:698:ASN:HD22	1:B:701:ALA:HB3	1.53	0.73
1:D:181:ARG:HB3	1:D:216:ASN:CB	2.19	0.73
1:A:465:ASP:OD1	1:A:513:SER:HB2	1.88	0.73
1:C:465:ASP:OD1	1:C:513:SER:HB2	1.88	0.73
1:C:192:MET:HE1	1:C:315:PRO:CG	2.17	0.73
1:C:261:LEU:O	1:C:262:ASN:C	2.32	0.73
1:D:261:LEU:O	1:D:262:ASN:C	2.32	0.73
1:A:261:LEU:O	1:A:262:ASN:C	2.31	0.73
1:A:503:SER:HB2	1:A:510:PRO:O	1.87	0.73
1:C:632:LEU:O	1:C:636:VAL:HG23	1.87	0.73
1:C:698:ASN:HD22	1:C:701:ALA:HB3	1.53	0.72
1:B:261:LEU:O	1:B:262:ASN:C	2.32	0.72
1:A:181:ARG:HB3	1:A:216:ASN:CB	2.19	0.72
1:A:730:ARG:O	1:A:733:TYR:HB3	1.90	0.72
1:D:465:ASP:OD1	1:D:513:SER:HB2	1.88	0.72
1:B:394:VAL:HG13	1:B:577:ALA:HB2	1.72	0.72
1:D:730:ARG:O	1:D:733:TYR:HB3	1.90	0.72
1:B:373:ILE:HD12	1:B:417:LEU:HB2	1.72	0.72
1:B:293:PRO:HB2	1:B:346:ILE:HD12	1.72	0.72
1:B:181:ARG:HB3	1:B:216:ASN:CB	2.19	0.71
1:B:730:ARG:O	1:B:733:TYR:HB3	1.90	0.71
1:D:77:PHE:CB	1:D:389:GLN:HG3	2.20	0.71
1:D:181:ARG:C	1:D:183:GLU:N	2.43	0.71
1:A:181:ARG:CB	1:A:216:ASN:HB3	2.21	0.71
1:C:181:ARG:HB3	1:C:216:ASN:CB	2.19	0.71
1:C:293:PRO:HB2	1:C:346:ILE:HD12	1.72	0.71
1:C:394:VAL:HG13	1:C:577:ALA:HB2	1.72	0.71
1:B:145:GLU:OE1	1:B:555:VAL:HG23	1.90	0.71
1:A:77:PHE:CB	1:A:389:GLN:HG3	2.20	0.71
1:A:394:VAL:HG13	1:A:577:ALA:HB2	1.72	0.71
1:C:181:ARG:C	1:C:183:GLU:N	2.42	0.71
1:C:730:ARG:O	1:C:733:TYR:HB3	1.90	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:145:GLU:OE1	1:C:555:VAL:HG23	1.90	0.71
1:C:373:ILE:HD12	1:C:417:LEU:HB2	1.72	0.71
1:A:145:GLU:OE1	1:A:555:VAL:HG23	1.90	0.71
1:D:181:ARG:HG2	1:D:183:GLU:HA	1.73	0.71
1:B:181:ARG:C	1:B:183:GLU:N	2.43	0.71
1:D:145:GLU:OE1	1:D:555:VAL:HG23	1.90	0.71
1:D:181:ARG:CB	1:D:216:ASN:HB3	2.21	0.71
1:D:293:PRO:HB2	1:D:346:ILE:HD12	1.72	0.71
1:B:113:TYR:HB3	1:B:274:ALA:HB3	1.73	0.71
1:C:113:TYR:HB3	1:C:274:ALA:HB3	1.73	0.71
1:B:735:ALA:O	1:B:739:VAL:HG23	1.91	0.70
1:C:181:ARG:CB	1:C:216:ASN:HB3	2.21	0.70
1:A:113:TYR:HB3	1:A:274:ALA:HB3	1.73	0.70
1:A:181:ARG:HG2	1:A:183:GLU:HA	1.73	0.70
1:B:174:LEU:HD12	1:B:174:LEU:N	2.06	0.70
1:D:394:VAL:HG13	1:D:577:ALA:HB2	1.72	0.70
1:B:77:PHE:CB	1:B:389:GLN:HG3	2.20	0.70
1:B:90:PHE:CZ	1:B:94:LYS:HE3	2.27	0.70
1:A:174:LEU:HD12	1:A:174:LEU:N	2.06	0.70
1:A:735:ALA:O	1:A:739:VAL:HG23	1.91	0.70
1:C:174:LEU:N	1:C:174:LEU:HD12	2.07	0.70
1:A:659:ILE:H	1:A:659:ILE:HD12	1.57	0.70
1:B:181:ARG:HG3	1:B:186:PHE:HB2	1.74	0.70
1:D:181:ARG:HG3	1:D:186:PHE:HB2	1.74	0.70
1:C:77:PHE:CB	1:C:389:GLN:HG3	2.20	0.70
1:D:90:PHE:CZ	1:D:94:LYS:HE3	2.27	0.70
1:A:181:ARG:HG3	1:A:186:PHE:HB2	1.74	0.70
1:B:659:ILE:H	1:B:659:ILE:HD12	1.56	0.70
1:C:659:ILE:HD12	1:C:659:ILE:H	1.57	0.70
1:C:735:ALA:O	1:C:739:VAL:HG23	1.91	0.70
1:A:90:PHE:CZ	1:A:94:LYS:HE3	2.27	0.70
1:C:181:ARG:HG3	1:C:186:PHE:HB2	1.74	0.70
1:D:735:ALA:O	1:D:739:VAL:HG23	1.91	0.70
1:D:174:LEU:HD12	1:D:174:LEU:N	2.06	0.69
1:D:659:ILE:H	1:D:659:ILE:HD12	1.56	0.69
1:A:293:PRO:HB2	1:A:346:ILE:HD12	1.72	0.69
1:A:373:ILE:HD12	1:A:417:LEU:HB2	1.72	0.69
1:D:70:ILE:HD11	1:D:573:HIS:HB3	1.74	0.69
1:A:70:ILE:HD11	1:A:573:HIS:HB3	1.74	0.69
1:C:90:PHE:CZ	1:C:94:LYS:HE3	2.27	0.69
1:D:373:ILE:HD12	1:D:417:LEU:HB2	1.72	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:187:LYS:HE3	1:A:190:ARG:HH22	1.58	0.69
1:B:187:LYS:HE3	1:B:190:ARG:HH22	1.58	0.69
1:D:113:TYR:HB3	1:D:274:ALA:HB3	1.73	0.69
1:B:656:SER:HA	1:D:655:LYS:O	1.93	0.69
1:A:541:TRP:HA	1:A:541:TRP:CE3	2.28	0.69
1:B:181:ARG:HG2	1:B:183:GLU:HA	1.73	0.69
1:B:181:ARG:CB	1:B:216:ASN:HB3	2.21	0.68
1:C:70:ILE:HD11	1:C:573:HIS:HB3	1.74	0.68
1:B:550:PRO:O	1:B:551:LEU:HB2	1.94	0.68
1:C:181:ARG:HG2	1:C:183:GLU:HA	1.73	0.68
1:D:187:LYS:HE3	1:D:190:ARG:HH22	1.58	0.68
1:A:377:HIS:NE2	1:A:453:ASP:OD1	2.27	0.68
1:B:591:ILE:HD11	1:D:654:ASP:HB2	1.74	0.68
1:D:689:HIS:HB3	1:D:692:TYR:O	1.94	0.68
1:B:504:PRO:O	1:B:505:GLU:HB3	1.93	0.68
1:D:377:HIS:NE2	1:D:453:ASP:OD1	2.27	0.68
1:A:181:ARG:C	1:A:183:GLU:N	2.43	0.68
1:A:550:PRO:O	1:A:551:LEU:HB2	1.93	0.68
1:B:214:VAL:O	1:B:217:ALA:HB3	1.94	0.68
1:C:115:VAL:CG1	1:C:429:LEU:HD13	2.24	0.68
1:C:214:VAL:O	1:C:217:ALA:HB3	1.94	0.68
1:C:550:PRO:O	1:C:551:LEU:HB2	1.93	0.68
1:C:377:HIS:NE2	1:C:453:ASP:OD1	2.27	0.68
1:C:541:TRP:HA	1:C:541:TRP:CE3	2.28	0.68
1:B:70:ILE:HD11	1:B:573:HIS:HB3	1.75	0.68
1:B:541:TRP:HA	1:B:541:TRP:CE3	2.28	0.68
1:A:214:VAL:O	1:A:217:ALA:HB3	1.94	0.67
1:A:504:PRO:O	1:A:505:GLU:HB3	1.93	0.67
1:B:610:LYS:O	1:B:614:ILE:HG12	1.94	0.67
1:C:325:VAL:CG2	1:C:326:PRO:HD2	2.22	0.67
1:C:610:LYS:O	1:C:614:ILE:HG12	1.94	0.67
1:B:689:HIS:HB3	1:B:692:TYR:O	1.94	0.67
1:B:377:HIS:NE2	1:B:453:ASP:OD1	2.27	0.67
1:C:123:THR:C	1:C:125:PRO:HD3	2.20	0.67
1:C:504:PRO:O	1:C:505:GLU:HB3	1.93	0.67
1:D:120:PRO:HB3	1:D:126:ASN:HD21	1.59	0.67
1:D:325:VAL:CG2	1:D:326:PRO:HD2	2.22	0.67
1:C:187:LYS:HE3	1:C:190:ARG:HH22	1.58	0.67
1:A:689:HIS:HB3	1:A:692:TYR:O	1.94	0.67
1:D:115:VAL:CG1	1:D:429:LEU:HD13	2.24	0.67
1:D:610:LYS:O	1:D:614:ILE:HG12	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:228:TYR:CB	1:C:297:ILE:HG22	2.24	0.67
1:C:689:HIS:HB3	1:C:692:TYR:O	1.94	0.67
1:D:541:TRP:HA	1:D:541:TRP:CE3	2.28	0.67
1:D:541:TRP:HA	1:D:541:TRP:HE3	1.60	0.67
1:A:123:THR:C	1:A:125:PRO:HD3	2.19	0.67
1:A:610:LYS:O	1:A:614:ILE:HG12	1.94	0.67
1:B:123:THR:C	1:B:125:PRO:HD3	2.19	0.67
1:C:120:PRO:HB3	1:C:126:ASN:HD21	1.59	0.67
1:D:79:GLN:O	1:D:80:ILE:HD13	1.95	0.67
1:D:214:VAL:O	1:D:217:ALA:HB3	1.94	0.67
1:A:140:ASN:CB	4:A:1760:NAG:H62	2.20	0.67
1:B:303:GLN:HE21	1:B:324:LYS:HB2	1.60	0.67
1:C:369:ASP:CG	1:D:663:MET:HG2	2.20	0.67
1:A:120:PRO:HB3	1:A:126:ASN:HD21	1.59	0.67
1:A:228:TYR:CB	1:A:297:ILE:HG22	2.24	0.67
1:C:79:GLN:O	1:C:80:ILE:HD13	1.95	0.67
1:C:241:SER:C	1:C:245:GLY:HA3	2.20	0.67
1:D:504:PRO:O	1:D:505:GLU:HB3	1.93	0.67
1:A:78:THR:HG21	1:A:559:TYR:H	1.60	0.66
1:B:241:SER:C	1:B:245:GLY:HA3	2.20	0.66
1:D:123:THR:C	1:D:125:PRO:HD3	2.20	0.66
1:D:550:PRO:O	1:D:551:LEU:HB2	1.94	0.66
1:A:141:THR:CG2	1:A:142:SER:N	2.58	0.66
1:B:115:VAL:CG1	1:B:429:LEU:HD13	2.24	0.66
1:B:228:TYR:CB	1:B:297:ILE:HG22	2.24	0.66
1:D:242:TYR:O	1:D:243:PRO:C	2.38	0.66
1:A:123:THR:O	1:A:125:PRO:HD3	1.96	0.66
1:B:141:THR:CG2	1:B:142:SER:N	2.58	0.66
1:C:242:TYR:O	1:C:243:PRO:C	2.38	0.66
1:D:141:THR:CG2	1:D:142:SER:N	2.58	0.66
1:A:241:SER:C	1:A:245:GLY:HA3	2.20	0.66
1:B:79:GLN:O	1:B:80:ILE:HD13	1.95	0.66
1:C:123:THR:O	1:C:125:PRO:HD3	1.96	0.66
1:C:239:VAL:HB	1:C:247:ASN:HD22	1.61	0.66
1:A:733:TYR:CE1	1:B:278:ALA:HA	2.31	0.66
1:B:174:LEU:HD11	1:B:342:VAL:CG1	2.26	0.66
1:C:141:THR:CG2	1:C:142:SER:N	2.58	0.66
1:C:337:PHE:HD2	1:C:340:GLN:HE21	1.43	0.66
1:D:337:PHE:HD2	1:D:340:GLN:HE21	1.43	0.66
1:A:218:GLN:HG2	1:A:292:ILE:HD12	1.76	0.66
1:B:123:THR:O	1:B:125:PRO:HD3	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:239:VAL:HB	1:B:247:ASN:HD22	1.61	0.66
1:B:246:TRP:CZ2	3:M:1:NAG:H82	2.28	0.66
1:A:173:ASP:HB3	1:A:332:GLY:N	2.10	0.66
1:A:263:GLY:CA	1:A:686:PHE:HB2	2.26	0.66
1:B:541:TRP:HA	1:B:541:TRP:HE3	1.60	0.66
1:C:78:THR:HG21	1:C:559:TYR:H	1.60	0.66
1:C:218:GLN:HG2	1:C:292:ILE:HD12	1.76	0.66
1:C:303:GLN:HE21	1:C:324:LYS:HB2	1.60	0.66
1:D:218:GLN:HG2	1:D:292:ILE:HD12	1.76	0.66
1:D:263:GLY:CA	1:D:686:PHE:HB2	2.26	0.66
1:C:174:LEU:HD11	1:C:342:VAL:CG1	2.26	0.66
1:C:460:TYR:O	1:C:461:THR:HG22	1.96	0.66
1:D:241:SER:C	1:D:245:GLY:HA3	2.20	0.66
1:D:303:GLN:HE21	1:D:324:LYS:HB2	1.60	0.66
1:A:79:GLN:O	1:A:80:ILE:HD13	1.95	0.66
1:A:242:TYR:O	1:A:243:PRO:C	2.38	0.66
1:B:120:PRO:HB3	1:B:126:ASN:HD21	1.59	0.66
1:B:218:GLN:HG2	1:B:292:ILE:HD12	1.76	0.66
1:B:78:THR:HG21	1:B:559:TYR:H	1.60	0.66
1:C:263:GLY:CA	1:C:686:PHE:HB2	2.26	0.66
1:C:541:TRP:HA	1:C:541:TRP:HE3	1.60	0.66
1:D:174:LEU:HD11	1:D:342:VAL:CG1	2.26	0.66
1:D:228:TYR:CB	1:D:297:ILE:HG22	2.24	0.66
1:A:239:VAL:HB	1:A:247:ASN:HD22	1.61	0.65
1:A:325:VAL:CG2	1:A:326:PRO:HD2	2.22	0.65
1:B:242:TYR:O	1:B:243:PRO:C	2.38	0.65
1:D:543:THR:HG22	1:D:544:ASN:ND2	2.12	0.65
1:B:264:ALA:HB3	1:B:527:ARG:HH11	1.61	0.65
1:D:78:THR:HG21	1:D:559:TYR:H	1.61	0.65
1:D:373:ILE:HB	1:D:449:TYR:HD1	1.62	0.65
1:A:187:LYS:HG2	1:A:190:ARG:NH2	2.12	0.65
1:A:460:TYR:O	1:A:461:THR:HG22	1.96	0.65
1:D:123:THR:O	1:D:125:PRO:HD3	1.96	0.65
1:A:174:LEU:HD11	1:A:342:VAL:CG1	2.26	0.65
1:B:173:ASP:HB3	1:B:332:GLY:N	2.10	0.65
1:B:187:LYS:HG2	1:B:190:ARG:NH2	2.12	0.65
1:B:373:ILE:HB	1:B:449:TYR:HD1	1.62	0.65
1:C:174:LEU:HD21	1:C:342:VAL:HG11	1.79	0.65
1:C:384:GLY:O	1:C:389:GLN:HB2	1.97	0.65
1:B:325:VAL:CG2	1:B:326:PRO:HD2	2.22	0.65
1:A:264:ALA:HB3	1:A:527:ARG:HH11	1.61	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:337:PHE:HD2	1:B:340:GLN:HE21	1.44	0.65
1:D:174:LEU:HD21	1:D:342:VAL:HG11	1.79	0.65
1:D:187:LYS:HG2	1:D:190:ARG:NH2	2.12	0.65
1:D:239:VAL:HB	1:D:247:ASN:HD22	1.61	0.65
1:A:255:ARG:HG2	1:A:255:ARG:HH11	1.62	0.65
1:A:373:ILE:HB	1:A:449:TYR:HD1	1.62	0.65
1:B:658:PRO:HG2	1:B:659:ILE:HD12	1.79	0.65
1:B:707:GLY:HA3	1:B:731:GLN:HG2	1.78	0.65
1:D:264:ALA:HB3	1:D:527:ARG:HH11	1.61	0.65
1:D:293:PRO:CB	1:D:346:ILE:HD12	2.27	0.65
1:A:115:VAL:CG1	1:A:429:LEU:HD13	2.24	0.65
1:B:263:GLY:CA	1:B:686:PHE:HB2	2.26	0.65
1:C:173:ASP:HB3	1:C:332:GLY:N	2.10	0.65
1:A:384:GLY:O	1:A:389:GLN:HB2	1.97	0.64
1:A:707:GLY:HA3	1:A:731:GLN:HG2	1.78	0.64
1:C:674:ALA:O	1:D:440:ARG:NH1	2.30	0.64
1:C:707:GLY:CA	1:C:731:GLN:HG2	2.28	0.64
1:A:337:PHE:HD2	1:A:340:GLN:HE21	1.44	0.64
1:A:541:TRP:HA	1:A:541:TRP:HE3	1.60	0.64
1:A:707:GLY:CA	1:A:731:GLN:HG2	2.28	0.64
1:B:174:LEU:HD21	1:B:342:VAL:HG11	1.79	0.64
1:B:543:THR:HG22	1:B:544:ASN:ND2	2.12	0.64
1:D:658:PRO:HG2	1:D:659:ILE:HD12	1.79	0.64
1:D:707:GLY:HA3	1:D:731:GLN:HG2	1.78	0.64
1:A:543:THR:HG22	1:A:544:ASN:ND2	2.12	0.64
1:B:65:LEU:O	1:B:574:LEU:HD11	1.98	0.64
1:B:266:ASP:OD2	1:B:269:THR:HG23	1.98	0.64
1:B:460:TYR:O	1:B:461:THR:HG22	1.96	0.64
1:C:266:ASP:OD2	1:C:269:THR:HG23	1.98	0.64
1:C:373:ILE:HB	1:C:449:TYR:HD1	1.62	0.64
1:A:65:LEU:O	1:A:574:LEU:HD11	1.98	0.64
1:A:303:GLN:HE21	1:A:324:LYS:HB2	1.60	0.64
1:B:503:SER:HB2	1:B:510:PRO:C	2.23	0.64
1:C:293:PRO:CB	1:C:346:ILE:HD12	2.27	0.64
1:C:503:SER:HB2	1:C:510:PRO:C	2.23	0.64
1:D:240:LYS:HD2	1:D:240:LYS:N	2.13	0.64
1:A:174:LEU:HD21	1:A:342:VAL:HG11	1.79	0.64
1:A:263:GLY:HA3	1:A:686:PHE:HB2	1.79	0.64
1:A:658:PRO:HG2	1:A:659:ILE:HD12	1.79	0.64
1:B:384:GLY:O	1:B:389:GLN:HB2	1.97	0.64
1:B:707:GLY:CA	1:B:731:GLN:HG2	2.28	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:255:ARG:HG2	1:D:255:ARG:HH11	1.62	0.64
1:A:293:PRO:CB	1:A:346:ILE:HD12	2.27	0.64
1:C:187:LYS:HG2	1:C:190:ARG:NH2	2.12	0.64
1:C:543:THR:HG22	1:C:544:ASN:ND2	2.12	0.64
1:C:658:PRO:HG2	1:C:659:ILE:HD12	1.79	0.64
1:D:384:GLY:O	1:D:389:GLN:HB2	1.97	0.64
1:D:503:SER:HB2	1:D:510:PRO:C	2.22	0.64
1:B:141:THR:HG22	1:B:142:SER:N	2.13	0.64
1:B:293:PRO:CB	1:B:346:ILE:HD12	2.27	0.64
1:B:382:VAL:CG2	1:B:383:PHE:H	2.08	0.64
1:C:255:ARG:HH11	1:C:255:ARG:HG2	1.62	0.64
1:D:141:THR:HG22	1:D:142:SER:N	2.13	0.64
1:D:460:TYR:O	1:D:461:THR:HG22	1.96	0.64
1:A:503:SER:HB2	1:A:510:PRO:C	2.22	0.64
1:B:228:TYR:CE1	1:B:230:ASP:HB2	2.33	0.64
1:A:266:ASP:OD2	1:A:269:THR:HG23	1.98	0.63
1:B:263:GLY:HA3	1:B:686:PHE:HB2	1.79	0.63
1:C:707:GLY:HA3	1:C:731:GLN:HG2	1.78	0.63
1:D:140:ASN:CB	4:D:4760:NAG:H62	2.20	0.63
1:A:128:ILE:HD13	1:A:226:ILE:CD1	2.21	0.63
1:B:683:ASP:C	1:B:684:ARG:HG3	2.23	0.63
1:C:263:GLY:HA3	1:C:686:PHE:HB2	1.79	0.63
1:D:266:ASP:OD2	1:D:269:THR:HG23	1.98	0.63
1:A:246:TRP:CZ2	3:H:1:NAG:H82	2.28	0.63
1:B:140:ASN:CB	4:B:2760:NAG:H62	2.20	0.63
1:C:65:LEU:O	1:C:574:LEU:HD11	1.98	0.63
1:C:683:ASP:C	1:C:684:ARG:HG3	2.23	0.63
1:C:705:PHE:N	1:C:706:PRO:HD3	2.14	0.63
1:D:263:GLY:HA3	1:D:686:PHE:HB2	1.79	0.63
1:D:707:GLY:CA	1:D:731:GLN:HG2	2.28	0.63
1:A:382:VAL:CG2	1:A:383:PHE:H	2.08	0.63
1:C:128:ILE:HD13	1:C:226:ILE:CD1	2.21	0.63
1:C:205:TYR:HE2	1:C:227:LEU:HD13	1.64	0.63
1:C:264:ALA:HB3	1:C:527:ARG:HH11	1.61	0.63
1:A:141:THR:HG22	1:A:142:SER:N	2.13	0.63
1:A:242:TYR:C	1:A:245:GLY:H	2.07	0.63
1:A:377:HIS:CE1	1:A:388:PRO:HB3	2.34	0.63
1:D:205:TYR:HE2	1:D:227:LEU:HD13	1.64	0.63
1:D:268:LEU:C	1:D:270:PRO:HD3	2.24	0.63
1:A:181:ARG:CG	1:A:186:PHE:HB2	2.29	0.63
1:A:205:TYR:HE2	1:A:227:LEU:HD13	1.64	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:181:ARG:CG	1:B:186:PHE:HB2	2.29	0.63
1:C:377:HIS:CE1	1:C:388:PRO:HB3	2.34	0.63
1:D:683:ASP:C	1:D:684:ARG:HG3	2.23	0.63
1:D:707:GLY:C	1:D:731:GLN:HG2	2.24	0.63
1:B:707:GLY:C	1:B:731:GLN:HG2	2.24	0.63
1:D:228:TYR:CE1	1:D:230:ASP:HB2	2.34	0.63
1:D:377:HIS:CE1	1:D:388:PRO:HB3	2.34	0.63
1:C:240:LYS:HD2	1:C:240:LYS:N	2.13	0.63
1:C:268:LEU:C	1:C:270:PRO:HD3	2.24	0.63
1:D:705:PHE:N	1:D:706:PRO:HD3	2.14	0.63
1:B:255:ARG:HG2	1:B:255:ARG:HH11	1.62	0.63
1:C:141:THR:HG22	1:C:142:SER:N	2.13	0.63
1:C:246:TRP:CZ2	3:R:1:NAG:H82	2.29	0.63
1:D:65:LEU:O	1:D:574:LEU:HD11	1.98	0.63
1:D:173:ASP:HB3	1:D:332:GLY:N	2.10	0.63
1:C:567:ASP:OD2	1:C:570:PHE:HA	1.99	0.62
1:D:77:PHE:HB3	1:D:389:GLN:CG	2.29	0.62
1:A:567:ASP:OD2	1:A:570:PHE:HA	1.99	0.62
1:A:707:GLY:C	1:A:731:GLN:HG2	2.24	0.62
1:C:228:TYR:CE1	1:C:230:ASP:HB2	2.33	0.62
1:D:246:TRP:CZ2	3:W:1:NAG:H82	2.28	0.62
1:A:228:TYR:CE1	1:A:230:ASP:HB2	2.33	0.62
1:C:77:PHE:HB3	1:C:389:GLN:CG	2.29	0.62
1:B:242:TYR:C	1:B:245:GLY:H	2.07	0.62
1:B:705:PHE:N	1:B:706:PRO:HD3	2.14	0.62
1:C:712:LEU:HD23	1:C:728:VAL:HG21	1.81	0.62
1:D:712:LEU:HD23	1:D:728:VAL:HG21	1.81	0.62
1:A:240:LYS:HD2	1:A:240:LYS:N	2.13	0.62
1:B:567:ASP:OD2	1:B:570:PHE:HA	1.99	0.62
1:C:707:GLY:C	1:C:731:GLN:HG2	2.24	0.62
1:A:683:ASP:C	1:A:684:ARG:HG3	2.23	0.62
1:A:705:PHE:N	1:A:706:PRO:HD3	2.14	0.62
1:C:140:ASN:CB	4:C:3760:NAG:H62	2.20	0.62
1:A:246:TRP:HE1	3:H:1:NAG:C7	2.13	0.62
1:B:245:GLY:O	1:B:246:TRP:CB	2.47	0.62
1:C:181:ARG:CG	1:C:186:PHE:HB2	2.29	0.62
1:C:242:TYR:C	1:C:245:GLY:H	2.07	0.62
1:C:673:ARG:HA	1:C:676:ILE:HD13	1.82	0.62
1:D:242:TYR:C	1:D:245:GLY:H	2.07	0.62
1:B:205:TYR:HE2	1:B:227:LEU:HD13	1.64	0.62
1:C:137:GLU:HB3	4:C:3760:NAG:O3	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:468:PRO:HA	1:C:471:TYR:CD1	2.35	0.62
1:D:181:ARG:CG	1:D:186:PHE:HB2	2.29	0.62
1:D:567:ASP:OD2	1:D:570:PHE:HA	1.99	0.62
1:A:356:TYR:O	1:A:422:ASP:HB2	2.00	0.62
1:B:268:LEU:C	1:B:270:PRO:HD3	2.24	0.62
1:D:120:PRO:HB3	1:D:126:ASN:ND2	2.15	0.62
1:D:246:TRP:HE1	3:W:1:NAG:C7	2.13	0.62
1:A:120:PRO:HB3	1:A:126:ASN:ND2	2.15	0.62
1:B:377:HIS:CE1	1:B:388:PRO:HB3	2.34	0.62
1:A:137:GLU:HB3	4:A:1760:NAG:O3	2.00	0.61
1:A:245:GLY:O	1:A:246:TRP:CB	2.47	0.61
1:A:268:LEU:C	1:A:270:PRO:HD3	2.24	0.61
1:B:246:TRP:HE1	3:M:1:NAG:C7	2.13	0.61
1:C:120:PRO:HB3	1:C:126:ASN:ND2	2.15	0.61
1:B:120:PRO:HB3	1:B:126:ASN:ND2	2.15	0.61
1:B:712:LEU:HD23	1:B:728:VAL:HG21	1.81	0.61
1:C:246:TRP:HE1	3:R:1:NAG:C7	2.13	0.61
1:C:483:SER:HB2	1:C:493:LEU:HA	1.82	0.61
1:A:468:PRO:HA	1:A:471:TYR:CD1	2.35	0.61
1:B:240:LYS:HD2	1:B:240:LYS:N	2.13	0.61
1:D:245:GLY:O	1:D:246:TRP:CB	2.48	0.61
1:C:245:GLY:O	1:C:246:TRP:CB	2.47	0.61
1:A:77:PHE:HB3	1:A:389:GLN:CG	2.29	0.61
1:C:356:TYR:O	1:C:422:ASP:HB2	2.00	0.61
1:D:182:THR:O	1:D:183:GLU:HB2	2.00	0.61
1:B:366:VAL:O	1:B:368:PRO:HD3	2.00	0.61
1:A:673:ARG:HA	1:A:676:ILE:HD13	1.82	0.61
1:D:137:GLU:HB3	4:D:4760:NAG:O3	2.00	0.61
1:A:402:PHE:HE2	1:A:585:PHE:HD1	1.49	0.61
1:B:356:TYR:O	1:B:422:ASP:HB2	2.00	0.61
1:B:402:PHE:HE2	1:B:585:PHE:HD1	1.49	0.61
1:D:128:ILE:HD13	1:D:226:ILE:CD1	2.21	0.61
1:B:673:ARG:HA	1:B:676:ILE:HD13	1.82	0.61
1:D:483:SER:HB2	1:D:493:LEU:HA	1.82	0.61
1:D:673:ARG:HA	1:D:676:ILE:HD13	1.82	0.61
1:B:137:GLU:HB3	4:B:2760:NAG:O3	2.00	0.60
1:A:712:LEU:HD23	1:A:728:VAL:HG21	1.81	0.60
1:B:483:SER:HB2	1:B:493:LEU:HA	1.82	0.60
1:D:303:GLN:NE2	1:D:324:LYS:HB2	2.16	0.60
1:C:303:GLN:NE2	1:C:324:LYS:HB2	2.16	0.60
1:D:468:PRO:HA	1:D:471:TYR:CD1	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:483:SER:HB2	1:A:493:LEU:HA	1.82	0.60
1:D:356:TYR:O	1:D:422:ASP:HB2	2.00	0.60
1:A:303:GLN:NE2	1:A:324:LYS:HB2	2.16	0.60
1:B:182:THR:O	1:B:183:GLU:HB2	2.00	0.60
1:C:182:THR:O	1:C:183:GLU:HB2	2.00	0.60
1:D:366:VAL:O	1:D:368:PRO:HD3	2.00	0.60
1:B:303:GLN:NE2	1:B:324:LYS:HB2	2.16	0.60
1:C:357:ASN:OD1	1:C:421:TRP:HA	2.02	0.60
1:A:357:ASN:OD1	1:A:421:TRP:HA	2.02	0.60
1:B:468:PRO:HA	1:B:471:TYR:CD1	2.35	0.60
1:D:242:TYR:N	1:D:245:GLY:HA3	2.17	0.60
1:D:357:ASN:OD1	1:D:421:TRP:HA	2.02	0.60
1:A:182:THR:O	1:A:183:GLU:HB2	2.00	0.60
1:A:242:TYR:N	1:A:245:GLY:HA3	2.17	0.60
1:A:366:VAL:O	1:A:368:PRO:HD3	2.00	0.60
1:A:517:SER:HB3	1:A:694:PRO:HG3	1.84	0.60
1:D:638:ASN:O	1:D:642:ILE:HG12	2.01	0.60
1:B:77:PHE:HB3	1:B:389:GLN:CG	2.29	0.60
1:B:517:SER:HB3	1:B:694:PRO:HG3	1.84	0.60
1:C:638:ASN:O	1:C:642:ILE:HG12	2.01	0.60
1:B:357:ASN:OD1	1:B:421:TRP:HA	2.02	0.59
1:D:402:PHE:HE2	1:D:585:PHE:HD1	1.49	0.59
1:A:59:LYS:O	1:A:60:ALA:C	2.46	0.59
1:A:598:ARG:O	1:A:602:VAL:HG23	2.03	0.59
1:B:370:ARG:HB2	1:B:414:ARG:HG2	1.85	0.59
1:C:517:SER:HB3	1:C:694:PRO:HG3	1.84	0.59
1:C:663:MET:HG2	1:D:369:ASP:OD1	2.02	0.59
1:D:517:SER:HB3	1:D:694:PRO:HG3	1.84	0.59
1:A:459:ASN:ND2	3:H:1:NAG:C7	2.66	0.59
1:B:242:TYR:N	1:B:245:GLY:HA3	2.17	0.59
1:B:598:ARG:O	1:B:602:VAL:HG23	2.03	0.59
1:C:242:TYR:N	1:C:245:GLY:HA3	2.17	0.59
1:C:598:ARG:O	1:C:602:VAL:HG23	2.03	0.59
1:B:638:ASN:O	1:B:642:ILE:HG12	2.01	0.59
1:C:272:TYR:CE2	1:D:734:VAL:HG13	2.37	0.59
1:C:366:VAL:O	1:C:368:PRO:HD3	2.00	0.59
1:D:459:ASN:ND2	3:W:1:NAG:C7	2.66	0.59
1:A:638:ASN:O	1:A:642:ILE:HG12	2.01	0.59
1:A:210:ARG:O	1:A:213:LYS:HB2	2.03	0.59
1:B:59:LYS:O	1:B:60:ALA:C	2.46	0.59
1:B:459:ASN:ND2	3:M:1:NAG:C7	2.66	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:377:HIS:NE2	1:C:388:PRO:HB3	2.18	0.59
1:C:59:LYS:O	1:C:60:ALA:C	2.46	0.59
1:D:382:VAL:CG2	1:D:383:PHE:H	2.08	0.59
1:A:574:LEU:O	1:A:578:GLN:HG3	2.03	0.59
1:B:210:ARG:O	1:B:213:LYS:HB2	2.03	0.59
1:D:377:HIS:NE2	1:D:388:PRO:HB3	2.18	0.59
1:A:264:ALA:HB3	1:A:527:ARG:NH1	2.18	0.59
1:B:574:LEU:O	1:B:578:GLN:HG3	2.03	0.58
1:C:402:PHE:HE2	1:C:585:PHE:HD1	1.49	0.58
1:D:598:ARG:O	1:D:602:VAL:HG23	2.03	0.58
1:A:377:HIS:NE2	1:A:388:PRO:HB3	2.18	0.58
1:C:155:SER:O	1:C:156:ASP:HB2	2.03	0.58
1:C:210:ARG:O	1:C:213:LYS:HB2	2.03	0.58
1:C:264:ALA:HB3	1:C:527:ARG:NH1	2.18	0.58
1:A:370:ARG:HB2	1:A:414:ARG:HG2	1.85	0.58
1:B:128:ILE:CD1	1:B:226:ILE:HD12	2.23	0.58
1:B:377:HIS:NE2	1:B:388:PRO:HB3	2.18	0.58
1:C:368:PRO:HD2	1:D:663:MET:SD	2.43	0.58
1:C:382:VAL:CG2	1:C:383:PHE:H	2.08	0.58
1:D:155:SER:O	1:D:156:ASP:HB2	2.03	0.58
1:D:264:ALA:HB3	1:D:527:ARG:NH1	2.18	0.58
1:B:269:THR:O	1:B:269:THR:OG1	2.20	0.58
1:D:210:ARG:O	1:D:213:LYS:HB2	2.03	0.58
1:D:574:LEU:O	1:D:578:GLN:HG3	2.03	0.58
1:C:459:ASN:ND2	3:R:1:NAG:C7	2.66	0.58
1:C:574:LEU:O	1:C:578:GLN:HG3	2.03	0.58
1:B:117:LEU:HD12	1:B:353:THR:HB	1.86	0.58
1:C:117:LEU:HD12	1:C:353:THR:HB	1.86	0.58
1:A:187:LYS:HG2	1:A:187:LYS:O	2.04	0.57
1:B:83:LEU:HB3	1:B:86:THR:CG2	2.34	0.57
1:C:437:GLU:HG2	1:C:438:ASN:ND2	2.19	0.57
1:C:187:LYS:HG2	1:C:187:LYS:O	2.04	0.57
1:C:370:ARG:HB2	1:C:414:ARG:HG2	1.85	0.57
1:D:437:GLU:HG2	1:D:438:ASN:ND2	2.19	0.57
1:A:155:SER:O	1:A:156:ASP:HB2	2.03	0.57
1:C:478:THR:HG23	1:C:494:TYR:CB	2.33	0.57
1:D:117:LEU:HD12	1:D:353:THR:HB	1.86	0.57
1:D:370:ARG:HB2	1:D:414:ARG:HG2	1.85	0.57
1:A:117:LEU:HD12	1:A:353:THR:HB	1.86	0.57
1:C:169:MET:HA	1:C:344:MET:O	2.05	0.57
1:D:550:PRO:O	1:D:551:LEU:CB	2.53	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:187:LYS:HG2	1:B:187:LYS:O	2.04	0.57
1:B:246:TRP:HB2	1:B:565:PHE:CD2	2.40	0.57
1:B:310:GLY:HA3	1:B:334:THR:HG23	1.87	0.57
1:B:437:GLU:HG2	1:B:438:ASN:ND2	2.19	0.57
1:C:83:LEU:HB3	1:C:86:THR:CG2	2.34	0.57
1:C:475:HIS:O	1:C:478:THR:HG22	2.05	0.57
1:C:749:VAL:HG12	1:D:445:ARG:CZ	2.34	0.57
1:D:187:LYS:HG2	1:D:187:LYS:O	2.04	0.57
1:A:242:TYR:CD2	1:A:556:TYR:HD2	2.22	0.57
1:B:169:MET:HA	1:B:344:MET:O	2.05	0.57
1:B:264:ALA:HB3	1:B:527:ARG:NH1	2.18	0.57
1:C:242:TYR:CD2	1:C:556:TYR:HD2	2.23	0.57
1:D:59:LYS:O	1:D:60:ALA:C	2.46	0.57
1:C:181:ARG:HD3	1:C:216:ASN:ND2	2.20	0.57
1:C:246:TRP:HB2	1:C:565:PHE:CD2	2.39	0.57
1:C:269:THR:OG1	1:C:269:THR:O	2.20	0.57
1:D:242:TYR:CD2	1:D:556:TYR:HD2	2.23	0.57
1:D:478:THR:HG23	1:D:494:TYR:CB	2.33	0.57
1:A:437:GLU:HG2	1:A:438:ASN:ND2	2.19	0.57
1:A:550:PRO:O	1:A:551:LEU:CB	2.53	0.57
1:B:242:TYR:CD2	1:B:556:TYR:HD2	2.22	0.57
1:A:131:ILE:O	1:A:340:GLN:HA	2.05	0.57
1:A:169:MET:HA	1:A:344:MET:O	2.05	0.57
1:A:246:TRP:HB2	1:A:565:PHE:CD2	2.40	0.57
1:C:128:ILE:CD1	1:C:226:ILE:HD12	2.23	0.57
1:C:131:ILE:O	1:C:340:GLN:HA	2.05	0.57
1:A:412:PRO:HB2	1:A:414:ARG:O	2.05	0.57
1:D:83:LEU:HB3	1:D:86:THR:CG2	2.34	0.57
1:D:543:THR:C	1:D:544:ASN:HD22	2.13	0.57
1:B:155:SER:O	1:B:156:ASP:HB2	2.03	0.56
1:D:131:ILE:O	1:D:340:GLN:HA	2.05	0.56
1:A:543:THR:C	1:A:544:ASN:HD22	2.13	0.56
1:B:475:HIS:O	1:B:478:THR:HG22	2.05	0.56
1:D:181:ARG:HD3	1:D:216:ASN:ND2	2.20	0.56
1:D:412:PRO:HB2	1:D:414:ARG:O	2.05	0.56
1:A:373:ILE:CD1	1:A:417:LEU:HB2	2.36	0.56
1:A:478:THR:HG23	1:A:494:TYR:CB	2.33	0.56
1:B:478:THR:HG23	1:B:494:TYR:CB	2.33	0.56
1:D:169:MET:HA	1:D:344:MET:O	2.05	0.56
1:D:246:TRP:HB2	1:D:565:PHE:CD2	2.39	0.56
1:D:683:ASP:O	1:D:684:ARG:HG3	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:266:ASP:HA	1:B:429:LEU:HD22	1.88	0.56
1:A:460:TYR:CD2	1:A:540:ASN:HA	2.41	0.56
1:A:683:ASP:O	1:A:684:ARG:HG3	2.06	0.56
1:B:550:PRO:O	1:B:551:LEU:CB	2.53	0.56
1:C:465:ASP:O	1:C:466:CYS:HB3	2.06	0.56
1:C:683:ASP:O	1:C:684:ARG:HG3	2.06	0.56
1:D:186:PHE:C	1:D:188:LEU:H	2.13	0.56
1:D:310:GLY:HA3	1:D:334:THR:HG23	1.87	0.56
1:B:412:PRO:HB2	1:B:414:ARG:O	2.05	0.56
1:C:460:TYR:CD2	1:C:540:ASN:HA	2.41	0.56
1:D:229:SER:HB3	1:D:234:TYR:HE1	1.71	0.56
1:D:363:ARG:HB3	1:D:411:ARG:HH21	1.71	0.56
1:C:550:PRO:O	1:C:551:LEU:CB	2.53	0.56
1:C:670:PHE:CE2	1:D:444:GLU:OE1	2.59	0.56
1:D:465:ASP:O	1:D:466:CYS:HB3	2.06	0.56
1:A:242:TYR:O	1:A:245:GLY:N	2.39	0.56
1:A:363:ARG:HB3	1:A:411:ARG:HH21	1.71	0.56
1:A:672:GLU:OE1	1:A:689:HIS:HE1	1.89	0.56
1:B:131:ILE:O	1:B:340:GLN:HA	2.05	0.56
1:B:460:TYR:CD2	1:B:540:ASN:HA	2.41	0.56
1:C:412:PRO:HB2	1:C:414:ARG:O	2.05	0.56
1:C:529:GLY:HA3	1:C:676:ILE:HD11	1.88	0.56
1:A:269:THR:O	1:A:269:THR:OG1	2.20	0.56
1:A:310:GLY:HA3	1:A:334:THR:HG23	1.87	0.56
1:A:475:HIS:O	1:A:478:THR:HG22	2.05	0.56
1:B:181:ARG:HD3	1:B:216:ASN:ND2	2.20	0.56
1:B:683:ASP:O	1:B:684:ARG:HG3	2.06	0.56
1:D:83:LEU:HB3	1:D:86:THR:HG21	1.88	0.56
1:D:475:HIS:O	1:D:478:THR:HG22	2.05	0.56
1:A:83:LEU:HB3	1:A:86:THR:CG2	2.34	0.56
1:B:465:ASP:O	1:B:466:CYS:HB3	2.06	0.56
1:C:543:THR:C	1:C:544:ASN:HD22	2.13	0.56
1:D:460:TYR:CD2	1:D:540:ASN:HA	2.41	0.56
1:A:83:LEU:HB3	1:A:86:THR:HG21	1.88	0.55
1:B:229:SER:HB3	1:B:234:TYR:HE1	1.71	0.55
1:C:83:LEU:HB3	1:C:86:THR:HG21	1.88	0.55
1:D:529:GLY:HA3	1:D:676:ILE:HD11	1.88	0.55
1:A:181:ARG:HD3	1:A:216:ASN:ND2	2.20	0.55
1:B:708:ILE:HG13	1:B:731:GLN:HB3	1.89	0.55
1:C:242:TYR:O	1:C:245:GLY:N	2.39	0.55
1:C:310:GLY:HA3	1:C:334:THR:HG23	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:543:THR:C	1:B:544:ASN:HD22	2.13	0.55
1:A:465:ASP:O	1:A:466:CYS:HB3	2.06	0.55
1:B:373:ILE:CD1	1:B:417:LEU:HB2	2.36	0.55
1:B:672:GLU:OE1	1:B:689:HIS:HE1	1.89	0.55
1:A:229:SER:HB3	1:A:234:TYR:HE1	1.71	0.55
1:A:266:ASP:HA	1:A:429:LEU:HD22	1.88	0.55
1:A:558:THR:O	1:A:561:LEU:HB3	2.07	0.55
1:B:363:ARG:HB3	1:B:411:ARG:HH21	1.71	0.55
1:B:558:THR:O	1:B:561:LEU:HB3	2.07	0.55
1:C:132:ASN:HB3	1:C:340:GLN:OE1	2.07	0.55
1:C:186:PHE:C	1:C:188:LEU:H	2.13	0.55
1:D:627:VAL:HG21	1:D:725:TRP:CE3	2.42	0.55
1:A:449:TYR:CE2	1:A:521:PHE:HA	2.42	0.55
1:A:737:PHE:CE1	1:B:273:PRO:HG2	2.42	0.55
1:B:128:ILE:HD13	1:B:226:ILE:CD1	2.21	0.55
1:B:529:GLY:HA3	1:B:676:ILE:HD11	1.88	0.55
1:C:672:GLU:OE1	1:C:689:HIS:HE1	1.89	0.55
1:A:497:TRP:CE2	1:A:510:PRO:HB3	2.42	0.55
1:B:497:TRP:CE2	1:B:510:PRO:HB3	2.42	0.55
1:C:78:THR:HG21	1:C:559:TYR:N	2.22	0.55
1:C:708:ILE:HG13	1:C:731:GLN:HB3	1.89	0.55
1:D:373:ILE:CD1	1:D:417:LEU:HB2	2.35	0.55
1:D:558:THR:O	1:D:561:LEU:HB3	2.07	0.55
1:B:186:PHE:C	1:B:188:LEU:H	2.13	0.55
1:B:627:VAL:HG21	1:B:725:TRP:CE3	2.42	0.55
1:A:178:ASN:O	1:A:180:ALA:N	2.40	0.55
1:A:186:PHE:C	1:A:188:LEU:H	2.13	0.55
1:A:529:GLY:HA3	1:A:676:ILE:HD11	1.88	0.55
1:C:363:ARG:HB3	1:C:411:ARG:HH21	1.71	0.55
1:C:473:LEU:HD13	1:C:594:PRO:HB3	1.89	0.55
1:C:488:PHE:HB3	1:C:491:LYS:HB2	1.89	0.55
1:D:266:ASP:HA	1:D:429:LEU:HD22	1.88	0.55
1:B:178:ASN:O	1:B:180:ALA:N	2.40	0.54
1:C:229:SER:HB3	1:C:234:TYR:HE1	1.71	0.54
1:A:657:ASN:OD1	1:A:660:VAL:HG23	2.07	0.54
1:B:449:TYR:CE2	1:B:521:PHE:HA	2.42	0.54
1:D:242:TYR:O	1:D:245:GLY:N	2.39	0.54
1:D:473:LEU:HD13	1:D:594:PRO:HB3	1.89	0.54
1:D:488:PHE:HB3	1:D:491:LYS:HB2	1.89	0.54
1:D:672:GLU:OE1	1:D:689:HIS:HE1	1.89	0.54
1:A:132:ASN:HB3	1:A:340:GLN:OE1	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:656:SER:O	1:D:656:SER:O	2.24	0.54
1:C:497:TRP:CE2	1:C:510:PRO:HB3	2.42	0.54
1:C:558:THR:O	1:C:561:LEU:HB3	2.07	0.54
1:D:192:MET:O	1:D:194:ILE:HG12	2.07	0.54
1:D:497:TRP:CE2	1:D:510:PRO:HB3	2.42	0.54
1:A:649:ARG:HD2	1:A:664:MET:HE1	1.90	0.54
1:B:83:LEU:HB3	1:B:86:THR:HG21	1.88	0.54
1:B:181:ARG:HG2	1:B:183:GLU:CA	2.38	0.54
1:C:181:ARG:HG2	1:C:183:GLU:CA	2.38	0.54
1:C:323:LEU:C	1:C:325:VAL:H	2.16	0.54
1:D:323:LEU:C	1:D:325:VAL:H	2.16	0.54
1:A:78:THR:HG21	1:A:559:TYR:N	2.22	0.54
1:B:428:LEU:HD21	1:B:518:GLY:O	2.08	0.54
1:B:488:PHE:HB3	1:B:491:LYS:HB2	1.89	0.54
1:B:657:ASN:OD1	1:B:660:VAL:HG23	2.07	0.54
1:C:178:ASN:O	1:C:180:ALA:N	2.41	0.54
1:C:373:ILE:CD1	1:C:417:LEU:HB2	2.35	0.54
1:C:428:LEU:HD21	1:C:518:GLY:O	2.08	0.54
1:C:627:VAL:HG21	1:C:725:TRP:CE3	2.42	0.54
1:D:132:ASN:HB3	1:D:340:GLN:OE1	2.07	0.54
1:D:178:ASN:O	1:D:180:ALA:N	2.40	0.54
1:D:449:TYR:CE2	1:D:521:PHE:HA	2.42	0.54
1:A:192:MET:O	1:A:194:ILE:HG12	2.07	0.54
1:A:627:VAL:HG21	1:A:725:TRP:CE3	2.42	0.54
1:B:192:MET:O	1:B:194:ILE:HG12	2.07	0.54
1:B:402:PHE:CE2	1:B:585:PHE:HD1	2.26	0.54
1:C:192:MET:O	1:C:194:ILE:HG12	2.07	0.54
1:D:428:LEU:HD21	1:D:518:GLY:O	2.08	0.54
1:B:242:TYR:O	1:B:245:GLY:N	2.39	0.54
1:C:266:ASP:HA	1:C:429:LEU:HD22	1.88	0.54
1:D:649:ARG:HD2	1:D:664:MET:HE1	1.90	0.54
1:D:657:ASN:OD1	1:D:660:VAL:HG23	2.07	0.54
1:C:449:TYR:CE2	1:C:521:PHE:HA	2.42	0.54
1:D:179:TYR:HA	1:D:204:ARG:O	2.08	0.54
1:D:708:ILE:HG13	1:D:731:GLN:HB3	1.89	0.54
1:B:107:SER:HB2	1:B:361:THR:HB	1.90	0.54
1:B:614:ILE:O	1:B:617:LYS:HB2	2.08	0.54
1:C:178:ASN:HB3	1:C:185:PHE:CD1	2.43	0.54
1:A:261:LEU:O	1:A:263:GLY:N	2.41	0.54
1:B:78:THR:HG21	1:B:559:TYR:N	2.22	0.54
1:B:132:ASN:HB3	1:B:340:GLN:OE1	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:529:GLY:HA3	1:B:676:ILE:CD1	2.38	0.54
1:D:337:PHE:HB3	1:D:340:GLN:HG3	1.90	0.54
1:D:614:ILE:O	1:D:617:LYS:HB2	2.08	0.54
1:A:428:LEU:HD21	1:A:518:GLY:O	2.08	0.53
1:A:614:ILE:O	1:A:617:LYS:HB2	2.08	0.53
1:A:715:ILE:HD13	1:A:725:TRP:CE2	2.44	0.53
1:B:473:LEU:HD13	1:B:594:PRO:HB3	1.89	0.53
1:D:78:THR:HG21	1:D:559:TYR:N	2.22	0.53
1:A:473:LEU:HD13	1:A:594:PRO:HB3	1.89	0.53
1:A:610:LYS:CD	1:A:614:ILE:HD11	2.38	0.53
1:B:178:ASN:HB3	1:B:185:PHE:CD1	2.43	0.53
1:B:261:LEU:O	1:B:263:GLY:N	2.41	0.53
1:B:323:LEU:C	1:B:325:VAL:H	2.16	0.53
1:C:377:HIS:CD2	1:C:453:ASP:OD1	2.61	0.53
1:D:181:ARG:HG2	1:D:183:GLU:CA	2.38	0.53
1:D:323:LEU:HB2	1:D:327:TYR:OH	2.08	0.53
1:A:174:LEU:HD11	1:A:342:VAL:HG22	1.91	0.53
1:A:488:PHE:HB3	1:A:491:LYS:HB2	1.89	0.53
1:B:625:TYR:CE2	1:B:722:SER:HA	2.44	0.53
1:C:261:LEU:O	1:C:263:GLY:N	2.41	0.53
1:C:273:PRO:HG2	1:D:737:PHE:CE1	2.43	0.53
1:D:261:LEU:O	1:D:263:GLY:N	2.41	0.53
1:D:625:TYR:CE2	1:D:722:SER:HA	2.44	0.53
1:B:323:LEU:HB2	1:B:327:TYR:OH	2.08	0.53
1:B:337:PHE:HB3	1:B:340:GLN:HG3	1.90	0.53
1:C:529:GLY:HA3	1:C:676:ILE:CD1	2.38	0.53
1:D:174:LEU:HD11	1:D:342:VAL:HG22	1.91	0.53
1:A:323:LEU:HB2	1:A:327:TYR:OH	2.08	0.53
1:A:337:PHE:HB3	1:A:340:GLN:HG3	1.90	0.53
1:A:529:GLY:HA3	1:A:676:ILE:CD1	2.39	0.53
1:A:625:TYR:CE2	1:A:722:SER:HA	2.44	0.53
1:A:708:ILE:HG13	1:A:731:GLN:HB3	1.89	0.53
1:B:610:LYS:CD	1:B:614:ILE:HD11	2.39	0.53
1:C:610:LYS:CD	1:C:614:ILE:HD11	2.39	0.53
1:D:715:ILE:HD13	1:D:725:TRP:CE2	2.43	0.53
1:A:160:PRO:HB3	1:A:253:VAL:HG11	1.91	0.53
1:B:160:PRO:HB3	1:B:253:VAL:HG11	1.91	0.53
1:B:179:TYR:HA	1:B:204:ARG:O	2.08	0.53
1:B:649:ARG:HD2	1:B:664:MET:HE1	1.90	0.53
1:C:179:TYR:HA	1:C:204:ARG:O	2.08	0.53
1:C:323:LEU:HB2	1:C:327:TYR:OH	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:337:PHE:HB3	1:C:340:GLN:HG3	1.90	0.53
1:D:178:ASN:HB3	1:D:185:PHE:CD1	2.43	0.53
1:D:377:HIS:CD2	1:D:453:ASP:OD1	2.61	0.53
1:D:402:PHE:CE2	1:D:585:PHE:HD1	2.26	0.53
1:A:107:SER:HB2	1:A:361:THR:HB	1.90	0.53
1:A:377:HIS:CD2	1:A:453:ASP:OD1	2.61	0.53
1:C:402:PHE:CE2	1:C:585:PHE:HD1	2.26	0.53
1:C:625:TYR:CE2	1:C:722:SER:HA	2.44	0.53
1:C:649:ARG:HD2	1:C:664:MET:HE1	1.90	0.53
1:C:657:ASN:OD1	1:C:660:VAL:HG23	2.07	0.53
1:D:529:GLY:HA3	1:D:676:ILE:CD1	2.38	0.53
1:C:715:ILE:HD13	1:C:725:TRP:CE2	2.43	0.53
1:D:107:SER:HB2	1:D:361:THR:HB	1.90	0.53
1:A:323:LEU:C	1:A:325:VAL:H	2.16	0.53
1:A:402:PHE:CE2	1:A:585:PHE:HD1	2.26	0.53
1:B:377:HIS:CD2	1:B:453:ASP:OD1	2.61	0.53
1:C:614:ILE:O	1:C:617:LYS:HB2	2.08	0.53
1:A:178:ASN:HB3	1:A:185:PHE:CD1	2.43	0.53
1:A:690:VAL:CG2	1:A:738:THR:HG21	2.38	0.53
1:B:715:ILE:HD13	1:B:725:TRP:CE2	2.44	0.53
1:C:107:SER:HB2	1:C:361:THR:HB	1.90	0.53
1:A:179:TYR:HA	1:A:204:ARG:O	2.08	0.52
1:B:314:PRO:HG3	1:B:328:ASN:HA	1.91	0.52
1:C:174:LEU:HD11	1:C:342:VAL:HG22	1.91	0.52
1:C:239:VAL:HG12	1:C:240:LYS:N	2.25	0.52
1:A:368:PRO:HD2	1:B:663:MET:SD	2.49	0.52
1:B:465:ASP:HB2	1:B:534:ARG:HG3	1.91	0.52
1:A:181:ARG:HG2	1:A:183:GLU:CA	2.38	0.52
1:A:465:ASP:HB2	1:A:534:ARG:HG3	1.92	0.52
1:A:670:PHE:CE2	1:B:444:GLU:CD	2.87	0.52
1:B:174:LEU:HD11	1:B:342:VAL:HG22	1.91	0.52
1:A:314:PRO:HG3	1:A:328:ASN:HA	1.91	0.52
1:C:160:PRO:HB3	1:C:253:VAL:HG11	1.91	0.52
1:D:110:LEU:CD2	1:D:358:VAL:HG22	2.40	0.52
1:B:110:LEU:CD2	1:B:358:VAL:HG22	2.40	0.52
1:B:269:THR:OG1	1:B:433:GLU:OE2	2.27	0.52
1:C:369:ASP:OD1	1:D:663:MET:HG2	2.08	0.52
1:C:465:ASP:HB2	1:C:534:ARG:HG3	1.91	0.52
1:B:616:MET:O	1:B:619:PRO:HD3	2.10	0.52
1:C:246:TRP:HD1	1:C:565:PHE:HB3	1.75	0.52
1:C:275:ASN:HD22	1:C:277:TYR:H	1.58	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:616:MET:O	1:A:619:PRO:HD3	2.10	0.52
1:D:275:ASN:HD22	1:D:277:TYR:H	1.58	0.52
1:D:610:LYS:CD	1:D:614:ILE:HD11	2.39	0.52
1:D:616:MET:O	1:D:619:PRO:HD3	2.10	0.52
1:C:239:VAL:HG11	1:C:246:TRP:HB3	1.92	0.51
1:C:269:THR:OG1	1:C:433:GLU:OE2	2.27	0.51
1:A:110:LEU:CD2	1:A:358:VAL:HG22	2.40	0.51
1:A:239:VAL:HG11	1:A:246:TRP:HB3	1.92	0.51
1:A:273:PRO:HA	1:A:433:GLU:OE1	2.10	0.51
1:A:638:ASN:O	1:A:639:PHE:C	2.53	0.51
1:B:424:GLU:HA	1:B:428:LEU:HA	1.92	0.51
1:C:314:PRO:HG3	1:C:328:ASN:HA	1.91	0.51
1:C:529:GLY:CA	1:C:676:ILE:HD11	2.41	0.51
1:C:737:PHE:CE1	1:D:273:PRO:HG2	2.45	0.51
1:D:246:TRP:HD1	1:D:565:PHE:HB3	1.75	0.51
1:A:246:TRP:HD1	1:A:565:PHE:HB3	1.75	0.51
1:D:465:ASP:HB2	1:D:534:ARG:HG3	1.91	0.51
1:D:521:PHE:CD1	1:D:521:PHE:C	2.88	0.51
1:A:269:THR:OG1	1:A:433:GLU:OE2	2.27	0.51
1:B:239:VAL:HG12	1:B:240:LYS:N	2.25	0.51
1:C:110:LEU:CD2	1:C:358:VAL:HG22	2.40	0.51
1:C:424:GLU:HA	1:C:428:LEU:HA	1.92	0.51
1:C:521:PHE:CD1	1:C:521:PHE:C	2.88	0.51
1:A:272:TYR:O	1:A:436:GLU:OE1	2.28	0.51
1:B:273:PRO:HA	1:B:433:GLU:OE1	2.10	0.51
1:C:178:ASN:HD21	1:C:204:ARG:HH21	1.59	0.51
1:C:273:PRO:HA	1:C:433:GLU:OE1	2.10	0.51
1:D:160:PRO:HB3	1:D:253:VAL:HG11	1.91	0.51
1:D:239:VAL:HG11	1:D:246:TRP:HB3	1.92	0.51
1:D:273:PRO:HA	1:D:433:GLU:OE1	2.10	0.51
1:A:239:VAL:HG12	1:A:240:LYS:N	2.25	0.51
1:A:521:PHE:C	1:A:521:PHE:CD1	2.88	0.51
1:B:246:TRP:HD1	1:B:565:PHE:HB3	1.75	0.51
1:B:272:TYR:O	1:B:436:GLU:OE1	2.28	0.51
1:B:521:PHE:CD1	1:B:521:PHE:C	2.88	0.51
1:C:616:MET:O	1:C:619:PRO:HD3	2.10	0.51
1:D:424:GLU:HA	1:D:428:LEU:HA	1.92	0.51
1:A:128:ILE:HG22	1:A:129:SER:H	1.76	0.51
1:A:145:GLU:HG3	1:A:160:PRO:HG2	1.93	0.51
1:A:529:GLY:CA	1:A:676:ILE:HD11	2.41	0.51
1:A:654:ASP:C	1:A:656:SER:H	2.19	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:128:ILE:HG22	1:B:129:SER:H	1.76	0.51
1:C:145:GLU:HB2	1:C:555:VAL:HG21	1.93	0.51
1:D:269:THR:OG1	1:D:433:GLU:OE2	2.27	0.51
1:D:314:PRO:HG3	1:D:328:ASN:HA	1.91	0.51
1:A:128:ILE:HG22	1:A:129:SER:N	2.26	0.51
1:B:275:ASN:HD22	1:B:277:TYR:N	2.09	0.51
1:D:178:ASN:HD21	1:D:204:ARG:HH21	1.59	0.51
1:D:275:ASN:HD22	1:D:277:TYR:N	2.09	0.51
1:B:690:VAL:CG2	1:B:738:THR:HG21	2.38	0.51
1:D:145:GLU:HG3	1:D:160:PRO:HG2	1.93	0.51
1:D:266:ASP:OD1	1:D:267:PRO:HD2	2.11	0.51
1:A:266:ASP:OD1	1:A:267:PRO:HD2	2.11	0.51
1:B:402:PHE:HE2	1:B:585:PHE:CD1	2.29	0.51
1:D:241:SER:O	1:D:243:PRO:CD	2.58	0.51
1:D:654:ASP:C	1:D:656:SER:H	2.19	0.51
1:B:626:SER:O	1:B:729:LYS:HD2	2.11	0.50
1:B:715:ILE:HD13	1:B:725:TRP:CZ2	2.46	0.50
1:D:242:TYR:HB3	1:D:243:PRO:HD3	1.93	0.50
1:A:626:SER:O	1:A:729:LYS:HD2	2.11	0.50
1:B:145:GLU:HG3	1:B:160:PRO:HG2	1.93	0.50
1:B:239:VAL:HG11	1:B:246:TRP:HB3	1.92	0.50
1:D:272:TYR:O	1:D:436:GLU:OE1	2.28	0.50
1:A:242:TYR:HB3	1:A:243:PRO:HD3	1.94	0.50
1:A:303:GLN:O	1:A:307:GLU:N	2.44	0.50
1:A:424:GLU:HA	1:A:428:LEU:HA	1.92	0.50
1:C:128:ILE:HG22	1:C:129:SER:H	1.76	0.50
1:D:715:ILE:HD13	1:D:725:TRP:CZ2	2.46	0.50
1:B:242:TYR:HB3	1:B:243:PRO:HD3	1.94	0.50
1:B:676:ILE:HG23	1:B:688:ARG:HB2	1.94	0.50
1:C:210:ARG:HA	1:C:213:LYS:HG3	1.93	0.50
1:C:310:GLY:H	1:C:333:PHE:HA	1.77	0.50
1:D:128:ILE:HG22	1:D:129:SER:N	2.26	0.50
1:D:128:ILE:HG22	1:D:129:SER:H	1.76	0.50
1:D:529:GLY:CA	1:D:676:ILE:HD11	2.41	0.50
1:A:178:ASN:HD21	1:A:204:ARG:HH21	1.59	0.50
1:B:497:TRP:CD2	1:B:510:PRO:HB3	2.47	0.50
1:C:128:ILE:HG22	1:C:129:SER:N	2.26	0.50
1:C:272:TYR:O	1:C:436:GLU:OE1	2.28	0.50
1:D:136:ASN:O	1:D:138:ILE:N	2.45	0.50
1:D:210:ARG:HA	1:D:213:LYS:HG3	1.94	0.50
1:D:626:SER:O	1:D:729:LYS:HD2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:145:GLU:HB2	1:A:555:VAL:HG21	1.93	0.50
1:A:268:LEU:O	1:A:270:PRO:HD3	2.12	0.50
1:A:275:ASN:HD22	1:A:277:TYR:H	1.58	0.50
1:A:497:TRP:CD2	1:A:510:PRO:HB3	2.47	0.50
1:B:275:ASN:HD22	1:B:277:TYR:H	1.58	0.50
1:C:136:ASN:O	1:C:138:ILE:N	2.45	0.50
1:D:145:GLU:HB2	1:D:555:VAL:HG21	1.93	0.50
1:D:239:VAL:HG12	1:D:240:LYS:N	2.24	0.50
1:A:297:ILE:HG23	1:A:298:GLY:O	2.12	0.50
1:A:715:ILE:HD13	1:A:725:TRP:CZ2	2.46	0.50
1:B:268:LEU:O	1:B:270:PRO:HD3	2.12	0.50
1:B:529:GLY:CA	1:B:676:ILE:HD11	2.41	0.50
1:B:575:THR:O	1:B:576:VAL:C	2.54	0.50
1:C:177:VAL:O	1:C:178:ASN:C	2.55	0.50
1:C:180:ALA:HB3	1:C:213:LYS:HG2	1.94	0.50
1:D:128:ILE:CD1	1:D:226:ILE:HD12	2.23	0.50
1:D:297:ILE:HG23	1:D:298:GLY:O	2.12	0.50
1:A:242:TYR:HA	1:A:246:TRP:H	1.77	0.50
1:A:676:ILE:HG23	1:A:688:ARG:HB2	1.94	0.50
1:D:325:VAL:HG22	1:D:326:PRO:CD	2.32	0.50
1:D:483:SER:OG	1:D:496:SER:HB2	2.12	0.50
1:A:310:GLY:H	1:A:333:PHE:HA	1.77	0.50
1:A:402:PHE:HE2	1:A:585:PHE:CD1	2.29	0.50
1:B:128:ILE:HG22	1:B:129:SER:N	2.26	0.50
1:B:145:GLU:HB2	1:B:555:VAL:HG21	1.93	0.50
1:B:177:VAL:O	1:B:178:ASN:C	2.55	0.50
1:C:145:GLU:HG3	1:C:160:PRO:HG2	1.93	0.50
1:C:734:VAL:HG13	1:D:272:TYR:CE2	2.45	0.50
1:D:303:GLN:O	1:D:307:GLU:N	2.44	0.50
1:D:310:GLY:H	1:D:333:PHE:HA	1.77	0.50
1:D:579:VAL:O	1:D:583:MET:HG2	2.12	0.50
1:D:676:ILE:HG23	1:D:688:ARG:HB2	1.94	0.50
1:A:483:SER:OG	1:A:496:SER:HB2	2.12	0.49
1:B:180:ALA:HB3	1:B:213:LYS:HG2	1.94	0.49
1:B:297:ILE:CG2	1:B:302:ALA:HB2	2.42	0.49
1:A:275:ASN:HD22	1:A:277:TYR:N	2.09	0.49
1:A:297:ILE:CG2	1:A:302:ALA:HB2	2.42	0.49
1:B:483:SER:OG	1:B:496:SER:HB2	2.12	0.49
1:D:269:THR:OG1	1:D:269:THR:O	2.20	0.49
1:A:663:MET:HG2	1:B:369:ASP:OD2	2.08	0.49
1:B:241:SER:O	1:B:243:PRO:CD	2.57	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:297:ILE:HG23	1:C:298:GLY:O	2.12	0.49
1:C:497:TRP:CD2	1:C:510:PRO:HB3	2.47	0.49
1:C:626:SER:O	1:C:729:LYS:HD2	2.11	0.49
1:D:575:THR:O	1:D:576:VAL:C	2.54	0.49
1:A:141:THR:CG2	1:A:142:SER:H	2.25	0.49
1:B:178:ASN:HD21	1:B:204:ARG:HH21	1.59	0.49
1:B:242:TYR:HA	1:B:246:TRP:H	1.77	0.49
1:C:242:TYR:HB3	1:C:243:PRO:HD3	1.94	0.49
1:C:266:ASP:OD1	1:C:267:PRO:HD2	2.11	0.49
1:C:375:GLY:O	1:C:451:ASN:HA	2.13	0.49
1:C:483:SER:OG	1:C:496:SER:HB2	2.12	0.49
1:C:676:ILE:HG23	1:C:688:ARG:HB2	1.94	0.49
1:C:690:VAL:CG2	1:C:738:THR:HG21	2.38	0.49
1:C:715:ILE:HD13	1:C:725:TRP:CZ2	2.46	0.49
1:D:242:TYR:HA	1:D:246:TRP:H	1.77	0.49
1:D:297:ILE:CG2	1:D:302:ALA:HB2	2.42	0.49
1:D:375:GLY:O	1:D:451:ASN:HA	2.13	0.49
1:D:497:TRP:CD2	1:D:510:PRO:HB3	2.47	0.49
1:B:654:ASP:HB2	1:D:591:ILE:CD1	2.34	0.49
1:C:268:LEU:O	1:C:270:PRO:HD3	2.12	0.49
1:C:402:PHE:HE2	1:C:585:PHE:CD1	2.29	0.49
1:D:131:ILE:HG22	1:D:132:ASN:N	2.28	0.49
1:D:268:LEU:O	1:D:270:PRO:HD3	2.12	0.49
1:A:131:ILE:HG22	1:A:132:ASN:N	2.28	0.49
1:A:180:ALA:HB3	1:A:213:LYS:HG2	1.94	0.49
1:A:579:VAL:O	1:A:583:MET:HG2	2.12	0.49
1:B:212:ASN:O	1:B:213:LYS:C	2.56	0.49
1:B:310:GLY:H	1:B:333:PHE:HA	1.77	0.49
1:C:241:SER:O	1:C:243:PRO:CD	2.58	0.49
1:C:297:ILE:CG2	1:C:302:ALA:HB2	2.42	0.49
1:A:375:GLY:O	1:A:451:ASN:HA	2.12	0.49
1:C:275:ASN:HD22	1:C:277:TYR:N	2.09	0.49
1:C:575:THR:O	1:C:576:VAL:C	2.54	0.49
1:C:733:TYR:CE1	1:D:278:ALA:HA	2.47	0.49
1:D:177:VAL:O	1:D:178:ASN:C	2.55	0.49
1:A:136:ASN:O	1:A:138:ILE:N	2.45	0.49
1:A:674:ALA:HB1	1:A:742:ALA:HA	1.95	0.49
1:B:136:ASN:O	1:B:138:ILE:N	2.45	0.49
1:B:297:ILE:HG23	1:B:298:GLY:O	2.12	0.49
1:B:579:VAL:O	1:B:583:MET:HG2	2.12	0.49
1:C:141:THR:CG2	1:C:142:SER:H	2.26	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:58:MET:HA	1:D:585:PHE:CE2	2.48	0.49
1:D:103:PHE:CD1	1:D:400:ARG:HG2	2.48	0.49
1:D:141:THR:CG2	1:D:142:SER:H	2.25	0.49
1:D:402:PHE:HE2	1:D:585:PHE:CD1	2.29	0.49
1:A:210:ARG:HA	1:A:213:LYS:HG3	1.94	0.49
1:B:103:PHE:CD1	1:B:400:ARG:HG2	2.48	0.49
1:B:206:GLY:H	1:B:213:LYS:NZ	2.11	0.49
1:B:266:ASP:OD1	1:B:267:PRO:HD2	2.11	0.49
1:C:579:VAL:O	1:C:583:MET:HG2	2.12	0.49
1:C:603:VAL:HG23	1:C:604:LEU:N	2.28	0.49
1:D:174:LEU:N	1:D:174:LEU:CD1	2.75	0.49
1:A:206:GLY:H	1:A:213:LYS:NZ	2.11	0.49
1:A:212:ASN:O	1:A:213:LYS:C	2.56	0.49
1:A:236:ALA:HB3	1:A:246:TRP:HZ3	1.78	0.49
1:A:598:ARG:O	1:A:601:ALA:HB3	2.13	0.49
1:C:212:ASN:O	1:C:213:LYS:C	2.56	0.49
1:C:440:ARG:NH1	1:D:674:ALA:O	2.45	0.49
1:D:359:ILE:CD1	1:D:434:TRP:NE1	2.76	0.49
1:A:128:ILE:CD1	1:A:226:ILE:HD12	2.23	0.48
1:A:602:VAL:HG12	1:A:606:LYS:HE3	1.95	0.48
1:B:359:ILE:CD1	1:B:434:TRP:NE1	2.76	0.48
1:B:674:ALA:HB1	1:B:742:ALA:HA	1.95	0.48
1:C:206:GLY:H	1:C:213:LYS:NZ	2.11	0.48
1:C:598:ARG:O	1:C:601:ALA:HB3	2.13	0.48
1:C:654:ASP:C	1:C:656:SER:H	2.19	0.48
1:D:180:ALA:HB3	1:D:213:LYS:HG2	1.94	0.48
1:D:602:VAL:HG12	1:D:606:LYS:HE3	1.95	0.48
1:A:174:LEU:N	1:A:174:LEU:CD1	2.75	0.48
1:B:598:ARG:O	1:B:601:ALA:HB3	2.13	0.48
1:B:654:ASP:C	1:B:656:SER:H	2.19	0.48
1:C:245:GLY:O	1:C:246:TRP:HB2	2.13	0.48
1:D:192:MET:O	1:D:193:LYS:C	2.56	0.48
1:A:603:VAL:HG23	1:A:604:LEU:N	2.28	0.48
1:B:210:ARG:HA	1:B:213:LYS:HG3	1.94	0.48
1:C:255:ARG:HG2	1:C:255:ARG:NH1	2.29	0.48
1:D:598:ARG:O	1:D:601:ALA:HB3	2.13	0.48
1:D:638:ASN:O	1:D:639:PHE:C	2.53	0.48
1:D:676:ILE:HD12	1:D:676:ILE:N	2.28	0.48
1:A:174:LEU:HA	1:A:200:ILE:O	2.14	0.48
1:A:259:LEU:CD2	1:A:289:LEU:HD23	2.44	0.48
1:A:670:PHE:CE2	1:B:444:GLU:OE1	2.66	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:58:MET:HA	1:B:585:PHE:CE2	2.48	0.48
1:B:449:TYR:O	1:B:532:SER:CB	2.62	0.48
1:B:603:VAL:HG23	1:B:604:LEU:N	2.28	0.48
1:B:638:ASN:O	1:B:639:PHE:C	2.53	0.48
1:C:593:LEU:C	1:C:595:PHE:H	2.22	0.48
1:C:600:TYR:O	1:C:604:LEU:HG	2.14	0.48
1:D:206:GLY:H	1:D:213:LYS:NZ	2.11	0.48
1:D:255:ARG:HG2	1:D:255:ARG:NH1	2.29	0.48
1:D:275:ASN:HD22	1:D:275:ASN:C	2.22	0.48
1:D:470:MET:HE3	1:D:587:LEU:HD11	1.95	0.48
1:D:630:ASP:O	1:D:634:SER:N	2.44	0.48
1:A:255:ARG:HG2	1:A:255:ARG:NH1	2.29	0.48
1:A:359:ILE:CD1	1:A:434:TRP:NE1	2.76	0.48
1:A:600:TYR:O	1:A:604:LEU:HG	2.14	0.48
1:A:631:SER:O	1:A:634:SER:HB3	2.14	0.48
1:B:422:ASP:O	1:B:430:GLY:HA3	2.13	0.48
1:B:470:MET:HE3	1:B:587:LEU:HD11	1.95	0.48
1:B:600:TYR:O	1:B:604:LEU:HG	2.14	0.48
1:B:631:SER:O	1:B:634:SER:HB3	2.14	0.48
1:B:676:ILE:N	1:B:676:ILE:HD12	2.28	0.48
1:B:692:TYR:O	1:B:693:ALA:HB2	2.14	0.48
1:C:174:LEU:HA	1:C:200:ILE:O	2.14	0.48
1:C:449:TYR:O	1:C:532:SER:CB	2.62	0.48
1:C:676:ILE:HD12	1:C:676:ILE:N	2.28	0.48
1:D:236:ALA:HB3	1:D:246:TRP:HZ3	1.78	0.48
1:D:245:GLY:O	1:D:246:TRP:HB2	2.13	0.48
1:D:593:LEU:C	1:D:595:PHE:H	2.22	0.48
1:A:103:PHE:CD1	1:A:400:ARG:HG2	2.48	0.48
1:B:184:ASP:O	1:B:187:LYS:N	2.47	0.48
1:B:275:ASN:HD22	1:B:275:ASN:C	2.22	0.48
1:B:375:GLY:O	1:B:451:ASN:HA	2.13	0.48
1:B:732:ILE:CD1	1:B:733:TYR:N	2.75	0.48
1:C:131:ILE:HG22	1:C:132:ASN:N	2.28	0.48
1:C:631:SER:O	1:C:634:SER:HB3	2.14	0.48
1:A:275:ASN:HD22	1:A:275:ASN:C	2.22	0.48
1:A:595:PHE:HB2	1:A:668:LEU:HG	1.96	0.48
1:A:676:ILE:HD12	1:A:676:ILE:N	2.29	0.48
1:A:692:TYR:O	1:A:693:ALA:HB2	2.14	0.48
1:B:131:ILE:HG22	1:B:132:ASN:N	2.28	0.48
1:B:141:THR:CG2	1:B:142:SER:H	2.25	0.48
1:C:174:LEU:N	1:C:174:LEU:CD1	2.75	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:184:ASP:O	1:C:187:LYS:N	2.47	0.48
1:C:630:ASP:O	1:C:634:SER:N	2.44	0.48
1:C:692:TYR:O	1:C:693:ALA:HB2	2.14	0.48
1:D:600:TYR:O	1:D:604:LEU:HG	2.14	0.48
1:A:689:HIS:HD2	1:A:691:ILE:H	1.62	0.48
1:B:240:LYS:C	1:B:245:GLY:HA2	2.39	0.48
1:D:174:LEU:HA	1:D:200:ILE:O	2.14	0.48
1:D:236:ALA:CB	1:D:246:TRP:HZ3	2.27	0.48
1:D:422:ASP:O	1:D:430:GLY:HA3	2.13	0.48
1:D:692:TYR:O	1:D:693:ALA:HB2	2.14	0.48
3:U:1:NAG:H62	3:U:2:NAG:C7	2.44	0.48
1:A:140:ASN:HB2	4:A:1760:NAG:C6	2.24	0.48
1:A:179:TYR:N	1:A:179:TYR:CD1	2.82	0.48
1:A:192:MET:O	1:A:193:LYS:C	2.57	0.48
1:A:268:LEU:HD13	1:A:280:ARG:HB3	1.96	0.48
1:A:705:PHE:HB3	1:A:708:ILE:CD1	2.44	0.48
1:B:593:LEU:C	1:B:595:PHE:H	2.22	0.48
1:C:58:MET:HA	1:C:585:PHE:CE2	2.48	0.48
1:C:174:LEU:HD11	1:C:342:VAL:CG2	2.44	0.48
1:C:303:GLN:O	1:C:307:GLU:N	2.44	0.48
1:C:359:ILE:CD1	1:C:434:TRP:NE1	2.76	0.48
1:C:422:ASP:O	1:C:430:GLY:HA3	2.13	0.48
1:C:705:PHE:HB3	1:C:708:ILE:CD1	2.44	0.48
1:D:259:LEU:CD2	1:D:289:LEU:HD23	2.44	0.48
3:K:1:NAG:H62	3:K:2:NAG:C7	2.44	0.48
1:A:506:PHE:C	1:A:508:GLY:H	2.22	0.48
1:B:236:ALA:HB3	1:B:246:TRP:HZ3	1.78	0.48
1:B:303:GLN:O	1:B:307:GLU:N	2.44	0.48
1:B:689:HIS:HD2	1:B:691:ILE:H	1.62	0.48
1:B:705:PHE:HB3	1:B:708:ILE:CD1	2.44	0.48
1:C:192:MET:O	1:C:193:LYS:C	2.57	0.48
1:C:242:TYR:HA	1:C:246:TRP:H	1.77	0.48
1:C:323:LEU:O	1:C:325:VAL:N	2.43	0.48
1:C:438:ASN:O	1:C:439:SER:C	2.57	0.48
3:F:1:NAG:H62	3:F:2:NAG:C7	2.44	0.48
1:A:95:GLN:HG2	1:A:99:GLN:OE1	2.14	0.47
1:A:240:LYS:CB	1:A:245:GLY:HA2	2.37	0.47
1:A:422:ASP:O	1:A:430:GLY:HA3	2.13	0.47
1:A:593:LEU:C	1:A:595:PHE:H	2.22	0.47
1:B:255:ARG:HG2	1:B:255:ARG:NH1	2.28	0.47
1:C:179:TYR:CD1	1:C:179:TYR:N	2.82	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:95:GLN:HG2	1:D:99:GLN:OE1	2.14	0.47
1:D:595:PHE:HB2	1:D:668:LEU:HG	1.96	0.47
3:P:1:NAG:H62	3:P:2:NAG:C7	2.44	0.47
1:A:240:LYS:C	1:A:245:GLY:HA2	2.39	0.47
1:A:442:LEU:HB3	1:A:530:ILE:HD11	1.96	0.47
1:B:192:MET:O	1:B:193:LYS:C	2.56	0.47
1:B:427:GLY:C	1:B:429:LEU:H	2.22	0.47
1:B:438:ASN:O	1:B:439:SER:C	2.57	0.47
1:B:602:VAL:HG12	1:B:606:LYS:HE3	1.95	0.47
1:C:236:ALA:CB	1:C:246:TRP:HZ3	2.27	0.47
1:C:470:MET:HE3	1:C:587:LEU:HD11	1.95	0.47
1:D:184:ASP:O	1:D:187:LYS:N	2.47	0.47
1:D:268:LEU:HD13	1:D:280:ARG:HB3	1.96	0.47
1:D:690:VAL:CG2	1:D:738:THR:HG21	2.38	0.47
1:A:58:MET:HA	1:A:585:PHE:CE2	2.48	0.47
1:A:178:ASN:O	1:A:179:TYR:C	2.58	0.47
1:A:184:ASP:O	1:A:187:LYS:N	2.47	0.47
1:A:727:GLU:O	1:A:730:ARG:HB3	2.15	0.47
1:B:442:LEU:HB3	1:B:530:ILE:HD11	1.96	0.47
1:C:103:PHE:CD1	1:C:400:ARG:HG2	2.48	0.47
1:C:236:ALA:HB3	1:C:246:TRP:HZ3	1.78	0.47
1:C:275:ASN:HD22	1:C:275:ASN:C	2.22	0.47
1:D:603:VAL:HG23	1:D:604:LEU:N	2.28	0.47
1:A:391:GLY:HA3	1:A:453:ASP:O	2.15	0.47
1:A:470:MET:HE3	1:A:587:LEU:HD11	1.95	0.47
1:B:95:GLN:HG2	1:B:99:GLN:OE1	2.14	0.47
1:B:174:LEU:HA	1:B:200:ILE:O	2.13	0.47
1:B:506:PHE:C	1:B:508:GLY:H	2.22	0.47
1:C:442:LEU:HB3	1:C:530:ILE:HD11	1.96	0.47
1:C:444:GLU:OE1	1:D:670:PHE:CE2	2.67	0.47
1:C:729:LYS:O	1:C:732:ILE:HG13	2.15	0.47
1:C:732:ILE:CD1	1:C:733:TYR:N	2.75	0.47
1:D:591:ILE:HG22	1:D:592:VAL:N	2.29	0.47
1:A:236:ALA:CB	1:A:246:TRP:HZ3	2.27	0.47
1:A:449:TYR:O	1:A:532:SER:CB	2.62	0.47
1:A:575:THR:O	1:A:576:VAL:C	2.54	0.47
1:B:174:LEU:HD11	1:B:342:VAL:CG2	2.44	0.47
1:B:179:TYR:N	1:B:179:TYR:CD1	2.82	0.47
1:B:259:LEU:CD2	1:B:289:LEU:HD23	2.44	0.47
1:B:268:LEU:HD13	1:B:280:ARG:HB3	1.96	0.47
1:B:470:MET:CE	1:B:587:LEU:HD11	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:595:PHE:HB2	1:B:668:LEU:HG	1.96	0.47
1:B:727:GLU:O	1:B:730:ARG:HB3	2.15	0.47
1:C:674:ALA:HB1	1:C:742:ALA:HA	1.95	0.47
1:C:705:PHE:N	1:C:706:PRO:CD	2.78	0.47
1:D:174:LEU:HD11	1:D:342:VAL:CG2	2.44	0.47
1:D:250:GLY:HA2	1:D:299:TYR:CZ	2.50	0.47
1:D:421:TRP:HH2	1:D:434:TRP:CE3	2.33	0.47
1:D:631:SER:O	1:D:634:SER:HB3	2.14	0.47
1:A:245:GLY:O	1:A:246:TRP:HB2	2.13	0.47
1:A:705:PHE:N	1:A:706:PRO:CD	2.78	0.47
1:B:245:GLY:O	1:B:246:TRP:HB2	2.13	0.47
1:C:240:LYS:C	1:C:245:GLY:HA2	2.39	0.47
1:C:638:ASN:O	1:C:639:PHE:C	2.53	0.47
1:A:174:LEU:HD11	1:A:342:VAL:CG2	2.44	0.47
1:A:428:LEU:HD23	1:A:520:ASP:HA	1.97	0.47
1:A:591:ILE:HG22	1:A:592:VAL:N	2.29	0.47
1:A:729:LYS:O	1:A:732:ILE:HG13	2.15	0.47
1:B:178:ASN:O	1:B:179:TYR:C	2.58	0.47
1:B:236:ALA:CB	1:B:246:TRP:HZ3	2.27	0.47
1:C:259:LEU:CD2	1:C:289:LEU:HD23	2.44	0.47
1:C:268:LEU:HD13	1:C:280:ARG:HB3	1.96	0.47
1:C:468:PRO:HG2	1:C:603:VAL:HG21	1.97	0.47
1:C:470:MET:CE	1:C:587:LEU:HD11	2.45	0.47
1:C:595:PHE:HB2	1:C:668:LEU:HG	1.96	0.47
1:C:602:VAL:HG12	1:C:606:LYS:HE3	1.95	0.47
1:C:727:GLU:O	1:C:730:ARG:HB3	2.15	0.47
1:D:391:GLY:HA3	1:D:453:ASP:O	2.15	0.47
1:D:674:ALA:HB1	1:D:742:ALA:HA	1.95	0.47
1:D:705:PHE:HB3	1:D:708:ILE:CD1	2.44	0.47
1:A:241:SER:O	1:A:243:PRO:CD	2.57	0.47
1:A:272:TYR:CE2	1:B:734:VAL:HG13	2.49	0.47
1:B:174:LEU:N	1:B:174:LEU:CD1	2.75	0.47
1:B:250:GLY:HA2	1:B:299:TYR:CZ	2.50	0.47
1:B:732:ILE:HD12	1:B:732:ILE:C	2.40	0.47
1:C:133:GLU:O	1:C:134:ASP:HB2	2.15	0.47
1:C:506:PHE:C	1:C:508:GLY:H	2.22	0.47
1:C:670:PHE:CE2	1:D:444:GLU:CD	2.93	0.47
1:D:470:MET:CE	1:D:587:LEU:HD11	2.45	0.47
1:A:177:VAL:O	1:A:178:ASN:C	2.55	0.47
1:A:250:GLY:HA2	1:A:299:TYR:CZ	2.50	0.47
1:A:427:GLY:C	1:A:429:LEU:H	2.22	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:538:THR:HG23	1:A:539:LYS:N	2.30	0.47
1:B:391:GLY:HA3	1:B:453:ASP:O	2.15	0.47
1:C:421:TRP:HH2	1:C:434:TRP:CE3	2.33	0.47
1:D:335:GLY:C	1:D:337:PHE:N	2.73	0.47
1:D:427:GLY:C	1:D:429:LEU:H	2.22	0.47
1:D:481:LEU:HA	1:D:481:LEU:HD23	1.70	0.47
1:D:729:LYS:O	1:D:732:ILE:HG13	2.15	0.47
1:A:661:LEU:O	1:A:664:MET:HB2	2.15	0.47
1:B:661:LEU:O	1:B:664:MET:HB2	2.15	0.47
1:D:178:ASN:O	1:D:179:TYR:C	2.58	0.47
1:D:449:TYR:O	1:D:532:SER:CB	2.62	0.47
1:A:282:GLY:O	1:A:283:ILE:C	2.58	0.46
1:A:438:ASN:O	1:A:439:SER:C	2.56	0.46
1:B:555:VAL:C	1:B:557:GLU:H	2.23	0.46
1:D:591:ILE:HG22	1:D:592:VAL:HG23	1.97	0.46
1:B:591:ILE:HG22	1:B:592:VAL:N	2.29	0.46
1:C:95:GLN:HG2	1:C:99:GLN:OE1	2.14	0.46
1:C:140:ASN:HB2	4:C:3760:NAG:C6	2.24	0.46
1:C:178:ASN:O	1:C:179:TYR:C	2.58	0.46
1:C:250:GLY:HA2	1:C:299:TYR:CZ	2.50	0.46
1:D:355:ILE:HB	1:D:422:ASP:OD2	2.15	0.46
1:D:442:LEU:HB3	1:D:530:ILE:HD11	1.96	0.46
1:D:727:GLU:O	1:D:730:ARG:HB3	2.15	0.46
1:A:470:MET:CE	1:A:587:LEU:HD11	2.45	0.46
1:B:676:ILE:HG23	1:B:688:ARG:CB	2.45	0.46
1:B:690:VAL:HG21	1:B:738:THR:CG2	2.41	0.46
1:C:106:ASP:CG	1:C:411:ARG:HH22	2.24	0.46
1:C:149:PRO:O	1:C:151:TYR:N	2.49	0.46
1:D:240:LYS:C	1:D:245:GLY:HA2	2.39	0.46
1:D:456:ILE:O	1:D:457:GLU:HG3	2.15	0.46
1:D:515:LEU:HB3	1:D:516:GLY:H	1.49	0.46
1:D:661:LEU:O	1:D:664:MET:HB2	2.15	0.46
1:D:689:HIS:HD2	1:D:691:ILE:H	1.62	0.46
1:A:369:ASP:OD2	1:A:662:ARG:NH2	2.44	0.46
1:A:708:ILE:HD11	1:A:735:ALA:CB	2.46	0.46
1:B:133:GLU:O	1:B:134:ASP:HB2	2.15	0.46
1:B:145:GLU:OE1	1:B:160:PRO:HG3	2.16	0.46
1:B:323:LEU:O	1:B:325:VAL:N	2.43	0.46
1:B:456:ILE:O	1:B:457:GLU:HG3	2.15	0.46
1:B:468:PRO:HG2	1:B:603:VAL:HG21	1.97	0.46
1:B:593:LEU:HA	1:B:594:PRO:HD3	1.64	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:708:ILE:HD11	1:B:735:ALA:CB	2.46	0.46
1:C:145:GLU:OE1	1:C:160:PRO:HG3	2.16	0.46
1:C:427:GLY:C	1:C:429:LEU:H	2.22	0.46
1:C:428:LEU:HD23	1:C:520:ASP:HA	1.97	0.46
1:C:608:ALA:O	1:C:611:ILE:HG22	2.16	0.46
1:D:179:TYR:N	1:D:179:TYR:CD1	2.82	0.46
1:A:421:TRP:HH2	1:A:434:TRP:CE3	2.33	0.46
1:A:468:PRO:HG2	1:A:603:VAL:HG21	1.97	0.46
1:A:574:LEU:O	1:A:577:ALA:HB3	2.16	0.46
1:A:676:ILE:HG23	1:A:688:ARG:CB	2.45	0.46
1:A:732:ILE:HD12	1:A:732:ILE:C	2.40	0.46
1:A:732:ILE:CD1	1:A:733:TYR:N	2.75	0.46
1:B:282:GLY:O	1:B:283:ILE:C	2.58	0.46
1:B:421:TRP:HH2	1:B:434:TRP:CE3	2.33	0.46
1:B:507:SER:C	1:B:509:MET:H	2.24	0.46
1:C:483:SER:OG	1:C:496:SER:CB	2.64	0.46
1:C:538:THR:HG23	1:C:539:LYS:N	2.30	0.46
1:C:689:HIS:HD2	1:C:691:ILE:H	1.62	0.46
1:D:212:ASN:O	1:D:213:LYS:C	2.56	0.46
1:D:676:ILE:HG23	1:D:688:ARG:CB	2.45	0.46
1:A:483:SER:OG	1:A:496:SER:CB	2.64	0.46
1:A:555:VAL:C	1:A:557:GLU:H	2.23	0.46
1:B:89:ASN:ND2	1:B:422:ASP:OD1	2.49	0.46
1:B:106:ASP:CG	1:B:411:ARG:HH22	2.24	0.46
1:C:391:GLY:HA3	1:C:453:ASP:O	2.15	0.46
1:C:661:LEU:O	1:C:664:MET:HB2	2.15	0.46
1:D:386:ILE:HA	1:D:390:SER:HB2	1.98	0.46
1:D:658:PRO:O	1:D:661:LEU:HB3	2.16	0.46
1:B:428:LEU:HD23	1:B:520:ASP:HA	1.97	0.46
1:B:574:LEU:O	1:B:577:ALA:HB3	2.16	0.46
1:B:729:LYS:O	1:B:732:ILE:HG13	2.15	0.46
1:C:89:ASN:ND2	1:C:422:ASP:OD1	2.49	0.46
1:C:591:ILE:HG22	1:C:592:VAL:N	2.29	0.46
1:D:133:GLU:O	1:D:134:ASP:HB2	2.15	0.46
1:D:178:ASN:HD22	1:D:178:ASN:HA	1.52	0.46
1:D:506:PHE:C	1:D:508:GLY:H	2.22	0.46
1:A:106:ASP:OD2	1:A:362:LEU:HD12	2.16	0.46
1:A:295:HIS:HA	1:A:296:PRO:HD3	1.66	0.46
1:B:526:GLN:HE21	1:B:692:TYR:C	2.24	0.46
1:B:591:ILE:HG22	1:B:592:VAL:HG23	1.97	0.46
1:C:355:ILE:HB	1:C:422:ASP:OD2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:456:ILE:O	1:C:457:GLU:HG3	2.15	0.46
1:D:149:PRO:O	1:D:151:TYR:N	2.49	0.46
1:D:438:ASN:O	1:D:439:SER:C	2.57	0.46
1:D:507:SER:C	1:D:509:MET:H	2.23	0.46
1:D:608:ALA:O	1:D:611:ILE:HG22	2.16	0.46
1:A:456:ILE:O	1:A:457:GLU:HG3	2.15	0.46
1:A:658:PRO:O	1:A:661:LEU:HB3	2.16	0.46
1:B:65:LEU:HD22	1:B:397:GLU:HG3	1.98	0.46
1:B:149:PRO:O	1:B:151:TYR:N	2.49	0.46
1:B:483:SER:OG	1:B:496:SER:CB	2.64	0.46
1:B:705:PHE:N	1:B:706:PRO:CD	2.78	0.46
1:D:65:LEU:HD22	1:D:397:GLU:HG3	1.98	0.46
1:D:145:GLU:OE1	1:D:160:PRO:HG3	2.16	0.46
1:D:468:PRO:HG2	1:D:603:VAL:HG21	1.97	0.46
1:D:555:VAL:C	1:D:557:GLU:H	2.23	0.46
1:D:732:ILE:HD12	1:D:732:ILE:C	2.40	0.46
1:A:146:PRO:HA	1:A:147:PRO:HD2	1.82	0.46
1:A:355:ILE:HB	1:A:422:ASP:OD2	2.16	0.46
1:A:386:ILE:HA	1:A:390:SER:HB2	1.98	0.46
1:B:214:VAL:HG21	1:B:258:ILE:HG21	1.98	0.46
1:B:658:PRO:O	1:B:661:LEU:HB3	2.16	0.46
1:C:386:ILE:HA	1:C:390:SER:HB2	1.98	0.46
1:C:555:VAL:C	1:C:557:GLU:H	2.23	0.46
1:C:708:ILE:HD11	1:C:735:ALA:CB	2.46	0.46
1:D:106:ASP:OD2	1:D:362:LEU:HD12	2.16	0.46
1:A:89:ASN:ND2	1:A:422:ASP:OD1	2.49	0.45
1:A:149:PRO:O	1:A:151:TYR:N	2.49	0.45
1:A:214:VAL:HG21	1:A:258:ILE:HG21	1.98	0.45
1:B:325:VAL:HG22	1:B:326:PRO:CD	2.32	0.45
1:B:427:GLY:C	1:B:429:LEU:N	2.74	0.45
1:B:608:ALA:O	1:B:611:ILE:HG22	2.16	0.45
1:C:627:VAL:HG21	1:C:725:TRP:HE3	1.81	0.45
1:D:483:SER:OG	1:D:496:SER:CB	2.64	0.45
1:A:133:GLU:O	1:A:134:ASP:HB2	2.15	0.45
1:A:608:ALA:O	1:A:611:ILE:HG22	2.16	0.45
1:A:663:MET:HG2	1:B:369:ASP:OD1	2.12	0.45
1:B:308:LYS:HD3	1:B:337:PHE:CD2	2.52	0.45
1:B:538:THR:HG23	1:B:539:LYS:N	2.30	0.45
1:B:698:ASN:ND2	1:B:701:ALA:C	2.75	0.45
1:C:65:LEU:HD22	1:C:397:GLU:HG3	1.98	0.45
1:C:275:ASN:C	1:C:275:ASN:ND2	2.74	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:567:ASP:CG	1:C:570:PHE:HA	2.41	0.45
1:C:574:LEU:O	1:C:577:ALA:HB3	2.16	0.45
1:D:106:ASP:CG	1:D:411:ARG:HH22	2.24	0.45
1:D:140:ASN:HB2	4:D:4760:NAG:C6	2.24	0.45
1:D:538:THR:HG23	1:D:539:LYS:N	2.30	0.45
1:A:567:ASP:CG	1:A:570:PHE:HA	2.41	0.45
1:A:591:ILE:HG22	1:A:592:VAL:HG23	1.98	0.45
1:A:630:ASP:O	1:A:634:SER:N	2.44	0.45
1:B:275:ASN:C	1:B:275:ASN:ND2	2.75	0.45
1:C:240:LYS:CB	1:C:245:GLY:HA2	2.37	0.45
1:C:732:ILE:HD12	1:C:732:ILE:C	2.40	0.45
1:D:89:ASN:ND2	1:D:422:ASP:OD1	2.49	0.45
1:A:467:THR:O	1:A:469:LEU:N	2.49	0.45
1:A:479:LYS:HG2	1:A:494:TYR:CG	2.52	0.45
1:B:131:ILE:HD12	1:B:136:ASN:HA	1.99	0.45
1:B:467:THR:HG21	1:B:531:ALA:HB1	1.99	0.45
1:B:708:ILE:HD11	1:B:735:ALA:HB2	1.99	0.45
1:C:79:GLN:C	1:C:80:ILE:HD13	2.42	0.45
1:C:593:LEU:HA	1:C:594:PRO:HD3	1.64	0.45
1:C:676:ILE:HG23	1:C:688:ARG:CB	2.45	0.45
1:C:708:ILE:HD11	1:C:735:ALA:HB2	1.99	0.45
1:D:214:VAL:HG21	1:D:258:ILE:HG21	1.98	0.45
1:D:240:LYS:H	1:D:240:LYS:CD	2.25	0.45
1:D:282:GLY:O	1:D:283:ILE:C	2.58	0.45
1:D:698:ASN:ND2	1:D:701:ALA:C	2.74	0.45
1:A:165:SER:OG	1:A:293:PRO:HA	2.17	0.45
1:B:240:LYS:CB	1:B:245:GLY:HA2	2.37	0.45
1:B:369:ASP:OD2	1:B:662:ARG:NH2	2.44	0.45
1:B:479:LYS:HG2	1:B:494:TYR:CG	2.52	0.45
1:B:610:LYS:HD2	1:B:614:ILE:HD11	1.98	0.45
1:C:308:LYS:HD3	1:C:337:PHE:CD2	2.52	0.45
1:C:507:SER:C	1:C:509:MET:H	2.23	0.45
1:C:728:VAL:C	1:C:730:ARG:N	2.75	0.45
1:D:79:GLN:C	1:D:80:ILE:HD13	2.42	0.45
1:D:427:GLY:C	1:D:429:LEU:N	2.74	0.45
1:D:441:LEU:O	1:D:445:ARG:N	2.50	0.45
1:D:732:ILE:CD1	1:D:733:TYR:N	2.75	0.45
1:A:131:ILE:HD12	1:A:136:ASN:HA	1.99	0.45
1:A:275:ASN:C	1:A:275:ASN:ND2	2.75	0.45
1:A:526:GLN:HE21	1:A:692:TYR:C	2.24	0.45
1:A:610:LYS:HD2	1:A:614:ILE:HD11	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:662:ARG:O	1:A:663:MET:C	2.59	0.45
1:B:79:GLN:C	1:B:80:ILE:HD13	2.42	0.45
1:B:355:ILE:HB	1:B:422:ASP:OD2	2.16	0.45
1:C:189:GLU:HB3	1:C:194:ILE:HB	1.98	0.45
1:C:214:VAL:HG21	1:C:258:ILE:HG21	1.98	0.45
1:C:335:GLY:C	1:C:337:PHE:N	2.73	0.45
1:C:509:MET:HE2	1:C:509:MET:HB3	1.79	0.45
1:C:658:PRO:O	1:C:661:LEU:HB3	2.16	0.45
1:D:574:LEU:O	1:D:577:ALA:HB3	2.16	0.45
1:A:145:GLU:OE1	1:A:160:PRO:HG3	2.16	0.45
1:A:308:LYS:HD3	1:A:337:PHE:CD2	2.52	0.45
1:A:441:LEU:O	1:A:445:ARG:N	2.50	0.45
1:A:690:VAL:HG21	1:A:738:THR:CG2	2.41	0.45
1:C:151:TYR:HB3	1:C:154:VAL:HG21	1.99	0.45
1:C:160:PRO:HB3	1:C:253:VAL:CG1	2.47	0.45
1:C:282:GLY:O	1:C:283:ILE:C	2.58	0.45
1:D:65:LEU:CD2	1:D:397:GLU:HG3	2.47	0.45
1:D:131:ILE:HD12	1:D:136:ASN:HA	1.99	0.45
1:D:467:THR:O	1:D:469:LEU:N	2.49	0.45
1:D:569:MET:O	1:D:570:PHE:HB2	2.16	0.45
1:A:65:LEU:HD22	1:A:397:GLU:HG3	1.98	0.45
1:A:106:ASP:CG	1:A:411:ARG:HH22	2.24	0.45
1:A:151:TYR:HB3	1:A:154:VAL:HG21	1.99	0.45
1:A:538:THR:HG23	1:A:539:LYS:O	2.17	0.45
1:B:106:ASP:OD2	1:B:362:LEU:HD12	2.16	0.45
1:B:189:GLU:HB3	1:B:194:ILE:HB	1.98	0.45
1:B:240:LYS:H	1:B:240:LYS:CD	2.25	0.45
1:B:387:ASP:HA	1:B:388:PRO:HA	1.84	0.45
1:C:106:ASP:OD2	1:C:362:LEU:HD12	2.16	0.45
1:C:467:THR:O	1:C:469:LEU:N	2.49	0.45
1:C:675:PHE:O	1:C:690:VAL:HG23	2.17	0.45
1:D:567:ASP:CG	1:D:570:PHE:HA	2.41	0.45
1:A:160:PRO:HB3	1:A:253:VAL:CG1	2.47	0.45
1:B:242:TYR:HD2	1:B:556:TYR:HD2	1.65	0.45
1:C:65:LEU:CD2	1:C:397:GLU:HG3	2.47	0.45
1:C:526:GLN:HE21	1:C:692:TYR:C	2.24	0.45
1:C:698:ASN:ND2	1:C:701:ALA:C	2.74	0.45
1:D:160:PRO:HB3	1:D:253:VAL:CG1	2.47	0.45
1:D:314:PRO:CG	1:D:327:TYR:O	2.65	0.45
1:D:708:ILE:HD11	1:D:735:ALA:CB	2.46	0.45
1:A:189:GLU:HB3	1:A:194:ILE:HB	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:728:VAL:C	1:A:730:ARG:N	2.75	0.45
1:B:160:PRO:HB3	1:B:253:VAL:CG1	2.47	0.45
1:B:669:MET:HE2	1:B:670:PHE:CE1	2.52	0.45
1:C:610:LYS:HD2	1:C:614:ILE:HD11	1.98	0.45
1:D:275:ASN:C	1:D:275:ASN:ND2	2.74	0.45
1:D:369:ASP:OD2	1:D:662:ARG:NH2	2.44	0.45
1:D:662:ARG:O	1:D:663:MET:C	2.59	0.45
1:A:314:PRO:CG	1:A:327:TYR:O	2.65	0.44
1:B:107:SER:O	1:B:108:VAL:CG2	2.66	0.44
1:C:441:LEU:O	1:C:445:ARG:N	2.50	0.44
1:C:569:MET:O	1:C:570:PHE:HB2	2.16	0.44
1:D:526:GLN:HE21	1:D:692:TYR:C	2.24	0.44
1:D:675:PHE:O	1:D:690:VAL:HG23	2.17	0.44
1:A:569:MET:O	1:A:570:PHE:HB2	2.16	0.44
1:B:182:THR:O	1:B:183:GLU:CB	2.65	0.44
1:B:362:LEU:HD12	1:B:362:LEU:HA	1.82	0.44
1:B:386:ILE:HA	1:B:390:SER:HB2	1.98	0.44
1:C:107:SER:O	1:C:108:VAL:CG2	2.66	0.44
1:C:314:PRO:CG	1:C:327:TYR:O	2.65	0.44
1:C:591:ILE:HG22	1:C:592:VAL:HG23	1.97	0.44
1:C:663:MET:SD	1:D:368:PRO:HD2	2.56	0.44
1:D:107:SER:O	1:D:108:VAL:CG2	2.66	0.44
1:D:428:LEU:HD23	1:D:520:ASP:HA	1.97	0.44
1:D:479:LYS:HG2	1:D:494:TYR:CG	2.52	0.44
1:D:538:THR:HG23	1:D:539:LYS:O	2.17	0.44
1:A:78:THR:HG21	1:A:559:TYR:HB2	1.99	0.44
1:A:79:GLN:C	1:A:80:ILE:HD13	2.42	0.44
1:A:323:LEU:O	1:A:325:VAL:N	2.43	0.44
1:A:669:MET:HE2	1:A:670:PHE:CE1	2.52	0.44
1:B:165:SER:OG	1:B:293:PRO:HA	2.17	0.44
1:C:292:ILE:HD13	1:C:292:ILE:H	1.83	0.44
1:D:189:GLU:HB3	1:D:194:ILE:HB	1.98	0.44
1:D:272:TYR:HA	1:D:273:PRO:HD3	1.77	0.44
1:A:242:TYR:HD2	1:A:556:TYR:HD2	1.65	0.44
1:A:245:GLY:O	1:A:246:TRP:HB3	2.18	0.44
1:A:427:GLY:C	1:A:429:LEU:N	2.74	0.44
1:A:515:LEU:HB3	1:A:516:GLY:H	1.49	0.44
1:A:698:ASN:ND2	1:A:701:ALA:C	2.74	0.44
1:A:708:ILE:HD11	1:A:735:ALA:HB2	1.99	0.44
1:B:78:THR:HG21	1:B:559:TYR:HB2	1.99	0.44
1:B:567:ASP:CG	1:B:570:PHE:HA	2.41	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:569:MET:O	1:B:570:PHE:HB2	2.16	0.44
1:C:78:THR:HG21	1:C:559:TYR:HB2	1.99	0.44
1:C:669:MET:HE2	1:C:670:PHE:CE1	2.52	0.44
1:D:151:TYR:HB3	1:D:154:VAL:HG21	1.99	0.44
1:D:165:SER:OG	1:D:293:PRO:HA	2.17	0.44
1:A:65:LEU:CD2	1:A:397:GLU:HG3	2.47	0.44
1:A:77:PHE:HB2	1:A:389:GLN:HG3	1.99	0.44
1:A:182:THR:O	1:A:183:GLU:CB	2.65	0.44
1:A:335:GLY:C	1:A:337:PHE:N	2.73	0.44
1:B:65:LEU:CD2	1:B:397:GLU:HG3	2.47	0.44
1:B:151:TYR:HB3	1:B:154:VAL:HG21	1.99	0.44
1:B:165:SER:HA	1:B:166:PRO:HD3	1.83	0.44
1:B:538:THR:HG23	1:B:539:LYS:O	2.17	0.44
1:C:159:PRO:O	1:C:160:PRO:C	2.61	0.44
1:C:725:TRP:O	1:C:729:LYS:HB2	2.18	0.44
1:D:78:THR:HG21	1:D:559:TYR:HB2	1.99	0.44
1:D:159:PRO:O	1:D:160:PRO:C	2.61	0.44
1:D:743:ALA:C	1:D:745:THR:N	2.75	0.44
1:A:656:SER:HB3	1:C:591:ILE:HD12	2.00	0.44
1:B:245:GLY:O	1:B:246:TRP:HB3	2.18	0.44
1:B:314:PRO:CG	1:B:327:TYR:O	2.65	0.44
1:B:441:LEU:O	1:B:445:ARG:N	2.50	0.44
1:B:467:THR:O	1:B:469:LEU:N	2.49	0.44
1:B:509:MET:HE2	1:B:509:MET:HB3	1.79	0.44
1:B:675:PHE:O	1:B:690:VAL:HG23	2.17	0.44
1:C:151:TYR:N	1:C:151:TYR:CD1	2.86	0.44
1:C:325:VAL:HG22	1:C:326:PRO:CD	2.32	0.44
1:C:538:THR:HG23	1:C:539:LYS:O	2.17	0.44
1:D:105:LEU:HD23	1:D:105:LEU:HA	1.66	0.44
1:D:610:LYS:HD2	1:D:614:ILE:HD11	1.98	0.44
1:A:107:SER:O	1:A:108:VAL:CG2	2.66	0.44
1:A:212:ASN:O	1:A:216:ASN:N	2.44	0.44
1:A:306:LEU:O	1:A:309:MET:HB3	2.18	0.44
1:A:675:PHE:O	1:A:690:VAL:HG23	2.17	0.44
1:C:616:MET:C	1:C:618:HIS:H	2.26	0.44
1:D:129:SER:O	1:D:342:VAL:HA	2.18	0.44
1:D:708:ILE:HD11	1:D:735:ALA:HB2	1.99	0.44
1:D:725:TRP:O	1:D:729:LYS:HB2	2.18	0.44
1:A:509:MET:HE2	1:A:509:MET:HB3	1.79	0.44
1:A:627:VAL:HG21	1:A:725:TRP:HE3	1.81	0.44
1:B:306:LEU:O	1:B:309:MET:HB3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:335:GLY:C	1:B:337:PHE:N	2.73	0.44
1:B:662:ARG:O	1:B:663:MET:C	2.59	0.44
1:B:743:ALA:C	1:B:745:THR:N	2.75	0.44
1:C:369:ASP:OD2	1:C:662:ARG:NH2	2.44	0.44
1:C:467:THR:HG21	1:C:531:ALA:HB1	1.98	0.44
1:A:458:GLY:HA2	3:H:1:NAG:H81	2.00	0.44
1:B:107:SER:O	1:B:108:VAL:HG23	2.18	0.44
1:B:728:VAL:C	1:B:730:ARG:N	2.75	0.44
1:C:131:ILE:HD12	1:C:136:ASN:HA	1.99	0.44
1:C:306:LEU:O	1:C:309:MET:HB3	2.18	0.44
4:C:3760:NAG:H83	4:C:3760:NAG:H3	2.00	0.44
1:D:107:SER:C	1:D:108:VAL:HG23	2.43	0.44
1:D:467:THR:HG21	1:D:531:ALA:HB1	1.99	0.44
1:A:107:SER:O	1:A:108:VAL:HG23	2.18	0.43
1:A:129:SER:O	1:A:342:VAL:HA	2.18	0.43
1:A:467:THR:HG21	1:A:531:ALA:HB1	1.99	0.43
1:B:141:THR:HG23	1:B:142:SER:H	1.83	0.43
1:B:698:ASN:ND2	1:B:701:ALA:O	2.51	0.43
1:C:107:SER:O	1:C:108:VAL:HG23	2.18	0.43
1:C:240:LYS:H	1:C:240:LYS:CD	2.25	0.43
1:C:245:GLY:O	1:C:246:TRP:HB3	2.18	0.43
1:C:427:GLY:C	1:C:429:LEU:N	2.74	0.43
1:C:479:LYS:HG2	1:C:494:TYR:CG	2.52	0.43
1:C:605:ARG:O	1:C:606:LYS:C	2.61	0.43
1:C:616:MET:HE2	1:C:622:MET:HE1	2.00	0.43
1:C:698:ASN:ND2	1:C:701:ALA:O	2.51	0.43
1:D:295:HIS:HA	1:D:296:PRO:HD3	1.66	0.43
1:D:616:MET:HE2	1:D:622:MET:HE1	2.00	0.43
1:A:605:ARG:O	1:A:606:LYS:C	2.61	0.43
1:B:151:TYR:N	1:B:151:TYR:CD1	2.86	0.43
1:C:107:SER:C	1:C:108:VAL:HG23	2.43	0.43
1:C:165:SER:OG	1:C:293:PRO:HA	2.17	0.43
1:C:261:LEU:O	1:C:263:GLY:C	2.61	0.43
1:C:458:GLY:HA2	3:R:1:NAG:H81	2.00	0.43
1:D:141:THR:HG23	1:D:142:SER:H	1.83	0.43
1:D:306:LEU:O	1:D:309:MET:HB3	2.18	0.43
1:D:308:LYS:HD3	1:D:337:PHE:CD2	2.52	0.43
1:D:618:HIS:HE1	1:D:716:GLU:HG2	1.83	0.43
1:D:669:MET:HE2	1:D:670:PHE:CE1	2.52	0.43
1:D:728:VAL:C	1:D:730:ARG:N	2.75	0.43
1:A:292:ILE:HD13	1:A:292:ILE:H	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:386:ILE:HG22	1:A:454:SER:HB3	1.99	0.43
1:A:698:ASN:ND2	1:A:701:ALA:O	2.51	0.43
1:B:77:PHE:HB2	1:B:389:GLN:HG3	1.99	0.43
1:C:114:ASP:O	1:C:274:ALA:HB1	2.18	0.43
1:C:129:SER:O	1:C:342:VAL:HA	2.18	0.43
1:C:743:ALA:C	1:C:745:THR:N	2.75	0.43
1:D:245:GLY:O	1:D:246:TRP:HB3	2.18	0.43
1:D:261:LEU:O	1:D:263:GLY:C	2.61	0.43
1:D:292:ILE:HD13	1:D:292:ILE:H	1.83	0.43
1:A:132:ASN:O	1:A:134:ASP:N	2.51	0.43
1:A:507:SER:C	1:A:509:MET:H	2.24	0.43
1:A:616:MET:HE2	1:A:622:MET:HE1	2.00	0.43
1:B:159:PRO:O	1:B:160:PRO:C	2.61	0.43
1:B:212:ASN:O	1:B:216:ASN:N	2.44	0.43
1:B:605:ARG:O	1:B:606:LYS:C	2.61	0.43
1:C:181:ARG:HD3	1:C:216:ASN:HD22	1.82	0.43
1:D:107:SER:O	1:D:108:VAL:HG23	2.18	0.43
1:D:250:GLY:HA2	1:D:299:TYR:CE1	2.54	0.43
1:D:449:TYR:HE2	1:D:521:PHE:HA	1.83	0.43
1:D:616:MET:C	1:D:618:HIS:H	2.26	0.43
1:A:114:ASP:O	1:A:274:ALA:HB1	2.18	0.43
1:A:151:TYR:N	1:A:151:TYR:CD1	2.86	0.43
1:A:569:MET:HE2	1:A:569:MET:HA	2.00	0.43
1:A:618:HIS:HE1	1:A:716:GLU:HG2	1.84	0.43
1:B:140:ASN:HB2	4:B:2760:NAG:C6	2.24	0.43
1:B:261:LEU:O	1:B:263:GLY:C	2.61	0.43
1:B:413:ARG:HG2	1:B:413:ARG:HH11	1.84	0.43
1:B:449:TYR:HE2	1:B:521:PHE:HA	1.83	0.43
1:C:569:MET:HE2	1:C:569:MET:HA	2.00	0.43
1:C:575:THR:O	1:C:578:GLN:N	2.51	0.43
1:C:605:ARG:HG2	1:C:605:ARG:HH11	1.84	0.43
1:C:662:ARG:O	1:C:663:MET:C	2.59	0.43
1:D:181:ARG:HD3	1:D:216:ASN:HD22	1.82	0.43
1:D:182:THR:O	1:D:183:GLU:CB	2.65	0.43
1:D:323:LEU:O	1:D:325:VAL:N	2.43	0.43
1:D:605:ARG:O	1:D:606:LYS:C	2.61	0.43
1:D:616:MET:HE2	1:D:622:MET:CE	2.49	0.43
1:A:141:THR:HG23	1:A:142:SER:H	1.83	0.43
1:A:159:PRO:O	1:A:160:PRO:C	2.61	0.43
1:A:738:THR:O	1:A:739:VAL:C	2.62	0.43
1:B:59:LYS:O	1:B:61:PHE:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:144:PHE:CD1	1:B:144:PHE:C	2.97	0.43
1:B:269:THR:OG1	1:B:433:GLU:CD	2.62	0.43
1:B:367:GLU:CD	1:B:413:ARG:HH12	2.27	0.43
1:B:382:VAL:CG2	1:B:383:PHE:N	2.68	0.43
1:B:616:MET:HE2	1:B:622:MET:HE1	2.00	0.43
1:B:618:HIS:HE1	1:B:716:GLU:HG2	1.84	0.43
1:C:132:ASN:O	1:C:134:ASP:N	2.51	0.43
1:C:146:PRO:HA	1:C:147:PRO:HD2	1.82	0.43
1:D:114:ASP:O	1:D:274:ALA:HB1	2.18	0.43
1:D:386:ILE:HG22	1:D:454:SER:HB3	1.99	0.43
1:D:443:GLN:O	1:D:673:ARG:NH1	2.46	0.43
1:D:605:ARG:HH11	1:D:605:ARG:HG2	1.84	0.43
1:A:107:SER:C	1:A:108:VAL:HG23	2.43	0.43
1:B:129:SER:O	1:B:342:VAL:HA	2.18	0.43
1:B:738:THR:O	1:B:739:VAL:C	2.62	0.43
1:C:59:LYS:O	1:C:61:PHE:N	2.51	0.43
1:C:295:HIS:HA	1:C:296:PRO:HD3	1.66	0.43
1:D:144:PHE:C	1:D:144:PHE:CD1	2.97	0.43
1:D:151:TYR:N	1:D:151:TYR:CD1	2.86	0.43
1:D:575:THR:O	1:D:578:GLN:N	2.51	0.43
1:D:690:VAL:HG21	1:D:738:THR:CG2	2.41	0.43
1:D:698:ASN:ND2	1:D:701:ALA:O	2.51	0.43
1:A:56:HIS:O	1:A:57:ASN:CB	2.67	0.43
1:A:206:GLY:H	1:A:213:LYS:HZ1	1.66	0.43
1:A:575:THR:O	1:A:578:GLN:N	2.51	0.43
1:A:733:TYR:CD1	1:B:278:ALA:HA	2.54	0.43
1:B:630:ASP:O	1:B:634:SER:N	2.44	0.43
1:B:725:TRP:O	1:B:729:LYS:HB2	2.18	0.43
1:C:269:THR:OG1	1:C:433:GLU:CD	2.61	0.43
1:D:467:THR:C	1:D:469:LEU:N	2.77	0.43
1:A:144:PHE:CD1	1:A:144:PHE:C	2.97	0.43
1:A:250:GLY:HA2	1:A:299:TYR:CE1	2.54	0.43
1:A:412:PRO:HA	1:A:589:ASN:OD1	2.19	0.43
1:A:467:THR:C	1:A:469:LEU:N	2.77	0.43
1:A:725:TRP:O	1:A:729:LYS:HB2	2.18	0.43
1:B:114:ASP:O	1:B:274:ALA:HB1	2.18	0.43
1:B:292:ILE:H	1:B:292:ILE:HD13	1.83	0.43
1:C:141:THR:HG23	1:C:142:SER:H	1.83	0.43
1:C:144:PHE:CD1	1:C:144:PHE:C	2.97	0.43
1:C:386:ILE:HG22	1:C:454:SER:HB3	1.99	0.43
1:C:506:PHE:O	1:C:508:GLY:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:229:SER:HB3	1:D:234:TYR:CE1	2.53	0.43
2:L:1:NAG:O3	2:L:2:NDG:N2	2.52	0.43
1:A:269:THR:OG1	1:A:433:GLU:CD	2.62	0.43
1:A:616:MET:HE2	1:A:622:MET:CE	2.49	0.43
1:A:718:LYS:HG2	1:A:724:ALA:HB2	2.01	0.43
4:A:1760:NAG:H3	4:A:1760:NAG:H83	2.00	0.43
1:B:412:PRO:HA	1:B:589:ASN:OD1	2.19	0.43
1:B:458:GLY:HA2	3:M:1:NAG:H81	2.00	0.43
1:B:467:THR:C	1:B:469:LEU:N	2.77	0.43
1:B:569:MET:HA	1:B:569:MET:HE2	2.00	0.43
1:B:575:THR:O	1:B:578:GLN:N	2.51	0.43
4:B:2760:NAG:H83	4:B:2760:NAG:H3	2.00	0.43
1:C:467:THR:C	1:C:469:LEU:N	2.77	0.43
1:C:618:HIS:HE1	1:C:716:GLU:HG2	1.84	0.43
1:C:738:THR:O	1:C:739:VAL:C	2.62	0.43
1:D:269:THR:OG1	1:D:433:GLU:CD	2.62	0.43
1:D:412:PRO:HA	1:D:589:ASN:OD1	2.19	0.43
1:D:413:ARG:HG2	1:D:413:ARG:HH11	1.84	0.43
1:A:174:LEU:CD1	1:A:342:VAL:HG22	2.49	0.42
1:A:261:LEU:O	1:A:263:GLY:C	2.61	0.42
1:B:107:SER:C	1:B:108:VAL:HG23	2.43	0.42
1:C:182:THR:O	1:C:182:THR:HG22	2.19	0.42
1:C:657:ASN:HA	1:C:658:PRO:HD2	1.88	0.42
1:D:59:LYS:O	1:D:61:PHE:N	2.51	0.42
1:D:367:GLU:CD	1:D:413:ARG:HH12	2.27	0.42
1:D:634:SER:O	1:D:637:LYS:N	2.52	0.42
1:A:59:LYS:O	1:A:61:PHE:N	2.51	0.42
1:A:158:VAL:HA	1:A:159:PRO:HD3	1.87	0.42
1:A:181:ARG:HD3	1:A:216:ASN:HD22	1.82	0.42
1:A:410:TRP:CH2	1:A:412:PRO:HG3	2.54	0.42
1:A:478:THR:OG1	1:A:493:LEU:HD13	2.19	0.42
1:B:443:GLN:O	1:B:673:ARG:NH1	2.46	0.42
1:B:671:LEU:O	1:B:674:ALA:HB3	2.19	0.42
1:C:367:GLU:CD	1:C:413:ARG:HH12	2.27	0.42
1:C:413:ARG:HG2	1:C:413:ARG:HH11	1.84	0.42
1:D:56:HIS:O	1:D:57:ASN:CB	2.67	0.42
1:D:182:THR:O	1:D:182:THR:HG22	2.19	0.42
1:D:253:VAL:HG11	1:D:296:PRO:HB2	2.01	0.42
1:D:506:PHE:O	1:D:508:GLY:N	2.52	0.42
4:D:4760:NAG:H3	4:D:4760:NAG:H83	2.00	0.42
1:A:387:ASP:HA	1:A:388:PRO:HA	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:410:TRP:CH2	1:B:412:PRO:HG3	2.54	0.42
1:B:616:MET:HE2	1:B:622:MET:CE	2.49	0.42
1:C:250:GLY:HA2	1:C:299:TYR:CE1	2.54	0.42
1:C:275:ASN:ND2	1:C:278:ALA:N	2.68	0.42
1:C:718:LYS:HG2	1:C:724:ALA:HB2	2.01	0.42
2:T:1:NAG:O3	2:T:2:NDG:C1	2.67	0.42
1:B:253:VAL:HG11	1:B:296:PRO:HB2	2.01	0.42
1:B:386:ILE:HG22	1:B:454:SER:HB3	1.99	0.42
1:B:605:ARG:HG2	1:B:605:ARG:HH11	1.84	0.42
1:B:634:SER:O	1:B:637:LYS:N	2.53	0.42
1:B:718:LYS:HG2	1:B:724:ALA:HB2	2.01	0.42
1:B:732:ILE:HD12	1:B:733:TYR:CA	2.50	0.42
1:C:77:PHE:HB2	1:C:389:GLN:HG3	1.98	0.42
1:C:111:ALA:HB3	1:C:357:ASN:HB2	2.01	0.42
1:C:515:LEU:HB3	1:C:516:GLY:H	1.49	0.42
1:D:205:TYR:HA	1:D:213:LYS:HZ3	1.83	0.42
1:A:190:ARG:C	1:A:192:MET:H	2.28	0.42
1:A:321:GLY:N	1:A:327:TYR:CZ	2.88	0.42
1:A:634:SER:O	1:A:637:LYS:N	2.53	0.42
1:B:506:PHE:O	1:B:508:GLY:N	2.52	0.42
1:C:365:ALA:HB2	1:C:411:ARG:HB2	2.02	0.42
1:C:671:LEU:O	1:C:674:ALA:HB3	2.19	0.42
1:D:240:LYS:CB	1:D:245:GLY:HA2	2.37	0.42
1:D:242:TYR:HD2	1:D:556:TYR:HD2	1.65	0.42
1:D:569:MET:HE2	1:D:569:MET:HA	2.00	0.42
1:D:708:ILE:O	1:D:711:ALA:HB3	2.19	0.42
2:E:1:NAG:O3	2:E:2:NDG:C1	2.67	0.42
1:A:261:LEU:HD13	1:A:265:GLY:O	2.19	0.42
1:A:365:ALA:HB2	1:A:411:ARG:HB2	2.02	0.42
1:A:506:PHE:O	1:A:508:GLY:N	2.52	0.42
1:A:708:ILE:O	1:A:711:ALA:HB3	2.19	0.42
1:B:250:GLY:HA2	1:B:299:TYR:CE1	2.54	0.42
1:C:382:VAL:CG2	1:C:383:PHE:N	2.68	0.42
1:D:544:ASN:HD22	1:D:544:ASN:N	2.17	0.42
1:D:671:LEU:O	1:D:674:ALA:HB3	2.19	0.42
1:D:718:LYS:HG2	1:D:724:ALA:HB2	2.01	0.42
2:J:1:NAG:O3	2:J:2:NDG:C1	2.67	0.42
1:A:367:GLU:CD	1:A:413:ARG:HH12	2.27	0.42
1:A:453:ASP:CG	1:A:454:SER:H	2.28	0.42
1:B:83:LEU:O	1:B:86:THR:HG23	2.20	0.42
1:B:708:ILE:O	1:B:711:ALA:HB3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:174:LEU:CD1	1:C:342:VAL:HG22	2.49	0.42
1:C:182:THR:O	1:C:183:GLU:CB	2.65	0.42
1:C:527:ARG:HD2	1:C:686:PHE:HB3	2.02	0.42
1:D:132:ASN:O	1:D:134:ASP:N	2.51	0.42
1:D:478:THR:OG1	1:D:493:LEU:HD13	2.20	0.42
2:G:1:NAG:O3	2:G:2:NDG:N2	2.52	0.42
1:A:182:THR:O	1:A:182:THR:HG22	2.19	0.42
1:A:275:ASN:ND2	1:A:278:ALA:N	2.68	0.42
1:A:413:ARG:HH11	1:A:413:ARG:HG2	1.84	0.42
1:B:97:GLN:HG3	1:B:108:VAL:HG12	2.02	0.42
1:B:137:GLU:O	1:B:139:PHE:N	2.53	0.42
1:B:381:TRP:NE1	1:B:425:GLU:HB3	2.35	0.42
1:B:654:ASP:C	1:B:656:SER:N	2.78	0.42
1:C:56:HIS:O	1:C:57:ASN:CB	2.67	0.42
1:C:321:GLY:N	1:C:327:TYR:CZ	2.88	0.42
1:C:708:ILE:O	1:C:711:ALA:HB3	2.19	0.42
1:D:83:LEU:O	1:D:86:THR:HG23	2.20	0.42
1:D:239:VAL:HG12	1:D:240:LYS:H	1.85	0.42
1:A:381:TRP:NE1	1:A:425:GLU:HB3	2.35	0.42
1:B:181:ARG:HD3	1:B:216:ASN:HD22	1.82	0.42
1:B:205:TYR:HA	1:B:213:LYS:HZ3	1.84	0.42
1:B:248:LEU:HA	1:B:249:PRO:HD3	1.88	0.42
1:B:527:ARG:HD2	1:B:686:PHE:HB3	2.02	0.42
1:C:206:GLY:H	1:C:213:LYS:HZ1	1.66	0.42
1:C:229:SER:HB3	1:C:234:TYR:CE1	2.53	0.42
1:C:412:PRO:HA	1:C:589:ASN:OD1	2.19	0.42
1:C:449:TYR:HE2	1:C:521:PHE:HA	1.83	0.42
1:C:616:MET:HE2	1:C:622:MET:CE	2.49	0.42
1:D:174:LEU:CD1	1:D:342:VAL:HG22	2.49	0.42
1:D:410:TRP:CH2	1:D:412:PRO:HG3	2.54	0.42
2:O:1:NAG:O3	2:O:2:NDG:C1	2.67	0.42
2:V:1:NAG:O3	2:V:2:NDG:N2	2.51	0.42
1:A:165:SER:HA	1:A:166:PRO:HD3	1.83	0.42
1:A:435:ALA:O	1:A:436:GLU:C	2.63	0.42
1:A:449:TYR:HE2	1:A:521:PHE:HA	1.83	0.42
1:A:616:MET:C	1:A:618:HIS:H	2.26	0.42
1:A:732:ILE:HD12	1:A:733:TYR:CA	2.50	0.42
1:B:365:ALA:HB2	1:B:411:ARG:HB2	2.02	0.42
1:B:544:ASN:HD22	1:B:544:ASN:N	2.17	0.42
1:C:277:TYR:OH	1:D:737:PHE:HA	2.20	0.42
1:D:212:ASN:O	1:D:216:ASN:N	2.44	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:111:ALA:HB3	1:A:357:ASN:HB2	2.01	0.41
1:B:182:THR:O	1:B:182:THR:HG22	2.19	0.41
1:B:323:LEU:C	1:B:325:VAL:N	2.78	0.41
1:B:478:THR:OG1	1:B:493:LEU:HD13	2.19	0.41
1:C:190:ARG:C	1:C:192:MET:H	2.28	0.41
1:C:370:ARG:HG2	1:C:370:ARG:NH1	2.35	0.41
1:C:453:ASP:CG	1:C:454:SER:H	2.28	0.41
1:D:323:LEU:C	1:D:325:VAL:N	2.78	0.41
1:D:330:GLY:HA2	1:D:331:PRO:HD3	1.79	0.41
1:D:527:ARG:HD2	1:D:686:PHE:HB3	2.02	0.41
1:A:240:LYS:H	1:A:240:LYS:CD	2.25	0.41
1:A:282:GLY:O	1:A:284:ALA:N	2.53	0.41
1:A:743:ALA:C	1:A:745:THR:N	2.75	0.41
1:B:56:HIS:O	1:B:57:ASN:CB	2.67	0.41
1:B:146:PRO:HA	1:B:147:PRO:HD2	1.82	0.41
1:B:174:LEU:CD1	1:B:342:VAL:HG22	2.49	0.41
1:B:615:SER:C	1:B:617:LYS:H	2.28	0.41
1:C:634:SER:O	1:C:637:LYS:N	2.53	0.41
1:D:111:ALA:HB3	1:D:357:ASN:HB2	2.01	0.41
1:D:275:ASN:ND2	1:D:278:ALA:N	2.68	0.41
1:D:715:ILE:CD1	1:D:725:TRP:CE2	3.03	0.41
1:D:738:THR:O	1:D:739:VAL:C	2.62	0.41
1:A:83:LEU:O	1:A:86:THR:HG23	2.20	0.41
1:A:544:ASN:HD22	1:A:544:ASN:N	2.17	0.41
1:A:605:ARG:HG2	1:A:605:ARG:HH11	1.84	0.41
1:A:671:LEU:O	1:A:674:ALA:HB3	2.19	0.41
1:A:695:SER:O	1:A:696:SER:C	2.64	0.41
1:A:715:ILE:CD1	1:A:725:TRP:CE2	3.03	0.41
1:B:242:TYR:CG	1:B:243:PRO:N	2.87	0.41
1:B:695:SER:O	1:B:696:SER:C	2.64	0.41
1:C:261:LEU:HD13	1:C:265:GLY:O	2.19	0.41
1:C:272:TYR:HA	1:C:273:PRO:HD3	1.77	0.41
1:C:410:TRP:CH2	1:C:412:PRO:HG3	2.54	0.41
1:D:248:LEU:HA	1:D:249:PRO:HD3	1.88	0.41
1:D:261:LEU:HD13	1:D:265:GLY:O	2.19	0.41
1:D:337:PHE:CB	1:D:340:GLN:HG3	2.50	0.41
1:D:365:ALA:HB2	1:D:411:ARG:HB2	2.02	0.41
1:D:627:VAL:HG21	1:D:725:TRP:HE3	1.81	0.41
1:A:137:GLU:O	1:A:139:PHE:N	2.53	0.41
1:A:615:SER:C	1:A:617:LYS:H	2.28	0.41
1:B:111:ALA:HB3	1:B:357:ASN:HB2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:239:VAL:HG12	1:B:240:LYS:H	1.85	0.41
1:B:321:GLY:N	1:B:327:TYR:CZ	2.88	0.41
1:B:470:MET:O	1:B:474:VAL:HG23	2.21	0.41
1:B:634:SER:O	1:B:635:ALA:C	2.64	0.41
1:C:394:VAL:O	1:C:395:VAL:C	2.63	0.41
1:C:654:ASP:C	1:C:656:SER:N	2.78	0.41
1:D:282:GLY:O	1:D:284:ALA:N	2.53	0.41
1:D:321:GLY:N	1:D:327:TYR:CZ	2.88	0.41
1:D:458:GLY:HA2	3:W:1:NAG:H81	2.00	0.41
1:D:470:MET:O	1:D:474:VAL:HG23	2.21	0.41
2:J:1:NAG:HO3	2:J:2:NDG:C1	2.32	0.41
1:A:113:TYR:O	1:A:355:ILE:HG12	2.21	0.41
1:A:128:ILE:HD12	1:A:297:ILE:HD13	2.02	0.41
1:A:634:SER:O	1:A:635:ALA:C	2.63	0.41
1:A:734:VAL:HG13	1:B:272:TYR:CE2	2.55	0.41
1:B:282:GLY:O	1:B:284:ALA:N	2.53	0.41
1:B:384:GLY:O	1:B:385:GLY:C	2.63	0.41
1:B:453:ASP:CG	1:B:454:SER:H	2.28	0.41
1:B:488:PHE:HE2	1:B:499:LYS:HD2	1.85	0.41
1:B:616:MET:C	1:B:618:HIS:H	2.26	0.41
1:B:627:VAL:HG21	1:B:725:TRP:HE3	1.81	0.41
1:B:736:ALA:O	1:B:737:PHE:C	2.64	0.41
1:C:83:LEU:O	1:C:86:THR:HG23	2.20	0.41
1:C:337:PHE:CB	1:C:340:GLN:HG3	2.50	0.41
1:C:478:THR:OG1	1:C:493:LEU:HD13	2.19	0.41
1:D:453:ASP:CG	1:D:454:SER:H	2.28	0.41
1:D:488:PHE:HE2	1:D:499:LYS:HD2	1.85	0.41
1:D:615:SER:C	1:D:617:LYS:H	2.28	0.41
1:D:634:SER:O	1:D:635:ALA:C	2.63	0.41
1:A:453:ASP:O	1:A:454:SER:C	2.63	0.41
1:A:481:LEU:HD23	1:A:481:LEU:HA	1.70	0.41
1:A:687:TYR:CZ	1:A:694:PRO:HG2	2.56	0.41
1:A:693:ALA:HB3	1:A:706:PRO:HG2	2.03	0.41
1:C:108:VAL:HG22	1:C:360:GLY:HA2	2.03	0.41
1:C:282:GLY:O	1:C:284:ALA:N	2.53	0.41
1:C:384:GLY:O	1:C:385:GLY:C	2.63	0.41
1:C:687:TYR:CZ	1:C:694:PRO:HG2	2.56	0.41
1:D:384:GLY:O	1:D:385:GLY:C	2.63	0.41
1:A:97:GLN:HG3	1:A:108:VAL:HG12	2.02	0.41
1:A:229:SER:HB3	1:A:234:TYR:CE1	2.53	0.41
1:A:253:VAL:HG11	1:A:296:PRO:HB2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:370:ARG:NH1	1:A:370:ARG:HG2	2.35	0.41
1:A:470:MET:O	1:A:474:VAL:HG23	2.21	0.41
1:A:610:LYS:HD3	1:A:614:ILE:HD11	2.03	0.41
1:B:261:LEU:HD13	1:B:265:GLY:O	2.19	0.41
1:B:394:VAL:O	1:B:395:VAL:C	2.63	0.41
1:D:108:VAL:HG22	1:D:360:GLY:HA2	2.03	0.41
1:D:137:GLU:O	1:D:139:PHE:N	2.53	0.41
1:D:370:ARG:NH1	1:D:370:ARG:HG2	2.35	0.41
1:D:377:HIS:CE1	1:D:424:GLU:OE1	2.74	0.41
1:D:611:ILE:HA	1:D:614:ILE:HG12	2.03	0.41
1:A:239:VAL:HG12	1:A:240:LYS:H	1.85	0.41
1:B:275:ASN:ND2	1:B:278:ALA:N	2.68	0.41
1:B:377:HIS:CE1	1:B:424:GLU:OE1	2.74	0.41
1:C:377:HIS:CE1	1:C:424:GLU:OE1	2.74	0.41
1:C:705:PHE:HB3	1:C:708:ILE:HD13	2.03	0.41
1:D:128:ILE:HD12	1:D:297:ILE:HD13	2.02	0.41
1:D:272:TYR:C	1:D:436:GLU:OE1	2.64	0.41
1:A:173:ASP:C	1:A:174:LEU:HD12	2.46	0.41
1:A:337:PHE:CB	1:A:340:GLN:HG3	2.50	0.41
1:A:449:TYR:HE2	1:A:521:PHE:CA	2.34	0.41
1:A:488:PHE:HE2	1:A:499:LYS:HD2	1.85	0.41
1:A:527:ARG:HD2	1:A:686:PHE:HB3	2.02	0.41
1:A:736:ALA:O	1:A:737:PHE:C	2.64	0.41
1:B:128:ILE:HD12	1:B:297:ILE:HD13	2.02	0.41
1:B:173:ASP:C	1:B:174:LEU:HD12	2.46	0.41
1:B:314:PRO:O	1:B:315:PRO:C	2.64	0.41
1:B:506:PHE:C	1:B:508:GLY:N	2.79	0.41
1:B:687:TYR:CZ	1:B:694:PRO:HG2	2.56	0.41
1:B:705:PHE:HB3	1:B:708:ILE:HD13	2.03	0.41
1:C:137:GLU:O	1:C:139:PHE:N	2.53	0.41
1:C:230:ASP:HA	1:C:231:PRO:HD3	1.91	0.41
1:C:253:VAL:HG11	1:C:296:PRO:HB2	2.01	0.41
1:C:272:TYR:C	1:C:436:GLU:OE1	2.64	0.41
1:C:314:PRO:O	1:C:315:PRO:C	2.64	0.41
1:C:381:TRP:NE1	1:C:425:GLU:HB3	2.35	0.41
1:C:470:MET:O	1:C:474:VAL:HG23	2.21	0.41
1:C:505:GLU:OE1	1:C:606:LYS:HE2	2.21	0.41
1:C:608:ALA:O	1:C:609:ASP:C	2.63	0.41
1:C:634:SER:O	1:C:635:ALA:C	2.64	0.41
1:D:97:GLN:HG3	1:D:108:VAL:HG12	2.02	0.41
1:D:681:LEU:HD23	1:D:681:LEU:HA	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:272:TYR:C	1:A:436:GLU:OE1	2.64	0.41
1:A:506:PHE:C	1:A:508:GLY:N	2.79	0.41
1:A:697:HIS:CG	1:A:713:PHE:CD2	3.09	0.41
1:A:705:PHE:HB3	1:A:708:ILE:HD13	2.03	0.41
1:B:164:PHE:CD1	1:B:259:LEU:HG	2.56	0.41
1:B:190:ARG:C	1:B:192:MET:H	2.28	0.41
1:B:272:TYR:C	1:B:436:GLU:OE1	2.64	0.41
1:B:295:HIS:HA	1:B:296:PRO:HD3	1.66	0.41
1:B:370:ARG:NH1	1:B:370:ARG:HG2	2.35	0.41
1:B:516:GLY:O	1:B:517:SER:O	2.39	0.41
1:C:128:ILE:HD12	1:C:297:ILE:HD13	2.02	0.41
1:C:205:TYR:HA	1:C:213:LYS:HZ3	1.86	0.41
1:C:516:GLY:O	1:C:517:SER:O	2.39	0.41
1:C:611:ILE:HA	1:C:614:ILE:HG12	2.03	0.41
1:C:715:ILE:CD1	1:C:725:TRP:CE2	3.03	0.41
1:D:381:TRP:NE1	1:D:425:GLU:HB3	2.35	0.41
1:D:453:ASP:O	1:D:454:SER:C	2.63	0.41
1:D:654:ASP:C	1:D:656:SER:N	2.78	0.41
1:D:657:ASN:HA	1:D:658:PRO:HD2	1.88	0.41
1:D:687:TYR:CZ	1:D:694:PRO:HG2	2.56	0.41
1:D:732:ILE:HD12	1:D:733:TYR:CA	2.50	0.41
1:D:736:ALA:O	1:D:737:PHE:C	2.64	0.41
1:A:108:VAL:HG22	1:A:360:GLY:HA2	2.03	0.40
1:B:337:PHE:CB	1:B:340:GLN:HG3	2.50	0.40
1:C:164:PHE:CD1	1:C:259:LEU:HG	2.56	0.40
1:C:539:LYS:H	1:C:539:LYS:HG2	1.74	0.40
1:C:695:SER:O	1:C:696:SER:C	2.64	0.40
1:D:173:ASP:C	1:D:174:LEU:HD12	2.46	0.40
1:D:190:ARG:C	1:D:192:MET:H	2.28	0.40
1:D:449:TYR:HE2	1:D:521:PHE:CA	2.34	0.40
1:A:323:LEU:C	1:A:325:VAL:N	2.78	0.40
1:A:362:LEU:HD12	1:A:362:LEU:HA	1.82	0.40
1:A:377:HIS:CE1	1:A:424:GLU:OE1	2.74	0.40
1:A:384:GLY:O	1:A:385:GLY:C	2.63	0.40
1:A:530:ILE:O	1:A:531:ALA:C	2.65	0.40
1:A:749:VAL:HG12	1:B:445:ARG:NH2	2.35	0.40
1:B:113:TYR:O	1:B:355:ILE:HG12	2.21	0.40
1:B:693:ALA:HB3	1:B:706:PRO:HG2	2.03	0.40
1:C:173:ASP:C	1:C:174:LEU:HD12	2.46	0.40
1:C:506:PHE:C	1:C:508:GLY:N	2.79	0.40
1:C:693:ALA:HB3	1:C:706:PRO:HG2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:697:HIS:CG	1:C:713:PHE:CD2	3.09	0.40
1:C:732:ILE:HD12	1:C:733:TYR:CA	2.50	0.40
1:D:314:PRO:O	1:D:315:PRO:C	2.64	0.40
2:Q:1:NAG:O3	2:Q:2:NDG:N2	2.52	0.40
1:A:164:PHE:CD1	1:A:259:LEU:HG	2.56	0.40
1:A:382:VAL:CG2	1:A:383:PHE:N	2.68	0.40
1:A:443:GLN:O	1:A:673:ARG:NH1	2.46	0.40
1:B:697:HIS:CG	1:B:713:PHE:CD2	3.09	0.40
1:B:715:ILE:CD1	1:B:725:TRP:CE2	3.03	0.40
4:B:2759:NAG:O7	4:B:2759:NAG:O3	2.32	0.40
1:C:97:GLN:HG3	1:C:108:VAL:HG12	2.02	0.40
1:C:163:ALA:HB3	1:C:257:ASN:HA	2.04	0.40
1:C:367:GLU:N	1:C:368:PRO:HD3	2.37	0.40
1:C:449:TYR:HE2	1:C:521:PHE:CA	2.34	0.40
1:C:488:PHE:HE2	1:C:499:LYS:HD2	1.85	0.40
1:C:681:LEU:HD23	1:C:681:LEU:HA	1.86	0.40
1:D:262:ASN:O	1:D:687:TYR:CZ	2.75	0.40
1:D:509:MET:HE2	1:D:509:MET:HB3	1.79	0.40
1:D:697:HIS:CG	1:D:713:PHE:CD2	3.09	0.40
2:E:1:NAG:HO3	2:E:2:NDG:C1	2.34	0.40
1:A:272:TYR:HA	1:A:273:PRO:HD3	1.77	0.40
1:A:427:GLY:O	1:A:429:LEU:N	2.55	0.40
1:B:83:LEU:HB3	1:B:86:THR:HG23	2.04	0.40
1:B:158:VAL:HA	1:B:159:PRO:HD3	1.86	0.40
1:B:611:ILE:HA	1:B:614:ILE:HG12	2.03	0.40
1:C:113:TYR:O	1:C:355:ILE:HG12	2.21	0.40
1:C:242:TYR:CG	1:C:243:PRO:N	2.87	0.40
1:C:615:SER:C	1:C:617:LYS:H	2.28	0.40
1:D:113:TYR:O	1:D:355:ILE:HG12	2.21	0.40
1:D:164:PHE:CD1	1:D:259:LEU:HG	2.56	0.40
1:D:516:GLY:O	1:D:517:SER:O	2.39	0.40
1:D:695:SER:O	1:D:696:SER:C	2.64	0.40
1:A:117:LEU:HD23	1:A:117:LEU:HA	1.88	0.40
1:A:314:PRO:O	1:A:315:PRO:C	2.64	0.40
1:A:397:GLU:OE2	1:A:400:ARG:NH2	2.55	0.40
1:B:105:LEU:HA	1:B:105:LEU:HD23	1.66	0.40
1:B:272:TYR:HA	1:B:273:PRO:HD3	1.77	0.40
1:B:427:GLY:O	1:B:429:LEU:N	2.55	0.40
1:B:515:LEU:HB3	1:B:516:GLY:H	1.49	0.40
1:B:551:LEU:HD13	1:B:561:LEU:CD2	2.52	0.40
1:B:657:ASN:OD1	1:B:657:ASN:C	2.64	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:676:ILE:HA	1:B:688:ARG:O	2.21	0.40
1:C:158:VAL:HA	1:C:159:PRO:HD3	1.87	0.40
1:C:239:VAL:HG12	1:C:240:LYS:H	1.85	0.40
1:C:453:ASP:O	1:C:454:SER:C	2.63	0.40
1:C:690:VAL:HG21	1:C:738:THR:CG2	2.42	0.40
1:D:236:ALA:HA	1:D:237:PRO:HD3	1.92	0.40
1:D:552:TYR:O	1:D:557:GLU:OE1	2.40	0.40
1:D:608:ALA:O	1:D:609:ASP:C	2.63	0.40

All (26) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:507:SER:OG	1:D:506:PHE:CE2[1_455]	0.99	1.21
1:C:507:SER:CB	1:D:506:PHE:CZ[1_455]	1.07	1.13
1:C:505:GLU:CA	1:D:507:SER:OG[1_455]	1.09	1.11
1:A:506:PHE:CZ	1:B:507:SER:OG[1_455]	1.18	1.02
1:C:505:GLU:N	1:D:507:SER:OG[1_455]	1.23	0.97
1:C:507:SER:OG	1:D:506:PHE:CZ[1_455]	1.37	0.83
1:A:506:PHE:CZ	1:B:507:SER:CB[1_455]	1.44	0.76
1:A:244:ASP:OD1	1:B:94:LYS:NZ[2_555]	1.49	0.71
2:G:2:NDG:C6	3:M:2:NAG:C8[2_655]	1.54	0.66
1:C:507:SER:CB	1:D:506:PHE:CE1[1_455]	1.55	0.65
1:A:508:GLY:CA	1:B:505:GLU:O[1_455]	1.63	0.57
1:C:505:GLU:O	1:D:508:GLY:N[1_455]	1.65	0.55
1:C:505:GLU:O	1:D:508:GLY:CA[1_455]	1.71	0.49
1:C:505:GLU:O	1:D:507:SER:C[1_455]	1.76	0.44
1:A:244:ASP:CG	1:B:94:LYS:NZ[2_555]	1.84	0.36
1:C:505:GLU:CB	1:D:507:SER:OG[1_455]	1.84	0.36
1:A:244:ASP:OD2	1:B:94:LYS:NZ[2_555]	1.85	0.35
1:A:506:PHE:CE2	1:B:507:SER:OG[1_455]	1.85	0.35
1:C:505:GLU:O	1:D:507:SER:O[1_455]	1.86	0.34
1:A:506:PHE:CE1	1:B:507:SER:CB[1_455]	1.90	0.30
1:C:507:SER:CB	1:D:506:PHE:CE2[1_455]	1.95	0.25
1:A:508:GLY:N	1:B:505:GLU:O[1_455]	1.98	0.22
1:C:505:GLU:CA	1:D:507:SER:CB[1_455]	1.98	0.22
1:A:334:THR:CG2	1:D:320:ARG:NH1[1_454]	1.99	0.21
1:C:507:SER:OG	1:D:506:PHE:CD2[1_455]	2.12	0.08
1:A:334:THR:CG2	1:D:320:ARG:CZ[1_454]	2.18	0.02

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 X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	693/695 (100%)	534 (77%)	115 (17%)	44 (6%)	1	12
1	B	693/695 (100%)	533 (77%)	116 (17%)	44 (6%)	1	12
1	C	693/695 (100%)	533 (77%)	116 (17%)	44 (6%)	1	12
1	D	693/695 (100%)	532 (77%)	117 (17%)	44 (6%)	1	12
All	All	2772/2780 (100%)	2132 (77%)	464 (17%)	176 (6%)	1	12

All (176) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	137	GLU
1	A	138	ILE
1	A	149	PRO
1	A	179	TYR
1	A	183	GLU
1	A	222	ALA
1	A	242	TYR
1	A	262	ASN
1	A	283	ILE
1	A	315	PRO
1	A	330	GLY
1	A	517	SER
1	A	547	SER
1	A	552	TYR
1	B	137	GLU
1	B	138	ILE
1	B	149	PRO
1	B	179	TYR
1	B	183	GLU
1	B	222	ALA
1	B	242	TYR
1	B	262	ASN

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Mol	Chain	Res	Type
1	B	283	ILE
1	B	315	PRO
1	B	330	GLY
1	B	517	SER
1	B	547	SER
1	B	552	TYR
1	C	137	GLU
1	C	138	ILE
1	C	149	PRO
1	C	179	TYR
1	C	183	GLU
1	C	222	ALA
1	C	242	TYR
1	C	262	ASN
1	C	283	ILE
1	C	315	PRO
1	C	330	GLY
1	C	517	SER
1	C	547	SER
1	C	552	TYR
1	D	137	GLU
1	D	138	ILE
1	D	149	PRO
1	D	179	TYR
1	D	183	GLU
1	D	222	ALA
1	D	242	TYR
1	D	262	ASN
1	D	283	ILE
1	D	315	PRO
1	D	330	GLY
1	D	517	SER
1	D	547	SER
1	D	552	TYR
1	A	150	GLY
1	A	181	ARG
1	A	192	MET
1	A	193	LYS
1	A	210	ARG
1	A	246	TRP
1	A	263	GLY
1	A	332	GLY

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Mol	Chain	Res	Type
1	A	440	ARG
1	A	507	SER
1	A	556	TYR
1	A	591	ILE
1	B	150	GLY
1	B	181	ARG
1	B	192	MET
1	B	193	LYS
1	B	210	ARG
1	B	246	TRP
1	B	263	GLY
1	B	332	GLY
1	B	440	ARG
1	B	507	SER
1	B	556	TYR
1	B	591	ILE
1	C	150	GLY
1	C	181	ARG
1	C	192	MET
1	C	193	LYS
1	C	210	ARG
1	C	246	TRP
1	C	263	GLY
1	C	332	GLY
1	C	440	ARG
1	C	507	SER
1	C	556	TYR
1	C	591	ILE
1	D	150	GLY
1	D	181	ARG
1	D	192	MET
1	D	193	LYS
1	D	210	ARG
1	D	246	TRP
1	D	263	GLY
1	D	332	GLY
1	D	440	ARG
1	D	507	SER
1	D	556	TYR
1	D	591	ILE
1	A	57	ASN
1	A	324	LYS

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Mol	Chain	Res	Type
1	A	382	VAL
1	A	520	ASP
1	B	57	ASN
1	B	324	LYS
1	B	382	VAL
1	B	520	ASP
1	B	551	LEU
1	C	57	ASN
1	C	324	LYS
1	C	382	VAL
1	C	520	ASP
1	C	551	LEU
1	D	57	ASN
1	D	324	LYS
1	D	382	VAL
1	D	520	ASP
1	D	551	LEU
1	A	133	GLU
1	A	180	ALA
1	A	428	LEU
1	A	457	GLU
1	A	515	LEU
1	A	551	LEU
1	A	594	PRO
1	B	133	GLU
1	B	180	ALA
1	B	428	LEU
1	B	457	GLU
1	B	515	LEU
1	B	594	PRO
1	C	133	GLU
1	C	180	ALA
1	C	428	LEU
1	C	457	GLU
1	C	515	LEU
1	D	133	GLU
1	D	180	ALA
1	D	428	LEU
1	D	457	GLU
1	D	515	LEU
1	A	60	ALA
1	A	139	PHE

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Mol	Chain	Res	Type
1	B	60	ALA
1	B	139	PHE
1	C	60	ALA
1	C	139	PHE
1	C	594	PRO
1	D	60	ALA
1	D	139	PHE
1	D	594	PRO
1	A	655	LYS
1	B	655	LYS
1	C	655	LYS
1	D	655	LYS
1	A	243	PRO
1	B	243	PRO
1	C	243	PRO
1	D	243	PRO
1	A	690	VAL
1	B	690	VAL
1	C	690	VAL
1	D	690	VAL
1	A	108	VAL
1	A	468	PRO
1	B	108	VAL
1	B	468	PRO
1	C	108	VAL
1	C	468	PRO
1	D	108	VAL
1	D	468	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	592/592 (100%)	551 (93%)	41 (7%)	14	39
1	B	592/592 (100%)	551 (93%)	41 (7%)	14	39
1	C	592/592 (100%)	551 (93%)	41 (7%)	14	39

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	592/592 (100%)	551 (93%)	41 (7%)	14	39
All	All	2368/2368 (100%)	2204 (93%)	164 (7%)	14	39

All (164) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	63	ASP
1	A	70	ILE
1	A	149	PRO
1	A	154	VAL
1	A	174	LEU
1	A	178	ASN
1	A	179	TYR
1	A	186	PHE
1	A	202	ILE
1	A	229	SER
1	A	260	ASN
1	A	266	ASP
1	A	275	ASN
1	A	292	ILE
1	A	297	ILE
1	A	301	ASP
1	A	315	PRO
1	A	325	VAL
1	A	370	ARG
1	A	388	PRO
1	A	389	GLN
1	A	440	ARG
1	A	456	ILE
1	A	461	THR
1	A	467	THR
1	A	475	HIS
1	A	478	THR
1	A	484	PRO
1	A	493	LEU
1	A	509	MET
1	A	519	ASN
1	A	523	VAL
1	A	526	GLN
1	A	538	THR
1	A	541	TRP
1	A	563	GLU

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Mol	Chain	Res	Type
1	A	600	TYR
1	A	631	SER
1	A	668	LEU
1	A	671	LEU
1	A	731	GLN
1	B	63	ASP
1	B	70	ILE
1	B	149	PRO
1	B	154	VAL
1	B	174	LEU
1	B	178	ASN
1	B	179	TYR
1	B	186	PHE
1	B	202	ILE
1	B	229	SER
1	B	260	ASN
1	B	266	ASP
1	B	275	ASN
1	B	292	ILE
1	B	297	ILE
1	B	301	ASP
1	B	315	PRO
1	B	325	VAL
1	B	370	ARG
1	B	388	PRO
1	B	389	GLN
1	B	440	ARG
1	B	456	ILE
1	B	461	THR
1	B	467	THR
1	B	475	HIS
1	B	478	THR
1	B	484	PRO
1	B	493	LEU
1	B	509	MET
1	B	519	ASN
1	B	523	VAL
1	B	526	GLN
1	B	538	THR
1	B	541	TRP
1	B	563	GLU
1	B	600	TYR

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Mol	Chain	Res	Type
1	B	631	SER
1	B	668	LEU
1	B	671	LEU
1	B	731	GLN
1	C	63	ASP
1	C	70	ILE
1	C	149	PRO
1	C	154	VAL
1	C	174	LEU
1	C	178	ASN
1	C	179	TYR
1	C	186	PHE
1	C	202	ILE
1	C	229	SER
1	C	260	ASN
1	C	266	ASP
1	C	275	ASN
1	C	292	ILE
1	C	297	ILE
1	C	301	ASP
1	C	315	PRO
1	C	325	VAL
1	C	370	ARG
1	C	388	PRO
1	C	389	GLN
1	C	440	ARG
1	C	456	ILE
1	C	461	THR
1	C	467	THR
1	C	475	HIS
1	C	478	THR
1	C	484	PRO
1	C	493	LEU
1	C	509	MET
1	C	519	ASN
1	C	523	VAL
1	C	526	GLN
1	C	538	THR
1	C	541	TRP
1	C	563	GLU
1	C	600	TYR
1	C	631	SER

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Mol	Chain	Res	Type
1	C	668	LEU
1	C	671	LEU
1	C	731	GLN
1	D	63	ASP
1	D	70	ILE
1	D	149	PRO
1	D	154	VAL
1	D	174	LEU
1	D	178	ASN
1	D	179	TYR
1	D	186	PHE
1	D	202	ILE
1	D	229	SER
1	D	260	ASN
1	D	266	ASP
1	D	275	ASN
1	D	292	ILE
1	D	297	ILE
1	D	301	ASP
1	D	315	PRO
1	D	325	VAL
1	D	370	ARG
1	D	388	PRO
1	D	389	GLN
1	D	440	ARG
1	D	456	ILE
1	D	461	THR
1	D	467	THR
1	D	475	HIS
1	D	478	THR
1	D	484	PRO
1	D	493	LEU
1	D	509	MET
1	D	519	ASN
1	D	523	VAL
1	D	526	GLN
1	D	538	THR
1	D	541	TRP
1	D	563	GLU
1	D	600	TYR
1	D	631	SER
1	D	668	LEU

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Mol	Chain	Res	Type
1	D	671	LEU
1	D	731	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (75) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	82	HIS
1	A	97	GLN
1	A	112	HIS
1	A	136	ASN
1	A	178	ASN
1	A	216	ASN
1	A	260	ASN
1	A	275	ASN
1	A	295	HIS
1	A	303	GLN
1	A	328	ASN
1	A	347	HIS
1	A	438	ASN
1	A	544	ASN
1	A	618	HIS
1	A	689	HIS
1	A	731	GLN
1	A	740	GLN
1	B	82	HIS
1	B	97	GLN
1	B	112	HIS
1	B	136	ASN
1	B	178	ASN
1	B	216	ASN
1	B	260	ASN
1	B	275	ASN
1	B	295	HIS
1	B	303	GLN
1	B	328	ASN
1	B	347	HIS
1	B	438	ASN
1	B	544	ASN
1	B	618	HIS
1	B	689	HIS
1	B	698	ASN
1	B	731	GLN

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Mol	Chain	Res	Type
1	B	740	GLN
1	C	82	HIS
1	C	97	GLN
1	C	112	HIS
1	C	136	ASN
1	C	178	ASN
1	C	216	ASN
1	C	260	ASN
1	C	275	ASN
1	C	295	HIS
1	C	303	GLN
1	C	328	ASN
1	C	347	HIS
1	C	438	ASN
1	C	544	ASN
1	C	618	HIS
1	C	689	HIS
1	C	697	HIS
1	C	731	GLN
1	C	740	GLN
1	D	82	HIS
1	D	97	GLN
1	D	112	HIS
1	D	136	ASN
1	D	178	ASN
1	D	216	ASN
1	D	260	ASN
1	D	275	ASN
1	D	295	HIS
1	D	303	GLN
1	D	328	ASN
1	D	347	HIS
1	D	438	ASN
1	D	544	ASN
1	D	618	HIS
1	D	689	HIS
1	D	698	ASN
1	D	731	GLN
1	D	740	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

40 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	E	1	2,1	14,14,15	0.79	0	17,19,21	1.07	2 (11%)
2	NDG	E	2	2	14,14,15	0.76	1 (7%)	17,19,21	0.68	0
3	NAG	F	1	3,1	14,14,15	0.75	1 (7%)	17,19,21	0.78	0
3	NAG	F	2	3	14,14,15	0.80	0	17,19,21	0.82	1 (5%)
2	NAG	G	1	2,1	14,14,15	0.65	0	17,19,21	0.95	0
2	NDG	G	2	2	14,14,15	0.69	0	17,19,21	0.62	0
3	NAG	H	1	3,1	14,14,15	0.63	0	17,19,21	0.95	2 (11%)
3	NAG	H	2	3	14,14,15	0.61	0	17,19,21	0.77	1 (5%)
3	NAG	I	1	3,1	14,14,15	0.61	0	17,19,21	0.99	1 (5%)
3	NAG	I	2	3	14,14,15	0.52	0	17,19,21	0.69	1 (5%)
2	NAG	J	1	2,1	14,14,15	0.78	0	17,19,21	1.08	2 (11%)
2	NDG	J	2	2	14,14,15	0.75	1 (7%)	17,19,21	0.68	0
3	NAG	K	1	3,1	14,14,15	0.75	1 (7%)	17,19,21	0.78	0
3	NAG	K	2	3	14,14,15	0.80	0	17,19,21	0.82	1 (5%)
2	NAG	L	1	2,1	14,14,15	0.65	0	17,19,21	0.95	0
2	NDG	L	2	2	14,14,15	0.68	0	17,19,21	0.62	0
3	NAG	M	1	3,1	14,14,15	0.62	0	17,19,21	0.95	2 (11%)
3	NAG	M	2	3	14,14,15	0.61	0	17,19,21	0.77	1 (5%)
3	NAG	N	1	3,1	14,14,15	0.61	0	17,19,21	0.99	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	N	2	3	14,14,15	0.52	0	17,19,21	0.69	1 (5%)
2	NAG	O	1	2,1	14,14,15	0.78	0	17,19,21	1.07	2 (11%)
2	NDG	O	2	2	14,14,15	0.77	1 (7%)	17,19,21	0.67	0
3	NAG	P	1	3,1	14,14,15	0.75	1 (7%)	17,19,21	0.78	0
3	NAG	P	2	3	14,14,15	0.82	0	17,19,21	0.82	1 (5%)
2	NAG	Q	1	2,1	14,14,15	0.65	0	17,19,21	0.95	0
2	NDG	Q	2	2	14,14,15	0.67	0	17,19,21	0.62	0
3	NAG	R	1	3,1	14,14,15	0.61	0	17,19,21	0.95	2 (11%)
3	NAG	R	2	3	14,14,15	0.60	0	17,19,21	0.77	1 (5%)
3	NAG	S	1	3,1	14,14,15	0.61	0	17,19,21	0.99	1 (5%)
3	NAG	S	2	3	14,14,15	0.53	0	17,19,21	0.70	1 (5%)
2	NAG	T	1	2,1	14,14,15	0.79	0	17,19,21	1.07	2 (11%)
2	NDG	T	2	2	14,14,15	0.75	1 (7%)	17,19,21	0.67	0
3	NAG	U	1	3,1	14,14,15	0.74	1 (7%)	17,19,21	0.78	0
3	NAG	U	2	3	14,14,15	0.81	0	17,19,21	0.82	1 (5%)
2	NAG	V	1	2,1	14,14,15	0.66	0	17,19,21	0.95	0
2	NDG	V	2	2	14,14,15	0.69	0	17,19,21	0.62	0
3	NAG	W	1	3,1	14,14,15	0.62	0	17,19,21	0.95	2 (11%)
3	NAG	W	2	3	14,14,15	0.60	0	17,19,21	0.77	1 (5%)
3	NAG	X	1	3,1	14,14,15	0.61	0	17,19,21	0.98	1 (5%)
3	NAG	X	2	3	14,14,15	0.53	0	17,19,21	0.70	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	E	1	2,1	-	4/6/23/26	0/1/1/1
2	NDG	E	2	2	-	3/6/23/26	0/1/1/1
3	NAG	F	1	3,1	-	5/6/23/26	0/1/1/1
3	NAG	F	2	3	-	2/6/23/26	0/1/1/1
2	NAG	G	1	2,1	1/1/5/7	4/6/23/26	0/1/1/1
2	NDG	G	2	2	-	3/6/23/26	0/1/1/1
3	NAG	H	1	3,1	-	4/6/23/26	0/1/1/1
3	NAG	H	2	3	-	5/6/23/26	0/1/1/1
3	NAG	I	1	3,1	-	4/6/23/26	0/1/1/1

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

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	1	NAG	C1-C2	2.16	1.55	1.52
3	K	1	NAG	C1-C2	2.14	1.55	1.52
2	O	2	NDG	C1-C2	2.13	1.55	1.52
2	E	2	NDG	C1-C2	2.13	1.55	1.52
3	P	1	NAG	C1-C2	2.10	1.55	1.52
2	J	2	NDG	C1-C2	2.08	1.55	1.52
2	T	2	NDG	C1-C2	2.06	1.55	1.52
3	U	1	NAG	C1-C2	2.03	1.55	1.52

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	1	NAG	C2-N2-C7	-3.24	118.56	122.90
3	S	1	NAG	C2-N2-C7	-3.24	118.56	122.90
3	N	1	NAG	C2-N2-C7	-3.23	118.57	122.90
3	X	1	NAG	C2-N2-C7	-3.22	118.59	122.90
2	J	1	NAG	C2-N2-C7	-2.65	119.35	122.90
2	T	1	NAG	C2-N2-C7	-2.63	119.38	122.90
2	E	1	NAG	C2-N2-C7	-2.62	119.39	122.90
2	O	1	NAG	C2-N2-C7	-2.62	119.39	122.90
2	J	1	NAG	C4-C3-C2	-2.45	107.42	111.02
2	O	1	NAG	C4-C3-C2	-2.45	107.43	111.02
2	E	1	NAG	C4-C3-C2	-2.45	107.43	111.02
2	T	1	NAG	C4-C3-C2	-2.44	107.44	111.02
3	W	2	NAG	C2-N2-C7	-2.30	119.82	122.90
3	R	2	NAG	C2-N2-C7	-2.29	119.83	122.90
3	M	2	NAG	C2-N2-C7	-2.28	119.85	122.90
3	H	2	NAG	C2-N2-C7	-2.25	119.89	122.90
3	U	2	NAG	C1-O5-C5	2.18	115.10	112.19
3	S	2	NAG	C2-N2-C7	-2.16	120.00	122.90
3	P	2	NAG	C1-O5-C5	2.15	115.07	112.19
3	X	2	NAG	C2-N2-C7	-2.15	120.02	122.90
3	N	2	NAG	C2-N2-C7	-2.12	120.06	122.90
3	K	2	NAG	C1-O5-C5	2.11	115.02	112.19
3	F	2	NAG	C1-O5-C5	2.11	115.01	112.19
3	I	2	NAG	C2-N2-C7	-2.10	120.08	122.90
3	W	1	NAG	C4-C3-C2	-2.08	107.97	111.02
3	M	1	NAG	C4-C3-C2	-2.08	107.97	111.02
3	H	1	NAG	C4-C3-C2	-2.07	107.98	111.02
3	R	1	NAG	C4-C3-C2	-2.06	108.00	111.02
3	W	1	NAG	C2-N2-C7	-2.03	120.17	122.90
3	R	1	NAG	C2-N2-C7	-2.03	120.18	122.90
3	M	1	NAG	C2-N2-C7	-2.03	120.18	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	1	NAG	C2-N2-C7	-2.01	120.20	122.90

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	G	1	NAG	C1
2	L	1	NAG	C1
2	Q	1	NAG	C1
2	V	1	NAG	C1

All (152) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	1	NAG	C8-C7-N2-C2
2	E	1	NAG	O7-C7-N2-C2
2	E	2	NDG	C1-C2-N2-C7
2	E	2	NDG	C8-C7-N2-C2
2	E	2	NDG	O7-C7-N2-C2
2	G	1	NAG	C8-C7-N2-C2
2	G	1	NAG	O7-C7-N2-C2
2	G	2	NDG	C8-C7-N2-C2
2	G	2	NDG	O7-C7-N2-C2
2	J	1	NAG	C8-C7-N2-C2
2	J	1	NAG	O7-C7-N2-C2
2	J	2	NDG	C1-C2-N2-C7
2	J	2	NDG	C8-C7-N2-C2
2	J	2	NDG	O7-C7-N2-C2
2	L	1	NAG	C8-C7-N2-C2
2	L	1	NAG	O7-C7-N2-C2
2	L	2	NDG	C8-C7-N2-C2
2	L	2	NDG	O7-C7-N2-C2
2	O	1	NAG	C8-C7-N2-C2
2	O	1	NAG	O7-C7-N2-C2
2	O	2	NDG	C1-C2-N2-C7
2	O	2	NDG	C8-C7-N2-C2
2	O	2	NDG	O7-C7-N2-C2
2	Q	1	NAG	C8-C7-N2-C2
2	Q	1	NAG	O7-C7-N2-C2
2	Q	2	NDG	C8-C7-N2-C2
2	Q	2	NDG	O7-C7-N2-C2
2	T	1	NAG	C8-C7-N2-C2
2	T	1	NAG	O7-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
2	T	2	NDG	C1-C2-N2-C7
2	T	2	NDG	C8-C7-N2-C2
2	T	2	NDG	O7-C7-N2-C2
2	V	1	NAG	C8-C7-N2-C2
2	V	1	NAG	O7-C7-N2-C2
2	V	2	NDG	C8-C7-N2-C2
2	V	2	NDG	O7-C7-N2-C2
3	F	1	NAG	C8-C7-N2-C2
3	F	1	NAG	O7-C7-N2-C2
3	F	2	NAG	C8-C7-N2-C2
3	F	2	NAG	O7-C7-N2-C2
3	H	1	NAG	C8-C7-N2-C2
3	H	1	NAG	O7-C7-N2-C2
3	H	2	NAG	C8-C7-N2-C2
3	H	2	NAG	O7-C7-N2-C2
3	I	1	NAG	C8-C7-N2-C2
3	I	1	NAG	O7-C7-N2-C2
3	K	1	NAG	C8-C7-N2-C2
3	K	1	NAG	O7-C7-N2-C2
3	K	2	NAG	C8-C7-N2-C2
3	K	2	NAG	O7-C7-N2-C2
3	M	1	NAG	C8-C7-N2-C2
3	M	1	NAG	O7-C7-N2-C2
3	M	2	NAG	C8-C7-N2-C2
3	M	2	NAG	O7-C7-N2-C2
3	N	1	NAG	C8-C7-N2-C2
3	N	1	NAG	O7-C7-N2-C2
3	P	1	NAG	C8-C7-N2-C2
3	P	1	NAG	O7-C7-N2-C2
3	P	2	NAG	C8-C7-N2-C2
3	P	2	NAG	O7-C7-N2-C2
3	R	1	NAG	C8-C7-N2-C2
3	R	1	NAG	O7-C7-N2-C2
3	R	2	NAG	C8-C7-N2-C2
3	R	2	NAG	O7-C7-N2-C2
3	S	1	NAG	C8-C7-N2-C2
3	S	1	NAG	O7-C7-N2-C2
3	U	1	NAG	C8-C7-N2-C2
3	U	1	NAG	O7-C7-N2-C2
3	U	2	NAG	C8-C7-N2-C2
3	U	2	NAG	O7-C7-N2-C2
3	W	1	NAG	C1-C2-N2-C7

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Mol	Chain	Res	Type	Atoms
3	W	1	NAG	C8-C7-N2-C2
3	W	1	NAG	O7-C7-N2-C2
3	W	2	NAG	C8-C7-N2-C2
3	W	2	NAG	O7-C7-N2-C2
3	X	1	NAG	C8-C7-N2-C2
3	X	1	NAG	O7-C7-N2-C2
3	I	2	NAG	O5-C5-C6-O6
3	N	2	NAG	O5-C5-C6-O6
3	S	2	NAG	O5-C5-C6-O6
3	X	2	NAG	O5-C5-C6-O6
3	I	1	NAG	O5-C5-C6-O6
3	N	1	NAG	O5-C5-C6-O6
3	S	1	NAG	O5-C5-C6-O6
3	X	1	NAG	O5-C5-C6-O6
2	E	1	NAG	O5-C5-C6-O6
2	J	1	NAG	O5-C5-C6-O6
2	O	1	NAG	O5-C5-C6-O6
2	T	1	NAG	O5-C5-C6-O6
3	I	2	NAG	O7-C7-N2-C2
3	N	2	NAG	O7-C7-N2-C2
3	S	2	NAG	O7-C7-N2-C2
3	X	2	NAG	O7-C7-N2-C2
3	I	1	NAG	C4-C5-C6-O6
3	N	1	NAG	C4-C5-C6-O6
3	S	1	NAG	C4-C5-C6-O6
3	X	1	NAG	C4-C5-C6-O6
3	I	2	NAG	C8-C7-N2-C2
3	N	2	NAG	C8-C7-N2-C2
3	S	2	NAG	C8-C7-N2-C2
3	X	2	NAG	C8-C7-N2-C2
3	I	2	NAG	C4-C5-C6-O6
3	N	2	NAG	C4-C5-C6-O6
3	S	2	NAG	C4-C5-C6-O6
3	X	2	NAG	C4-C5-C6-O6
3	F	1	NAG	O5-C5-C6-O6
3	K	1	NAG	O5-C5-C6-O6
3	P	1	NAG	O5-C5-C6-O6
3	U	1	NAG	O5-C5-C6-O6
3	F	1	NAG	C4-C5-C6-O6
3	K	1	NAG	C4-C5-C6-O6
3	P	1	NAG	C4-C5-C6-O6
3	U	1	NAG	C4-C5-C6-O6

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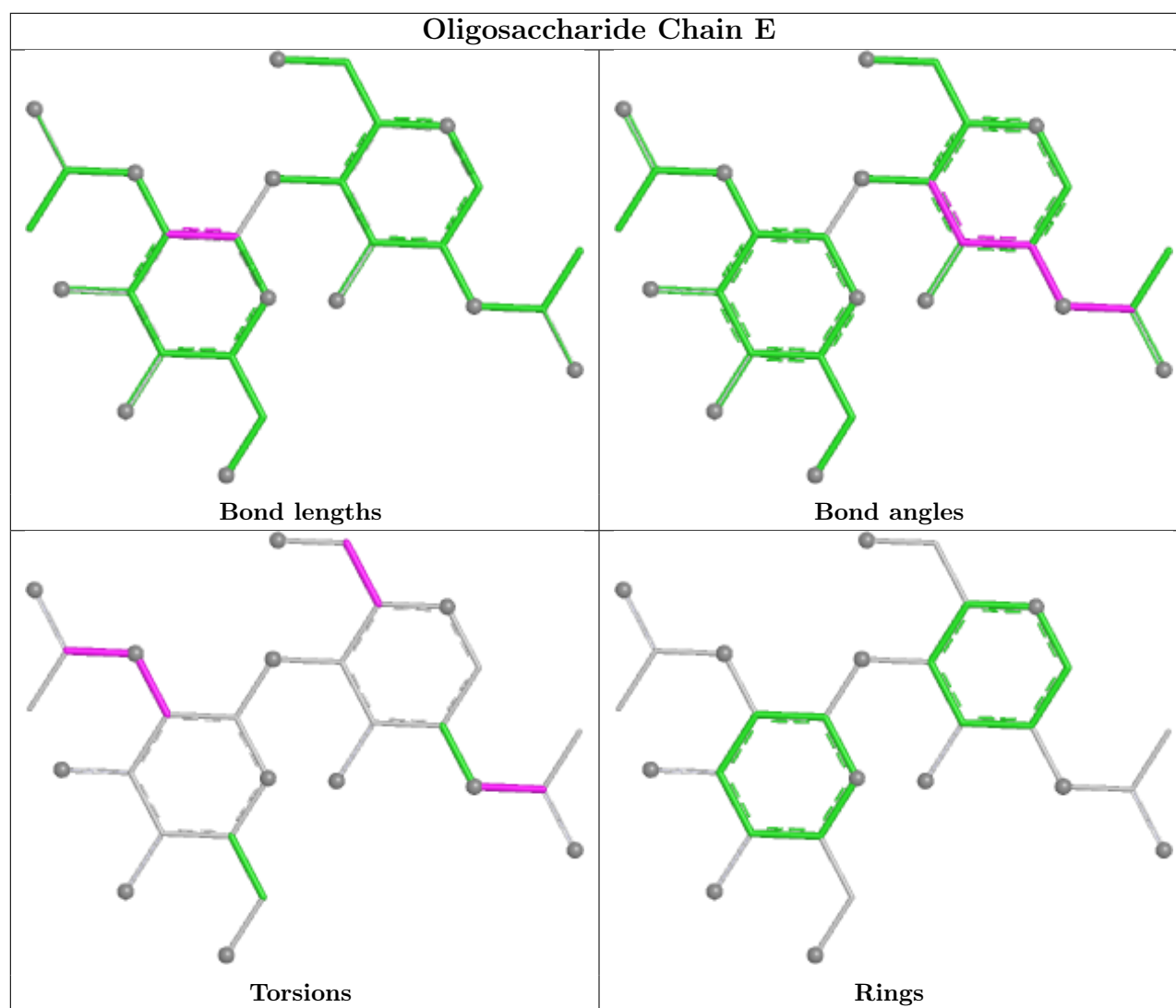
Mol	Chain	Res	Type	Atoms
2	E	1	NAG	C4-C5-C6-O6
2	J	1	NAG	C4-C5-C6-O6
2	O	1	NAG	C4-C5-C6-O6
2	T	1	NAG	C4-C5-C6-O6
3	H	1	NAG	C3-C2-N2-C7
3	M	1	NAG	C3-C2-N2-C7
3	R	1	NAG	C3-C2-N2-C7
3	W	1	NAG	C3-C2-N2-C7
3	H	1	NAG	C1-C2-N2-C7
3	M	1	NAG	C1-C2-N2-C7
3	R	1	NAG	C1-C2-N2-C7
3	H	2	NAG	C4-C5-C6-O6
3	M	2	NAG	C4-C5-C6-O6
3	R	2	NAG	C4-C5-C6-O6
3	W	2	NAG	C4-C5-C6-O6
2	L	2	NDG	C4-C5-C6-O6
2	Q	2	NDG	C4-C5-C6-O6
2	V	2	NDG	C4-C5-C6-O6
2	G	2	NDG	C4-C5-C6-O6
3	F	1	NAG	C3-C2-N2-C7
3	H	2	NAG	C3-C2-N2-C7
3	K	1	NAG	C3-C2-N2-C7
3	M	2	NAG	C3-C2-N2-C7
3	P	1	NAG	C3-C2-N2-C7
3	R	2	NAG	C3-C2-N2-C7
3	U	1	NAG	C3-C2-N2-C7
3	W	2	NAG	C3-C2-N2-C7
2	Q	1	NAG	C4-C5-C6-O6
2	V	1	NAG	C4-C5-C6-O6
2	G	1	NAG	C4-C5-C6-O6
2	L	1	NAG	C4-C5-C6-O6
3	H	2	NAG	C1-C2-N2-C7
3	M	2	NAG	C1-C2-N2-C7
3	R	2	NAG	C1-C2-N2-C7
3	W	2	NAG	C1-C2-N2-C7
2	G	1	NAG	C3-C2-N2-C7
2	L	1	NAG	C3-C2-N2-C7
2	Q	1	NAG	C3-C2-N2-C7
2	V	1	NAG	C3-C2-N2-C7

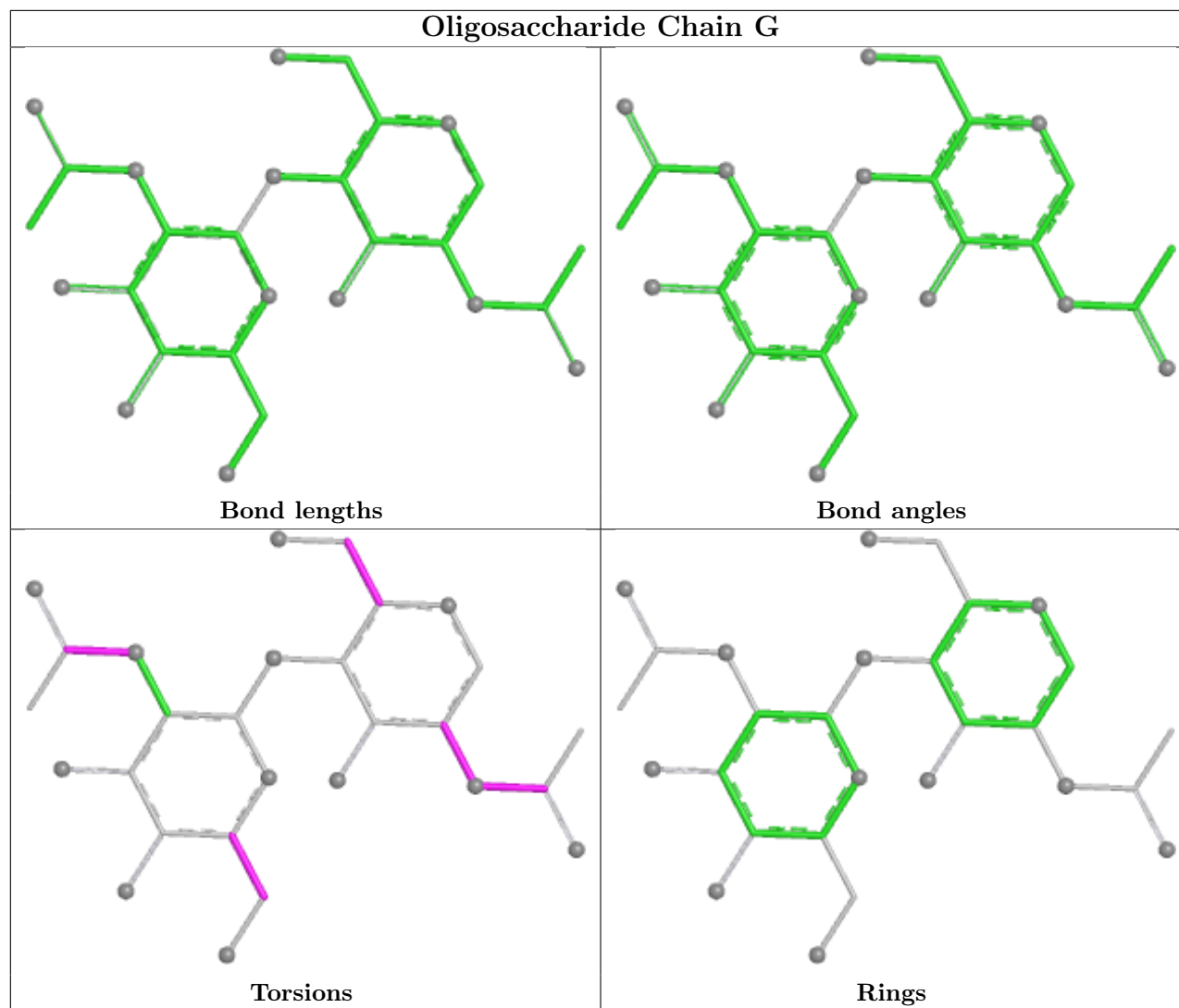
There are no ring outliers.

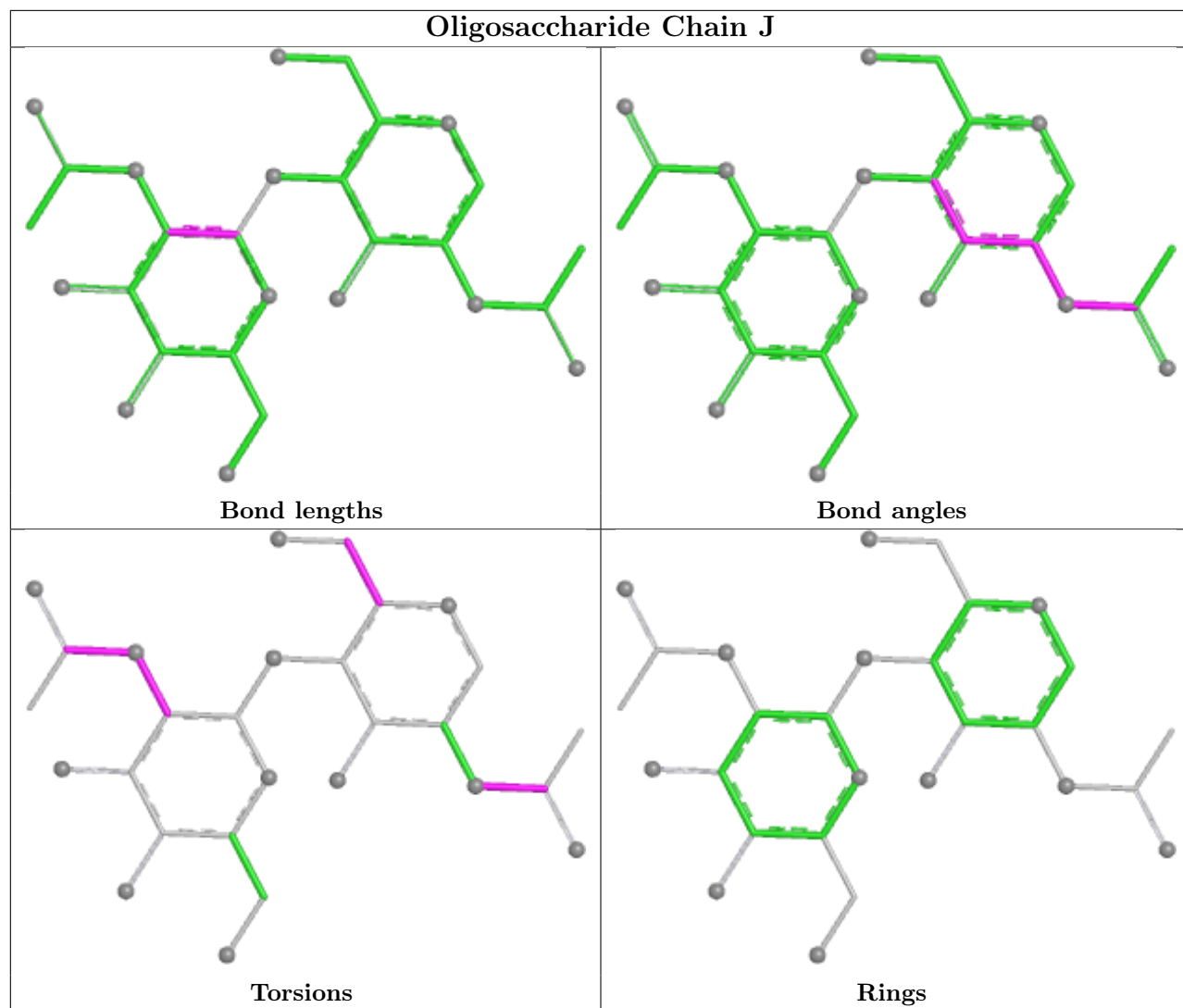
29 monomers are involved in 35 short contacts:

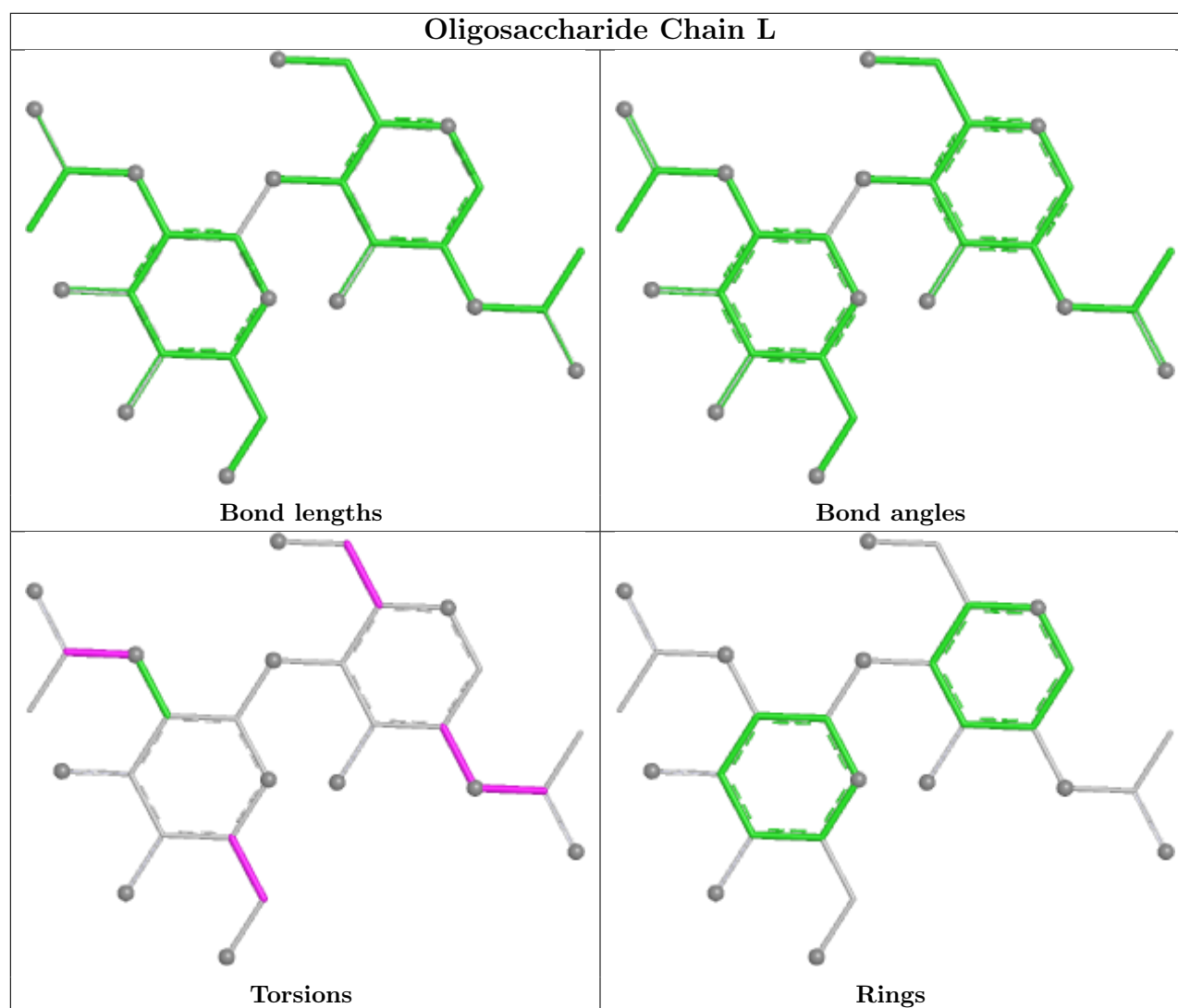
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	P	1	NAG	1	0
3	W	1	NAG	5	0
2	Q	2	NDG	1	0
3	F	2	NAG	1	0
2	L	1	NAG	1	0
2	E	1	NAG	2	0
3	H	1	NAG	5	0
3	U	2	NAG	1	0
2	O	2	NDG	1	0
2	Q	1	NAG	1	0
3	F	1	NAG	1	0
2	V	1	NAG	1	0
2	G	1	NAG	1	0
3	K	2	NAG	1	0
3	P	2	NAG	1	0
2	L	2	NDG	1	0
2	E	2	NDG	2	0
3	R	1	NAG	5	0
2	J	1	NAG	2	0
2	T	1	NAG	1	0
3	U	1	NAG	1	0
2	J	2	NDG	2	0
2	O	1	NAG	1	0
2	T	2	NDG	1	0
2	V	2	NDG	1	0
2	G	2	NDG	1	1
3	M	1	NAG	5	0
3	M	2	NAG	0	1
3	K	1	NAG	1	0

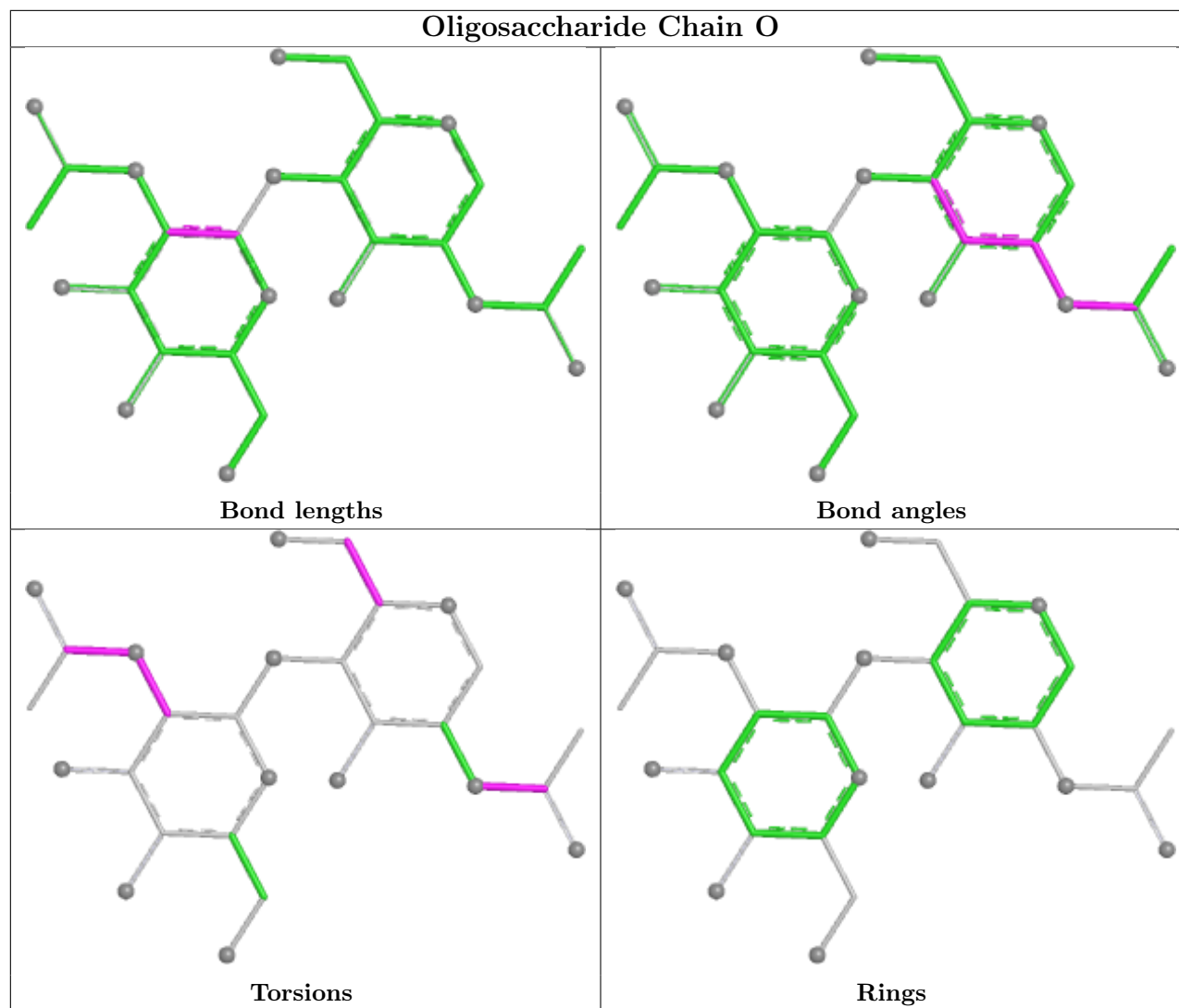
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

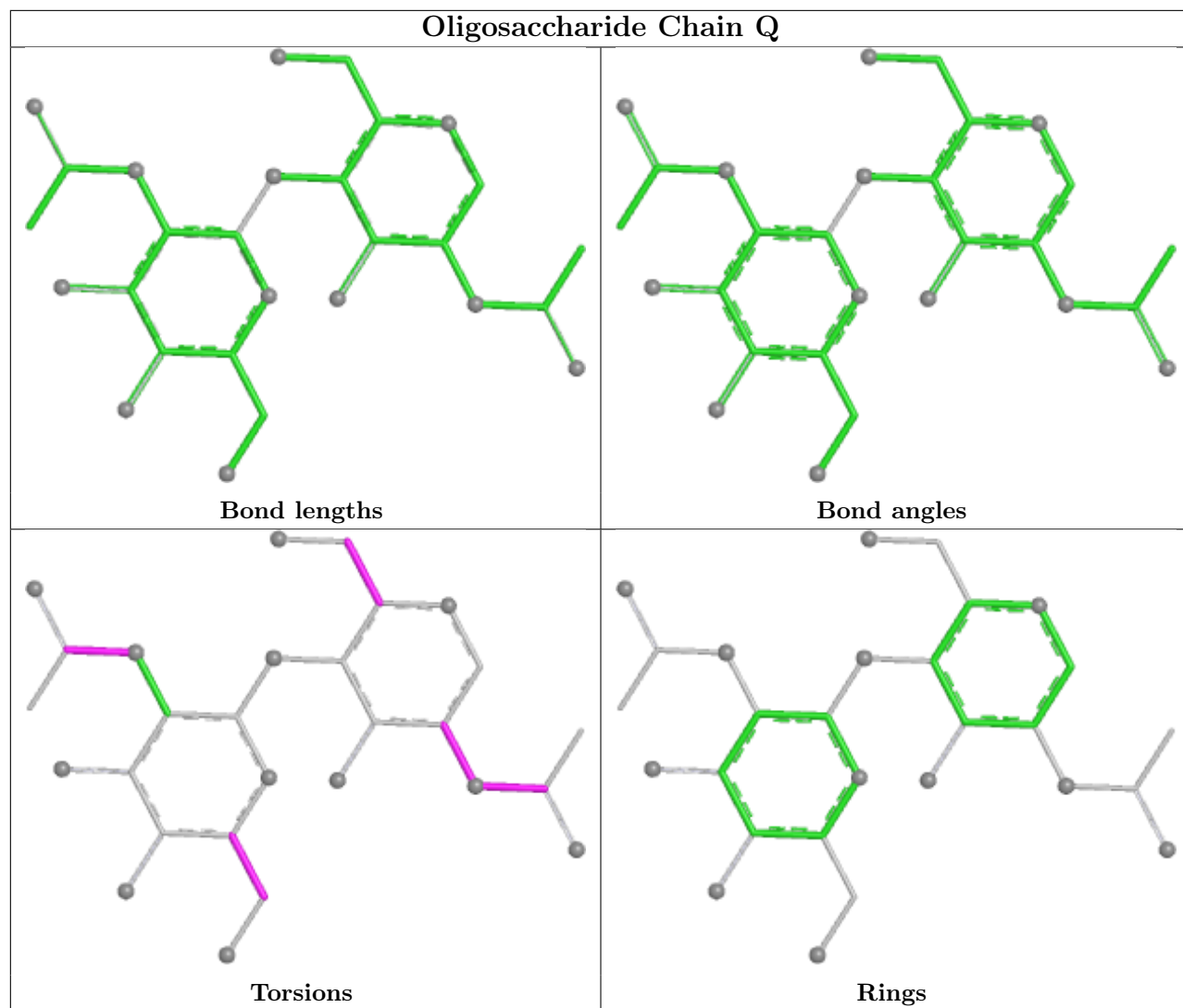


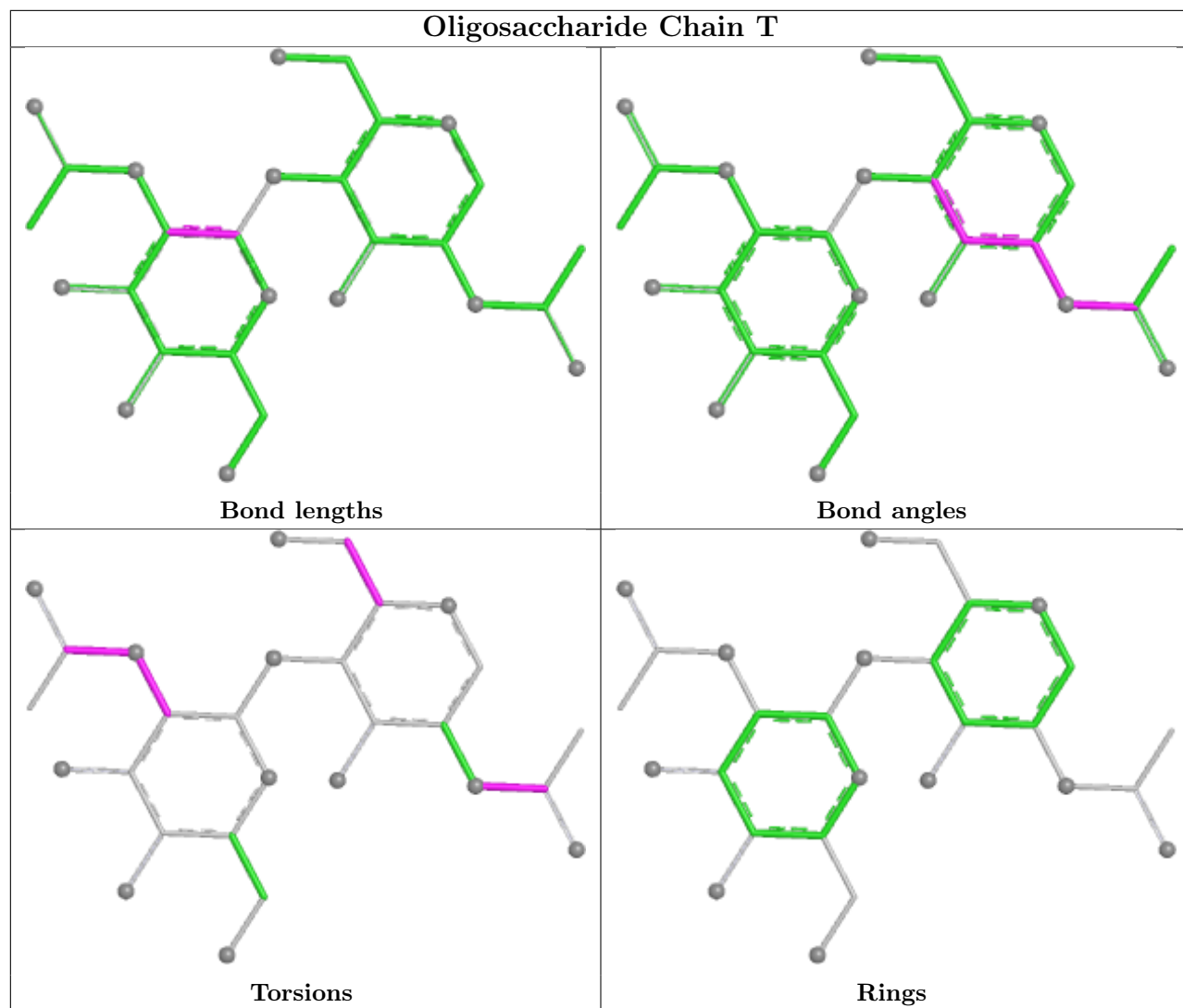


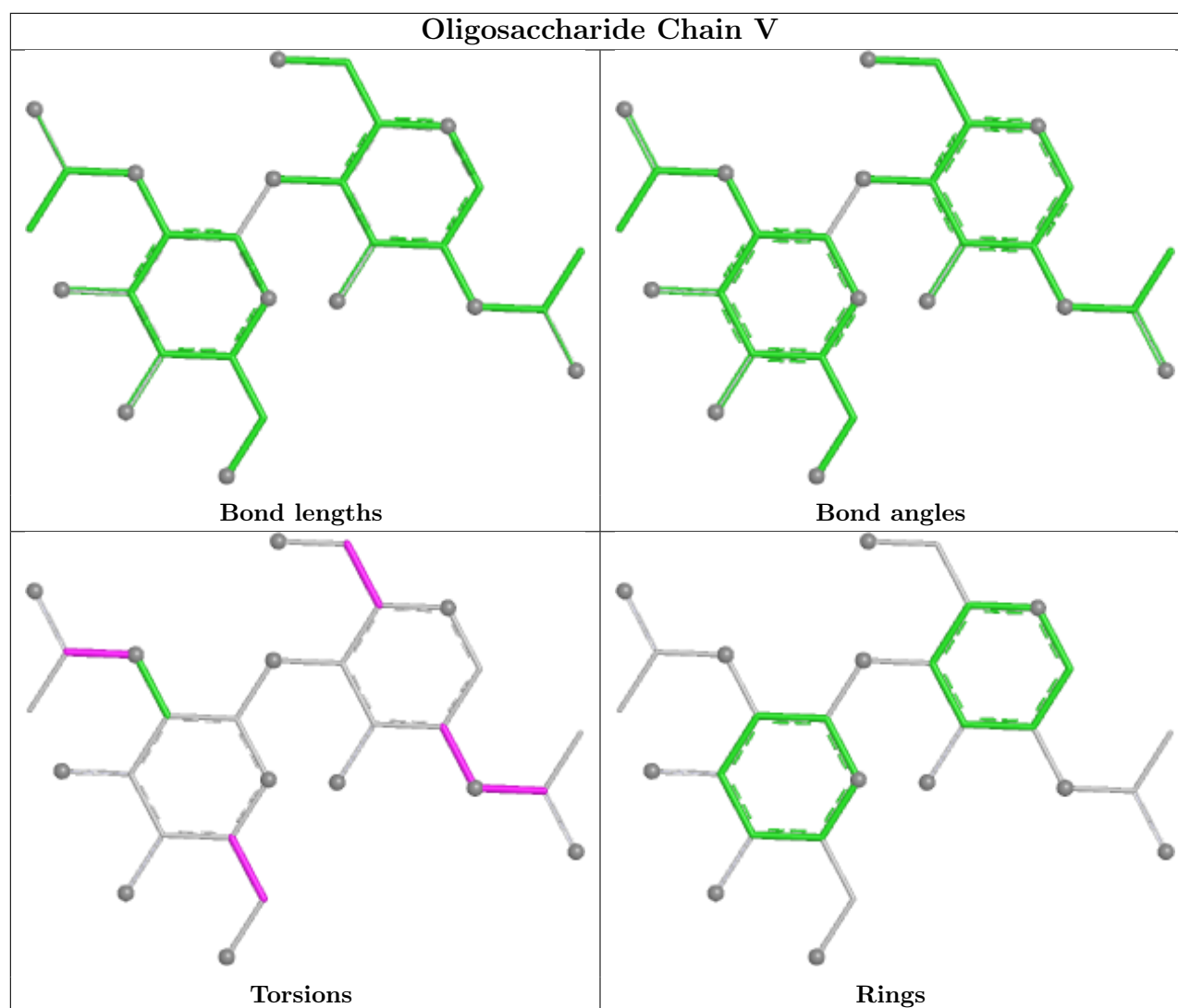


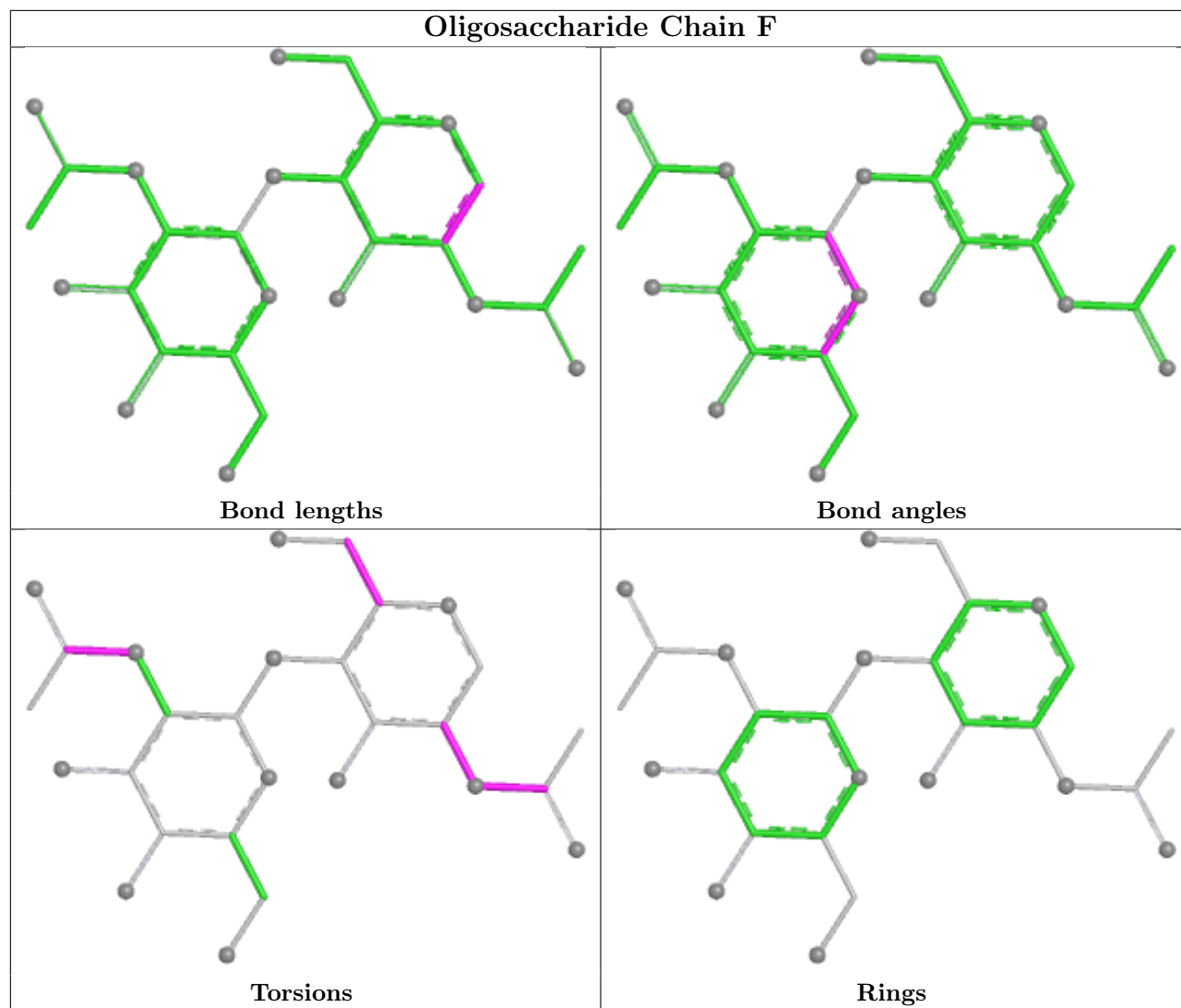


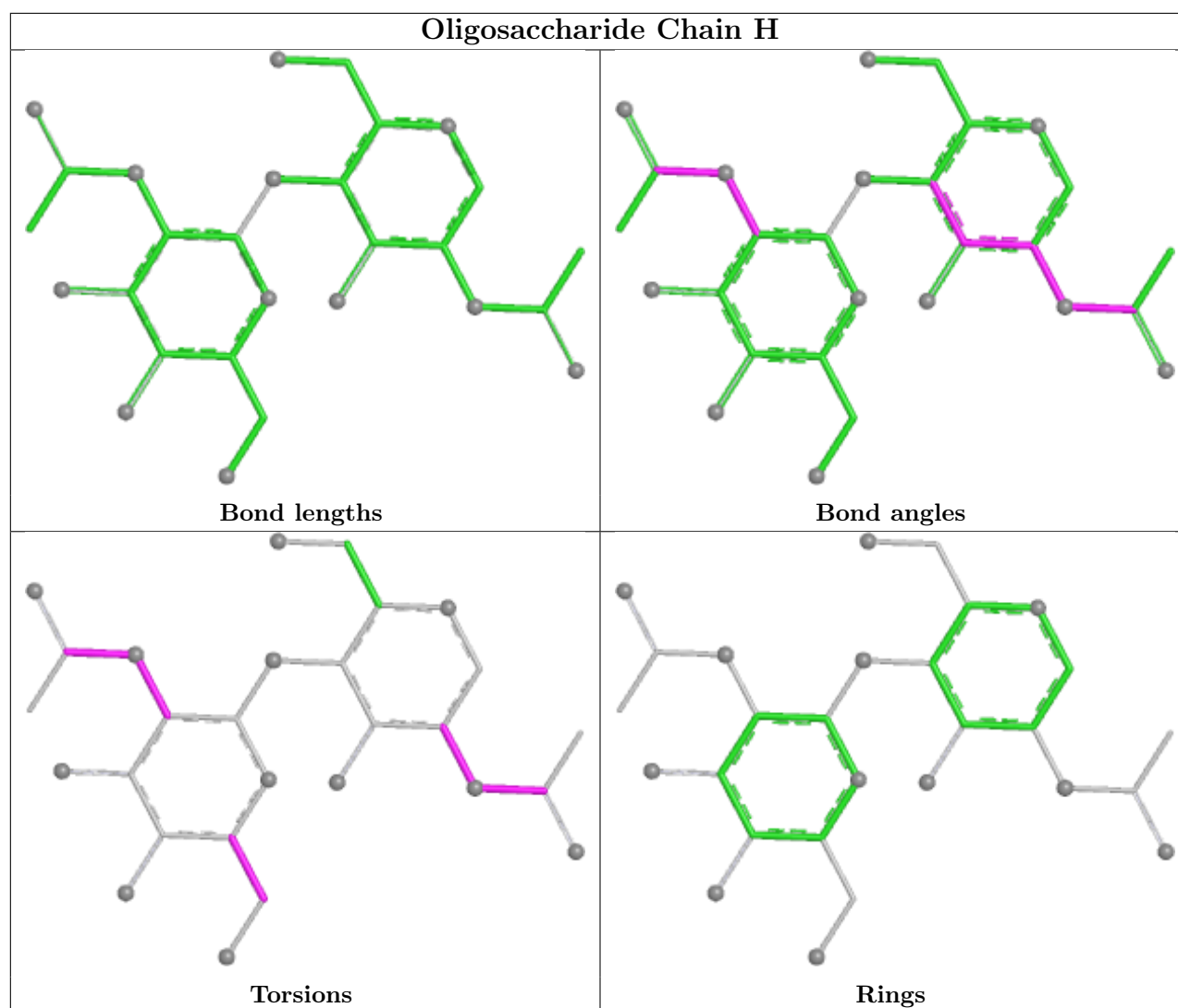


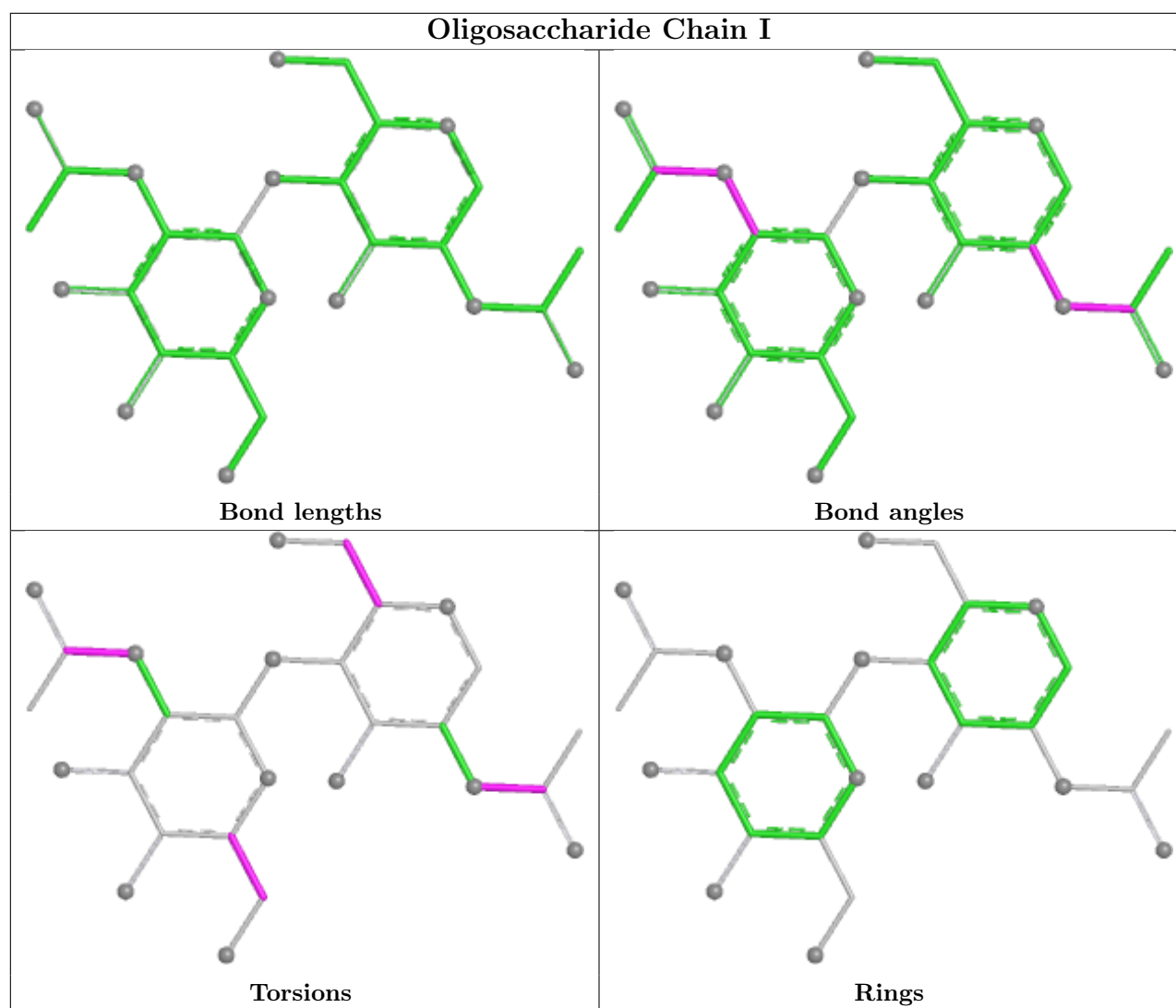


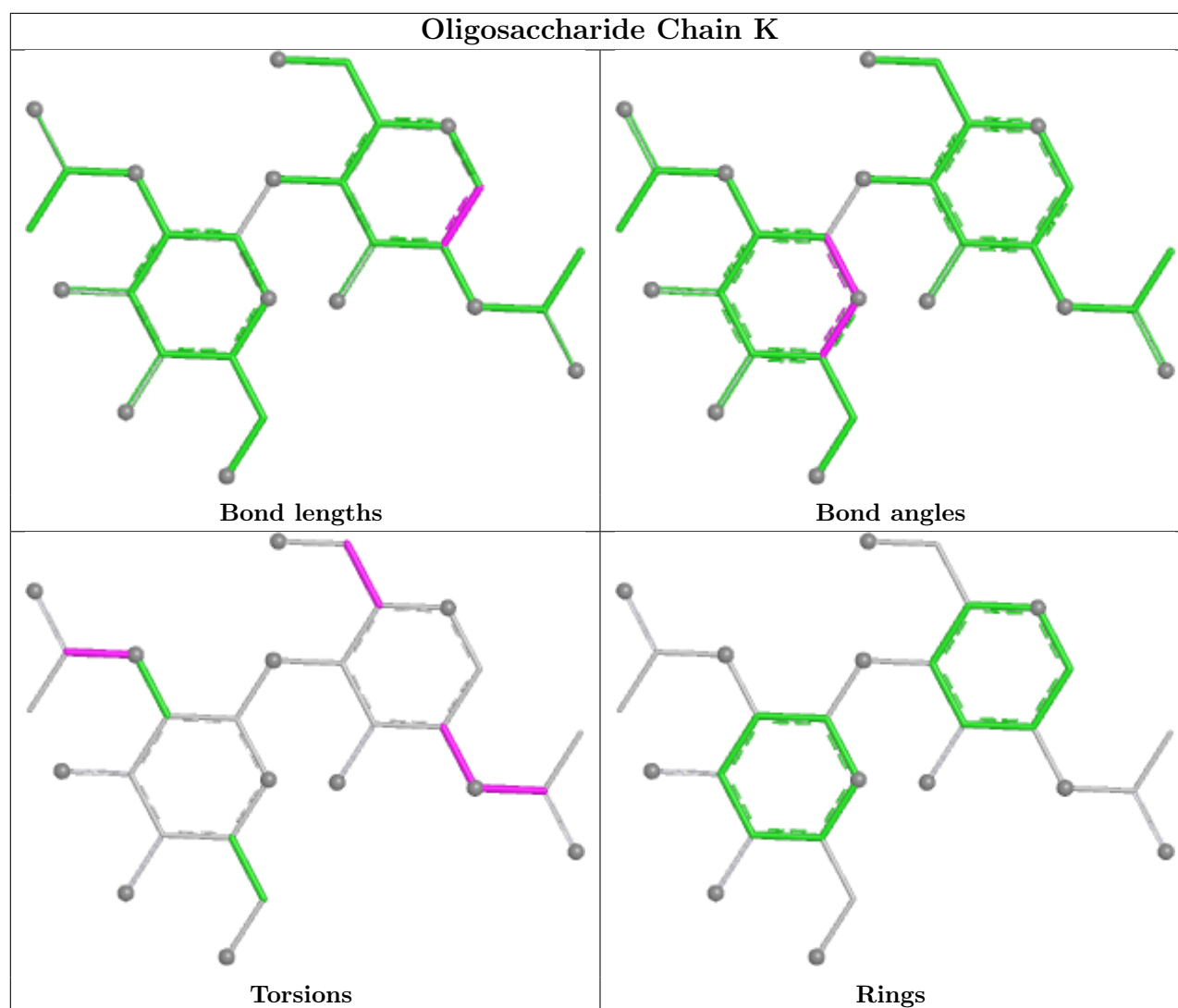


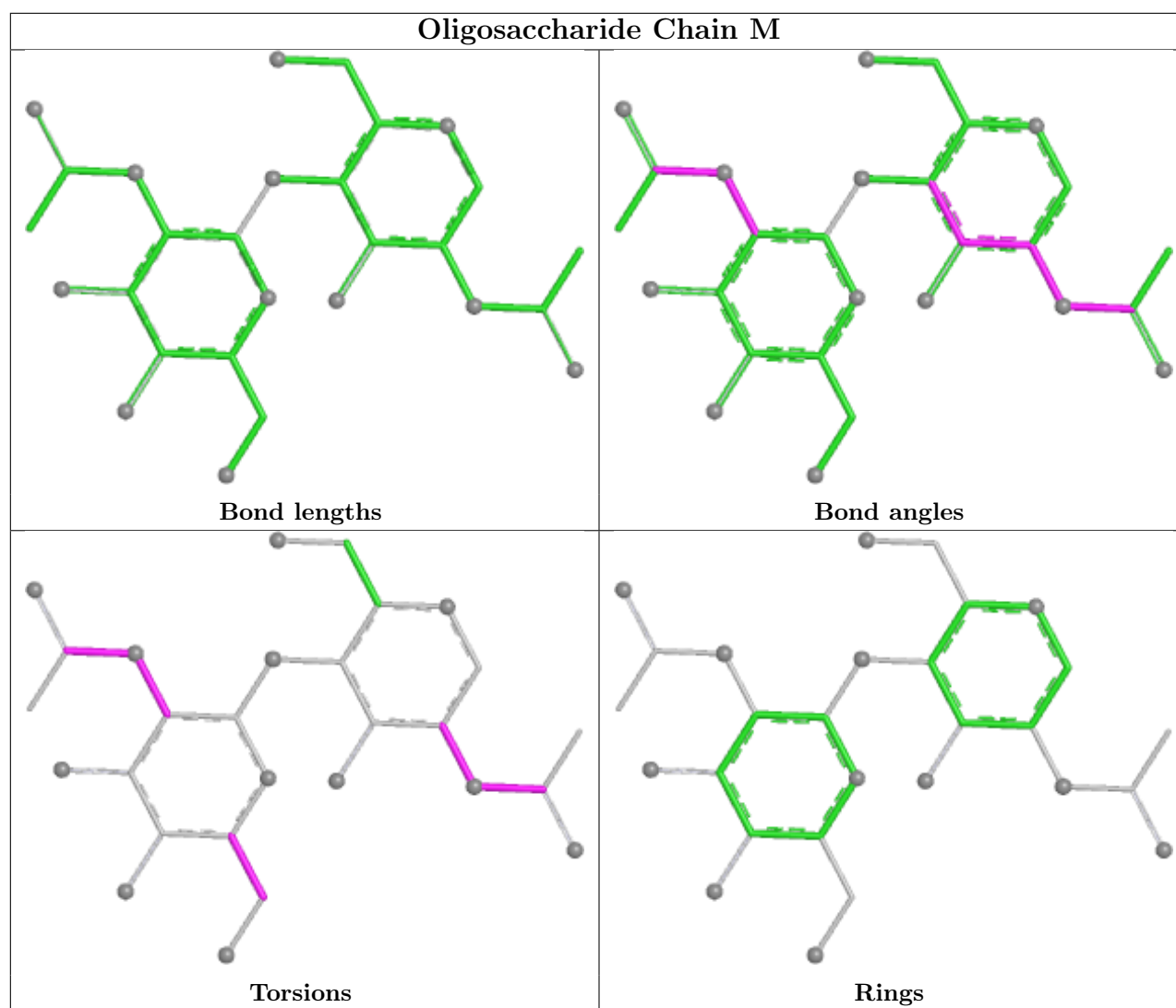


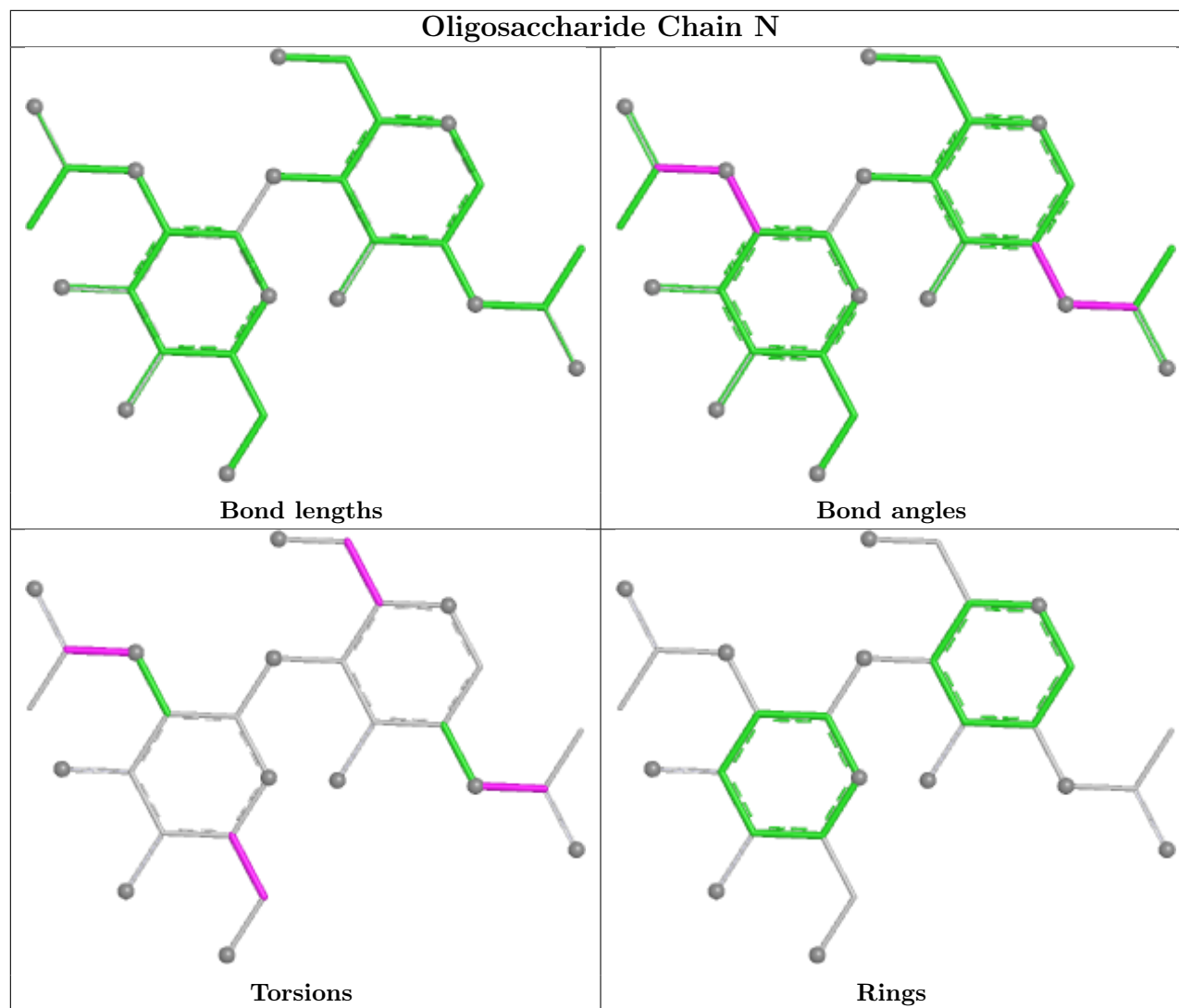


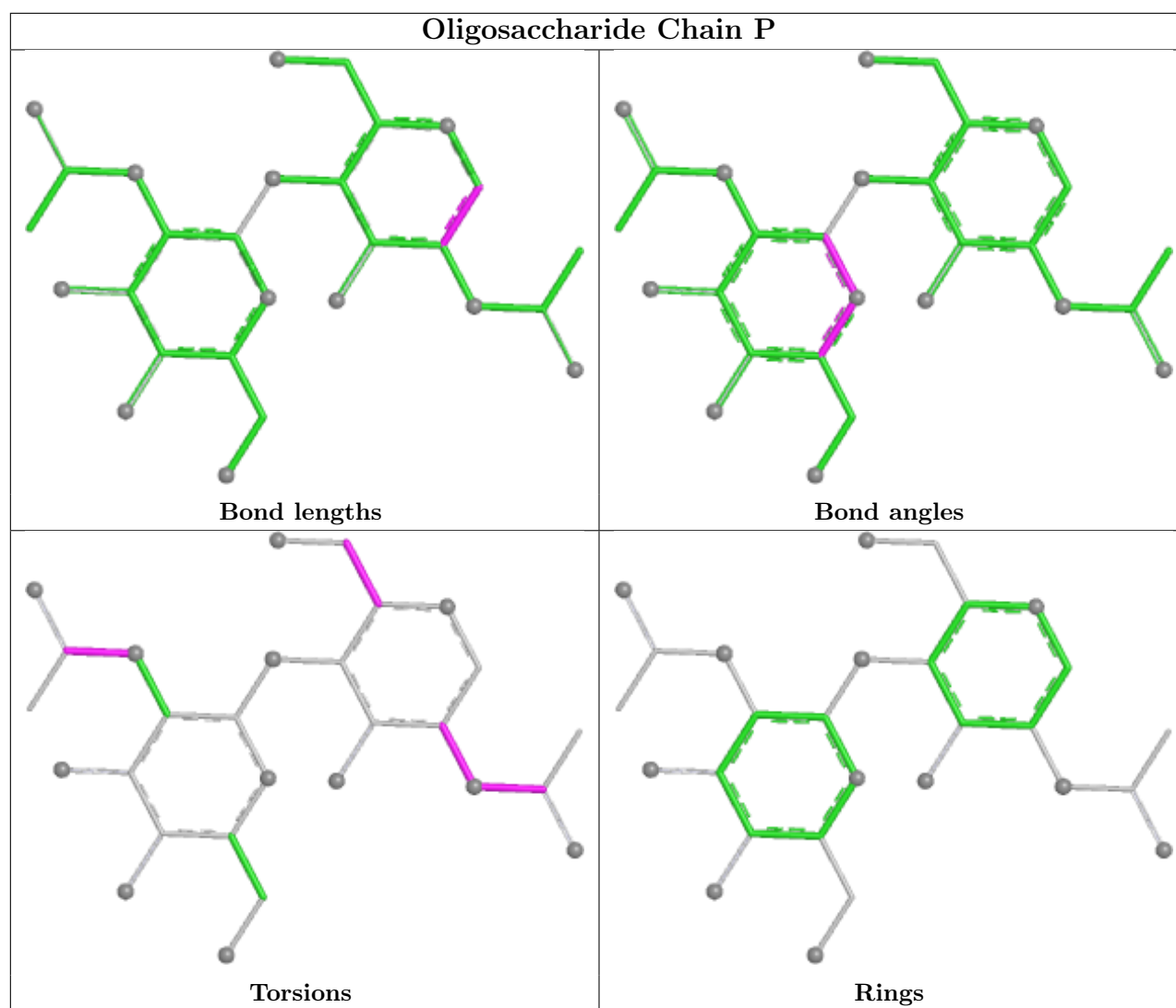


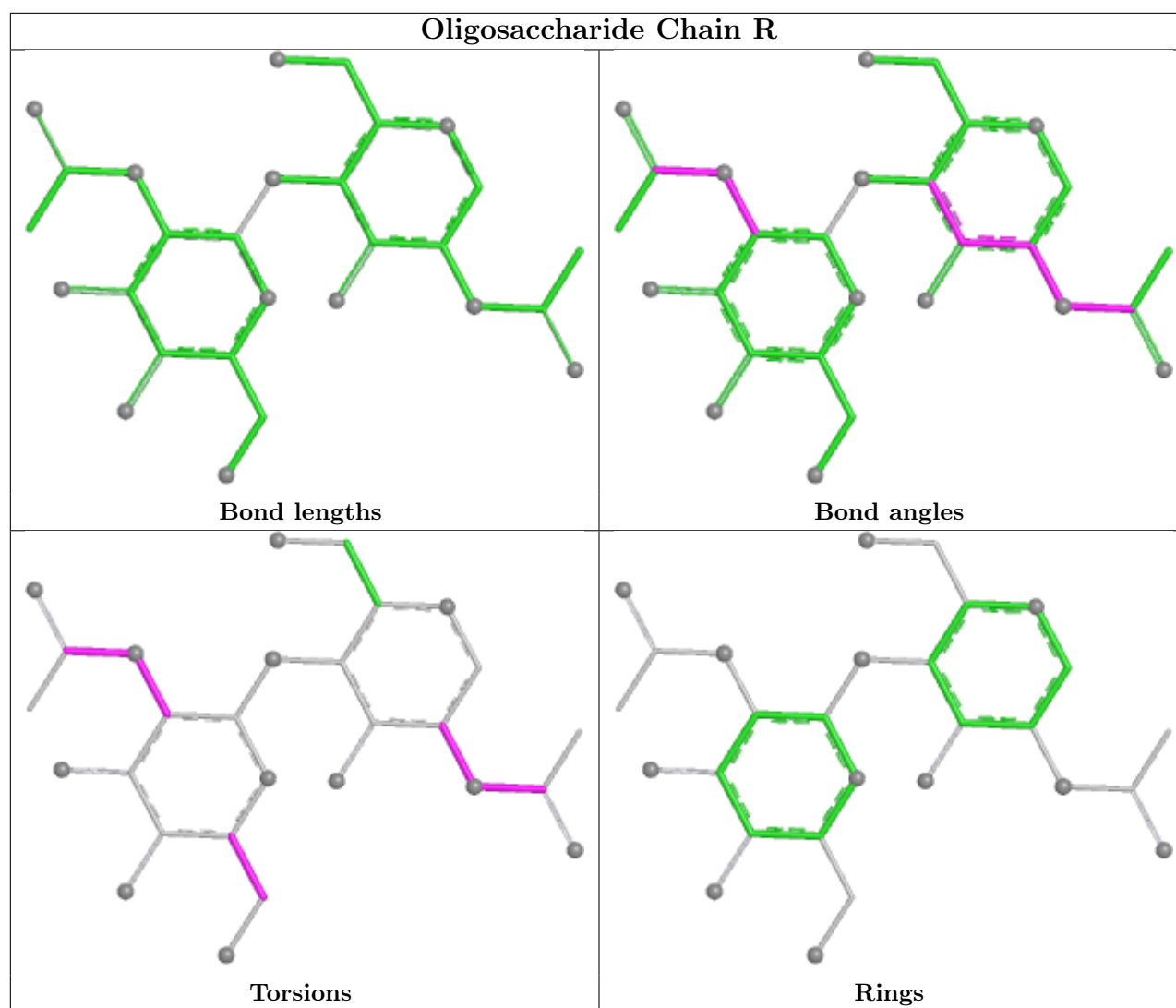


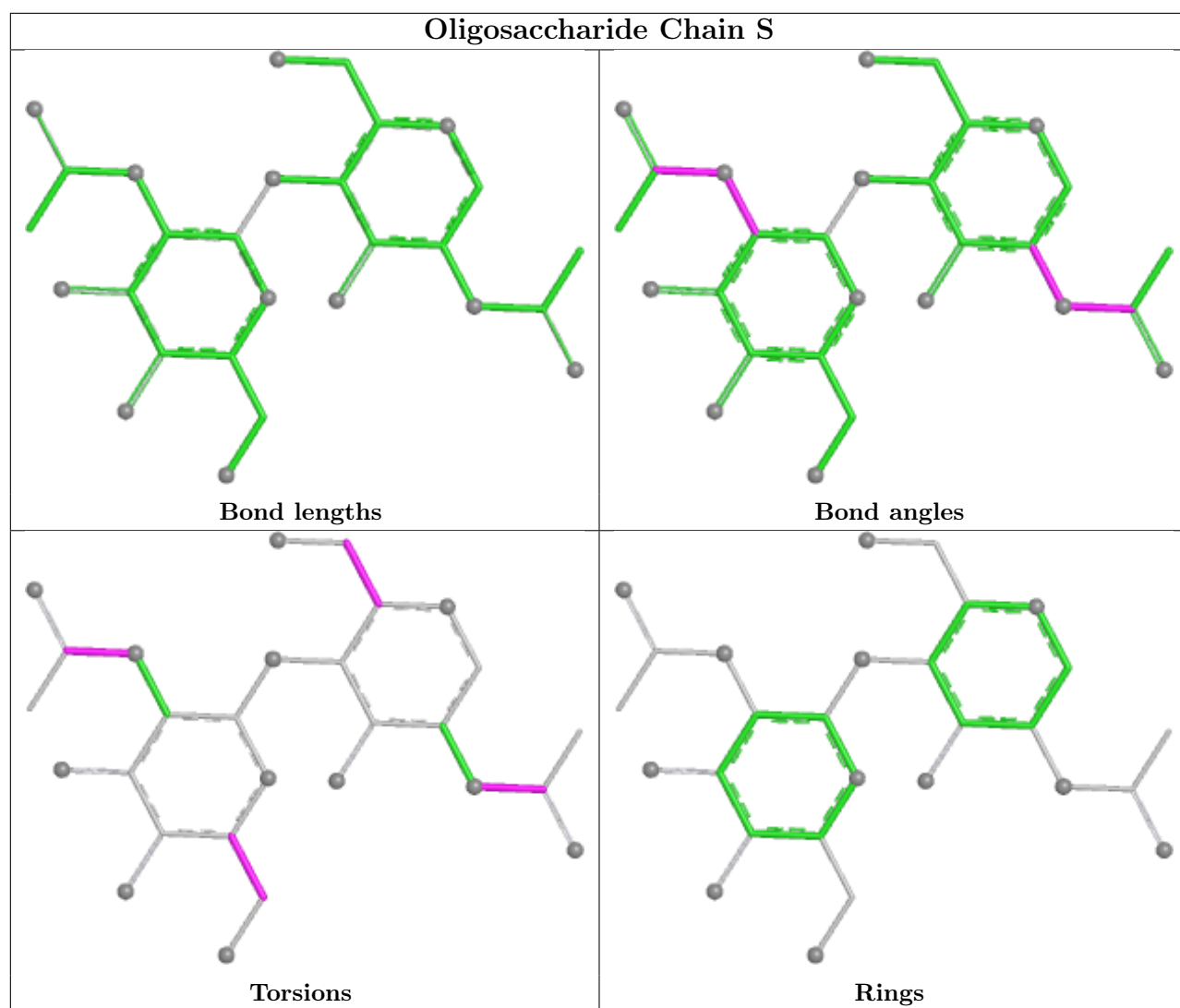


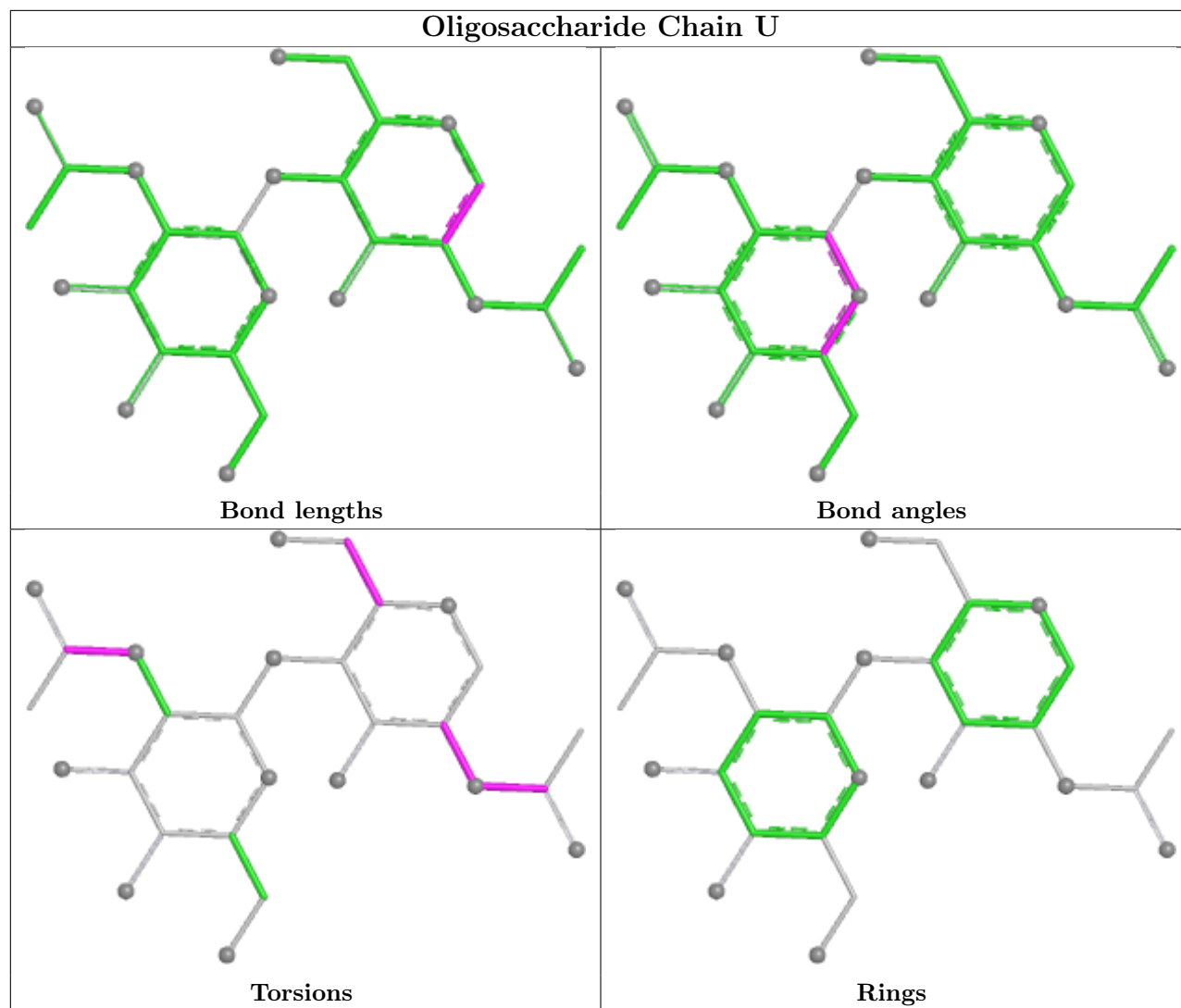


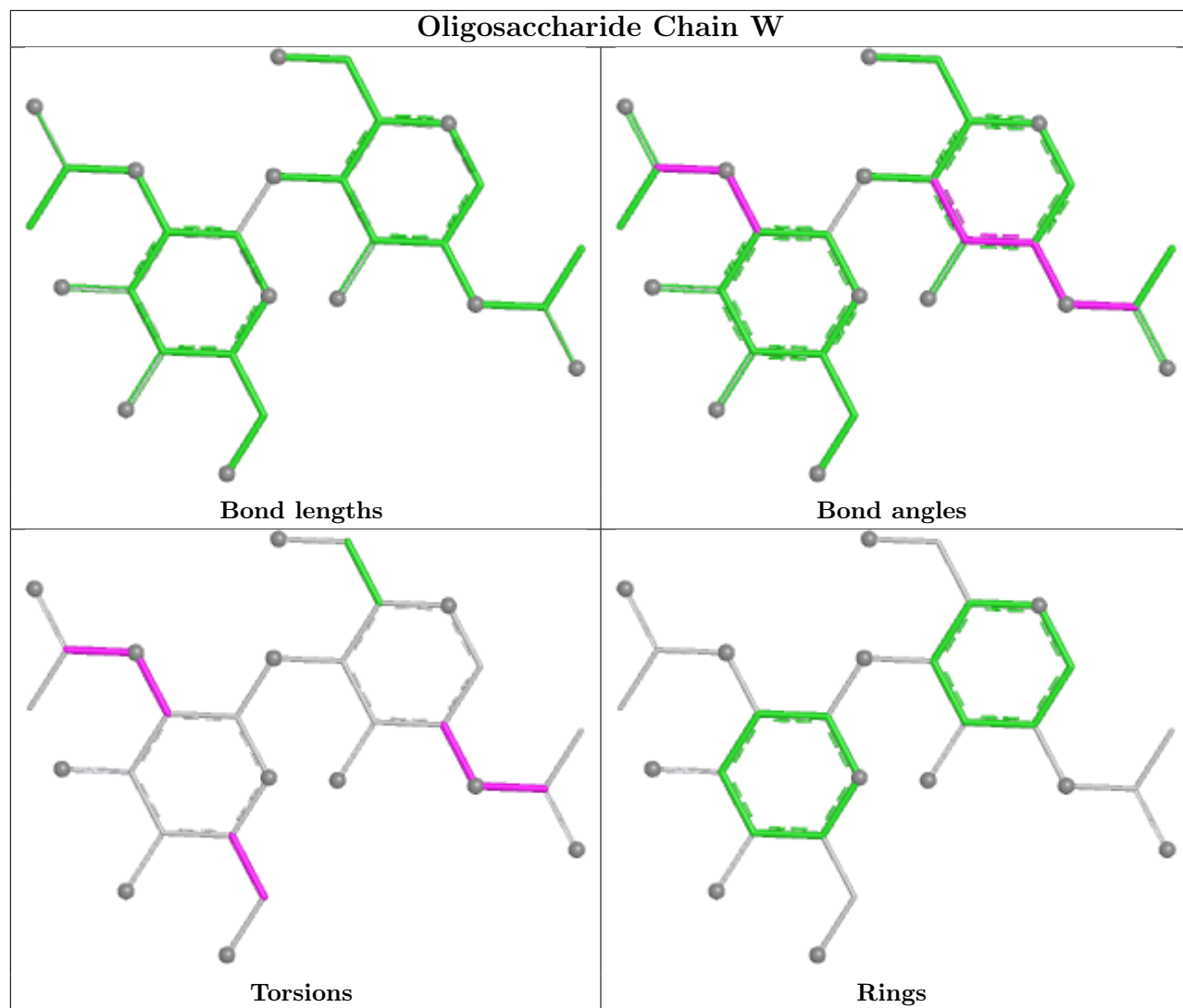


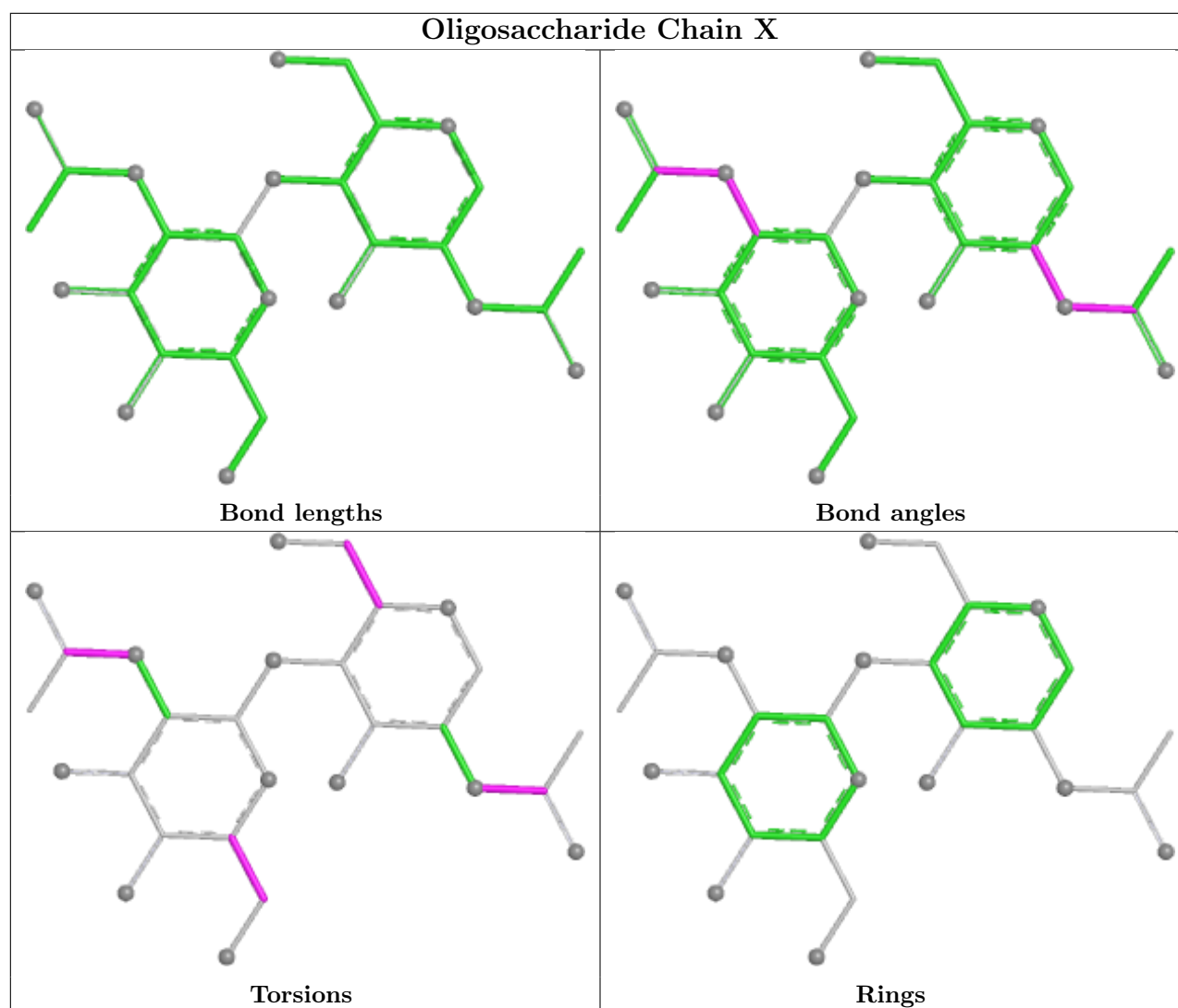












5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 8 are monoatomic - leaving 8 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	NAG	C	3759	1	14,14,15	0.82	0	17,19,21	0.76	0
4	NAG	B	2760	1	14,14,15	0.97	1 (7%)	17,19,21	0.72	0
4	NAG	A	1759	1	14,14,15	0.82	0	17,19,21	0.76	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	C	3760	1	14,14,15	0.98	1 (7%)	17,19,21	0.73	0
4	NAG	D	4759	1	14,14,15	0.82	0	17,19,21	0.76	0
4	NAG	D	4760	1	14,14,15	0.98	1 (7%)	17,19,21	0.73	0
4	NAG	B	2759	1	14,14,15	0.82	0	17,19,21	0.75	0
4	NAG	A	1760	1	14,14,15	0.97	1 (7%)	17,19,21	0.72	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
4	NAG	C	3759	1	-	5/6/23/26	0/1/1/1
4	NAG	B	2760	1	-	5/6/23/26	0/1/1/1
4	NAG	A	1759	1	-	5/6/23/26	0/1/1/1
4	NAG	C	3760	1	-	5/6/23/26	0/1/1/1
4	NAG	D	4759	1	-	5/6/23/26	0/1/1/1
4	NAG	D	4760	1	-	5/6/23/26	0/1/1/1
4	NAG	B	2759	1	-	5/6/23/26	0/1/1/1
4	NAG	A	1760	1	-	5/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	4760	NAG	C1-C2	2.95	1.56	1.52
4	C	3760	NAG	C1-C2	2.92	1.56	1.52
4	B	2760	NAG	C1-C2	2.90	1.56	1.52
4	A	1760	NAG	C1-C2	2.90	1.56	1.52

There are no bond angle outliers.

There are no chirality outliers.

All (40) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1759	NAG	C8-C7-N2-C2
4	A	1759	NAG	O7-C7-N2-C2
4	A	1760	NAG	C8-C7-N2-C2
4	A	1760	NAG	O7-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
4	B	2759	NAG	C8-C7-N2-C2
4	B	2759	NAG	O7-C7-N2-C2
4	B	2760	NAG	C8-C7-N2-C2
4	B	2760	NAG	O7-C7-N2-C2
4	C	3759	NAG	C8-C7-N2-C2
4	C	3759	NAG	O7-C7-N2-C2
4	C	3760	NAG	C8-C7-N2-C2
4	C	3760	NAG	O7-C7-N2-C2
4	D	4759	NAG	C8-C7-N2-C2
4	D	4759	NAG	O7-C7-N2-C2
4	D	4760	NAG	C8-C7-N2-C2
4	D	4760	NAG	O7-C7-N2-C2
4	A	1759	NAG	O5-C5-C6-O6
4	B	2759	NAG	O5-C5-C6-O6
4	C	3759	NAG	O5-C5-C6-O6
4	D	4759	NAG	O5-C5-C6-O6
4	A	1759	NAG	C4-C5-C6-O6
4	B	2759	NAG	C4-C5-C6-O6
4	C	3759	NAG	C4-C5-C6-O6
4	D	4759	NAG	C4-C5-C6-O6
4	A	1760	NAG	O5-C5-C6-O6
4	B	2760	NAG	O5-C5-C6-O6
4	C	3760	NAG	O5-C5-C6-O6
4	D	4760	NAG	O5-C5-C6-O6
4	A	1760	NAG	C3-C2-N2-C7
4	B	2760	NAG	C3-C2-N2-C7
4	C	3760	NAG	C3-C2-N2-C7
4	D	4760	NAG	C3-C2-N2-C7
4	A	1759	NAG	C3-C2-N2-C7
4	B	2759	NAG	C3-C2-N2-C7
4	C	3759	NAG	C3-C2-N2-C7
4	D	4759	NAG	C3-C2-N2-C7
4	D	4760	NAG	C4-C5-C6-O6
4	A	1760	NAG	C4-C5-C6-O6
4	B	2760	NAG	C4-C5-C6-O6
4	C	3760	NAG	C4-C5-C6-O6

There are no ring outliers.

5 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	2760	NAG	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	3760	NAG	5	0
4	D	4760	NAG	5	0
4	B	2759	NAG	1	0
4	A	1760	NAG	5	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	695/695 (100%)	0.16	8 (1%) 76 52	2, 51, 143, 197	0
1	B	695/695 (100%)	0.14	3 (0%) 88 72	2, 51, 143, 197	0
1	C	695/695 (100%)	0.06	0 100 100	2, 51, 143, 197	0
1	D	695/695 (100%)	0.18	20 (2%) 53 31	2, 51, 143, 197	0
All	All	2780/2780 (100%)	0.14	31 (1%) 78 54	2, 51, 144, 197	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	180	ALA	4.7
1	D	319	TRP	4.0
1	D	214	VAL	3.8
1	D	305	LEU	3.2
1	D	315	PRO	3.2
1	D	307	GLU	2.9
1	D	309	MET	2.8
1	D	224	GLY	2.8
1	A	698	ASN	2.7
1	A	302	ALA	2.5
1	D	308	LYS	2.5
1	B	489	GLU	2.4
1	D	186	PHE	2.4
1	D	328	ASN	2.4
1	D	326	PRO	2.2
1	D	316	ASP	2.2
1	D	208	VAL	2.2
1	D	330	GLY	2.2
1	A	209	PHE	2.2
1	D	313	ALA	2.2
1	A	171	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	699	LYS	2.1
1	B	227	LEU	2.1
1	D	174	LEU	2.1
1	A	175	VAL	2.1
1	A	182	THR	2.1
1	D	189	GLU	2.1
1	D	202	ILE	2.1
1	B	725	TRP	2.1
1	A	343	LYS	2.1
1	D	718	LYS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	NAG	F	2	14/15	0.06	0.15	196,196,196,196	0
2	NAG	L	1	14/15	0.09	0.15	197,197,197,197	0
2	NDG	G	2	14/15	0.09	0.12	189,189,189,189	0
2	NAG	V	1	14/15	0.22	0.14	197,197,197,197	0
2	NDG	V	2	14/15	0.27	0.14	189,189,189,189	0
2	NDG	L	2	14/15	0.35	0.13	189,189,189,189	0
3	NAG	K	1	14/15	0.36	0.13	173,173,173,173	0
3	NAG	K	2	14/15	0.38	0.14	196,196,196,196	0
3	NAG	P	1	14/15	0.38	0.13	173,173,173,173	0
3	NAG	U	2	14/15	0.38	0.14	196,196,196,196	0
3	NAG	P	2	14/15	0.40	0.14	196,196,196,196	0
2	NDG	Q	2	14/15	0.40	0.12	189,189,189,189	0
3	NAG	U	1	14/15	0.44	0.14	173,173,173,173	0
3	NAG	M	2	14/15	0.45	0.15	197,197,197,197	0
3	NAG	F	1	14/15	0.51	0.13	173,173,173,173	0
2	NAG	Q	1	14/15	0.54	0.13	197,197,197,197	0
2	NAG	G	1	14/15	0.55	0.10	197,197,197,197	0
3	NAG	W	2	14/15	0.58	0.17	197,197,197,197	0

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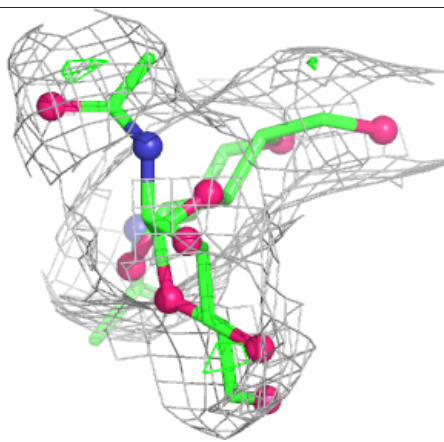
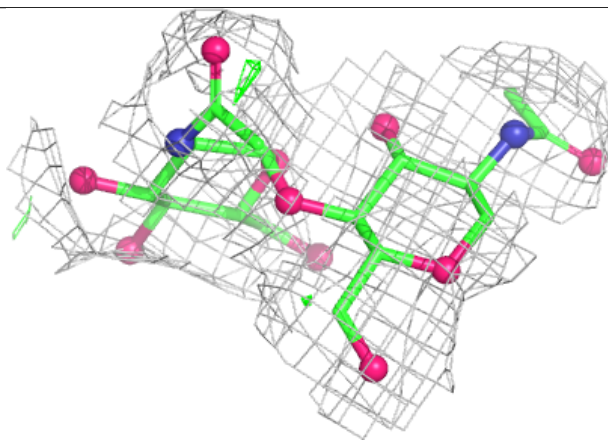
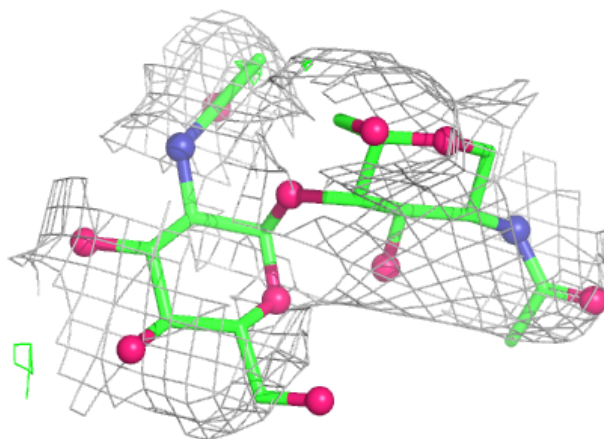
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	NAG	H	2	14/15	0.59	0.15	197,197,197,197	0
2	NDG	E	2	14/15	0.62	0.12	142,142,142,142	0
3	NAG	R	2	14/15	0.64	0.14	197,197,197,197	0
3	NAG	I	2	14/15	0.71	0.15	111,111,111,111	0
3	NAG	N	2	14/15	0.71	0.11	111,111,111,111	0
2	NDG	T	2	14/15	0.72	0.14	142,142,142,142	0
3	NAG	R	1	14/15	0.74	0.13	117,117,117,117	0
2	NAG	E	1	14/15	0.75	0.12	77,77,77,77	0
3	NAG	S	2	14/15	0.78	0.10	111,111,111,111	0
2	NDG	O	2	14/15	0.78	0.11	142,142,142,142	0
3	NAG	M	1	14/15	0.79	0.14	117,117,117,117	0
2	NAG	T	1	14/15	0.80	0.10	77,77,77,77	0
2	NDG	J	2	14/15	0.81	0.14	142,142,142,142	0
3	NAG	S	1	14/15	0.81	0.11	88,88,88,88	0
3	NAG	N	1	14/15	0.81	0.11	88,88,88,88	0
3	NAG	H	1	14/15	0.83	0.12	117,117,117,117	0
3	NAG	W	1	14/15	0.83	0.13	117,117,117,117	0
2	NAG	J	1	14/15	0.83	0.10	77,77,77,77	0
3	NAG	X	2	14/15	0.83	0.13	111,111,111,111	0
3	NAG	X	1	14/15	0.84	0.12	88,88,88,88	0
2	NAG	O	1	14/15	0.84	0.10	77,77,77,77	0
3	NAG	I	1	14/15	0.86	0.12	88,88,88,88	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

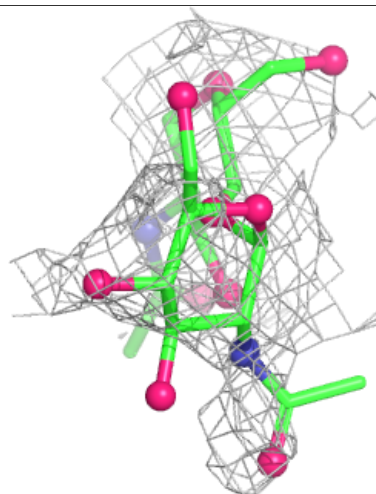
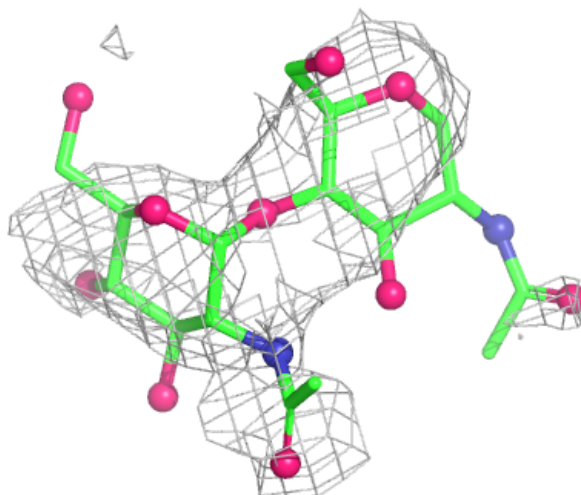
Electron density around Chain E:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



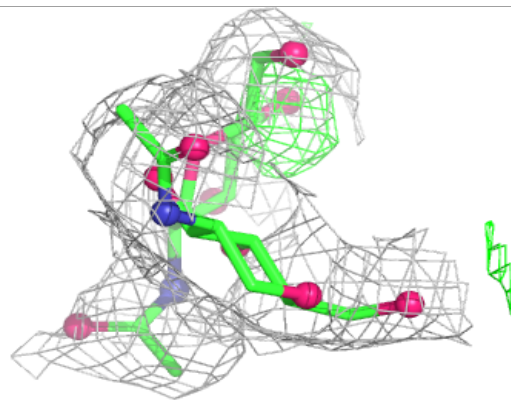
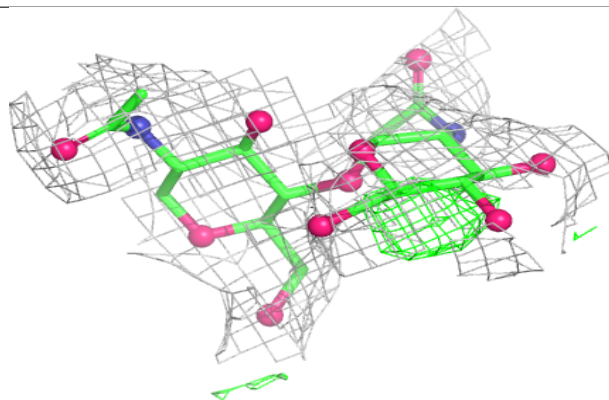
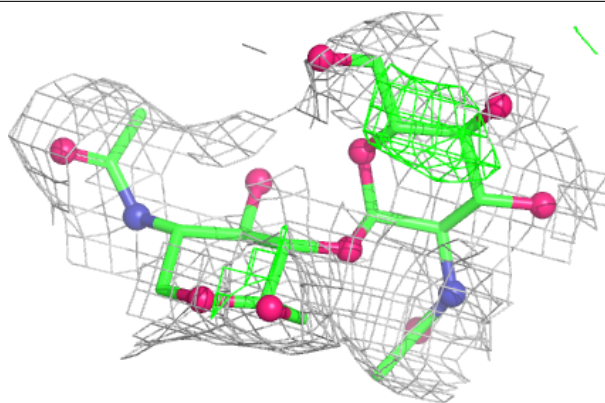
Electron density around Chain G:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



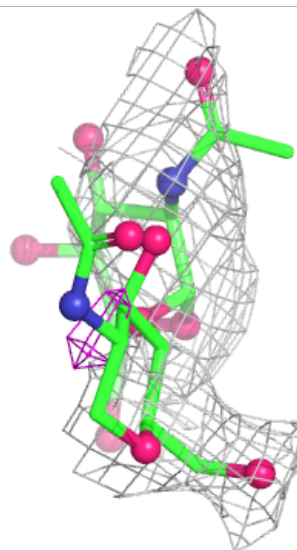
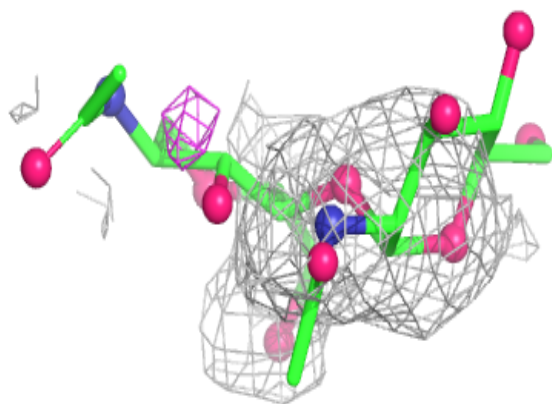
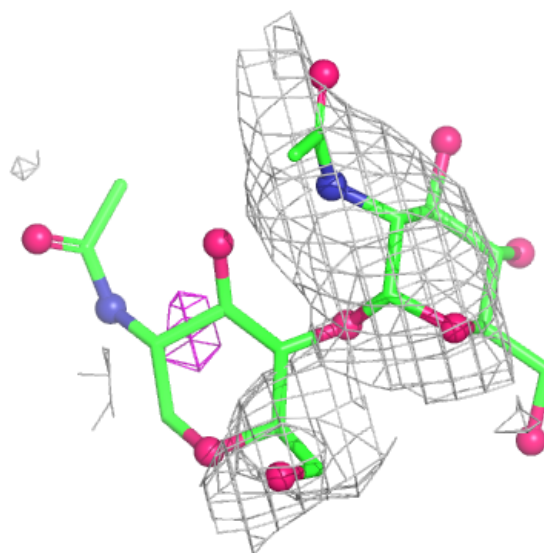
Electron density around Chain J:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



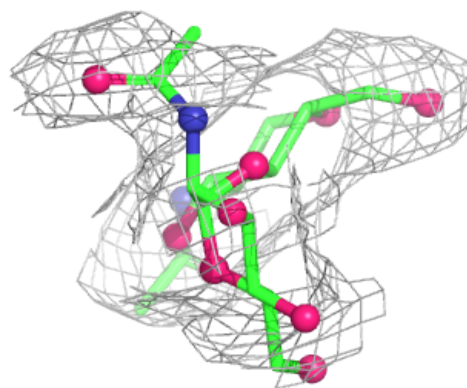
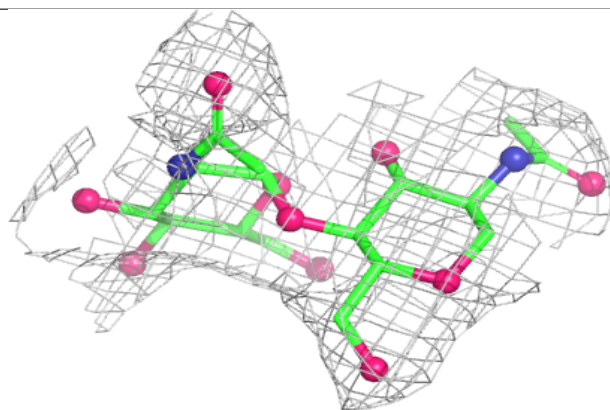
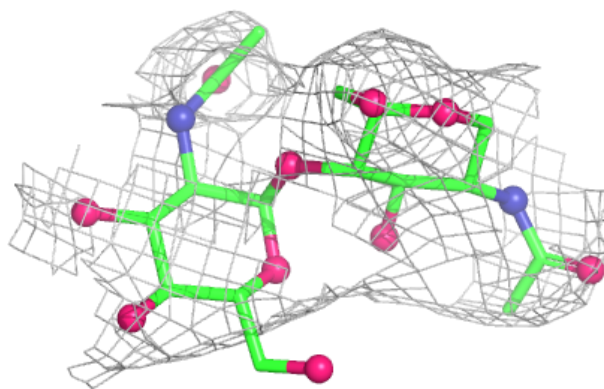
Electron density around Chain L:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



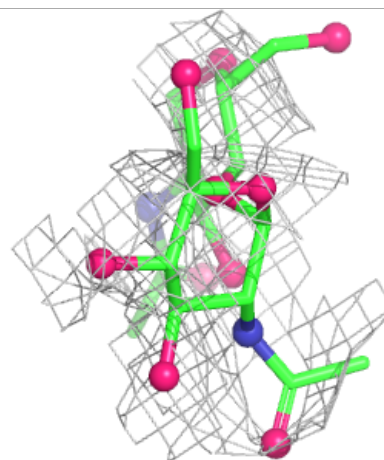
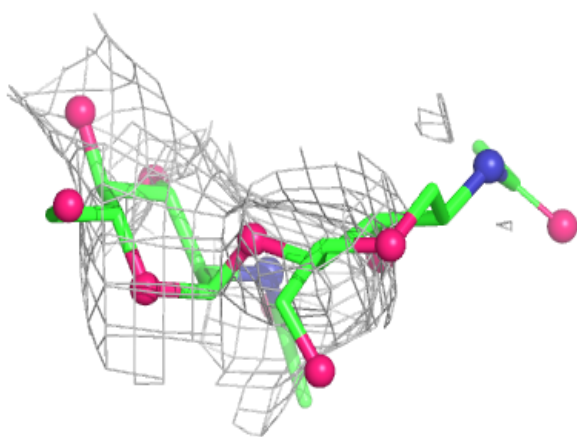
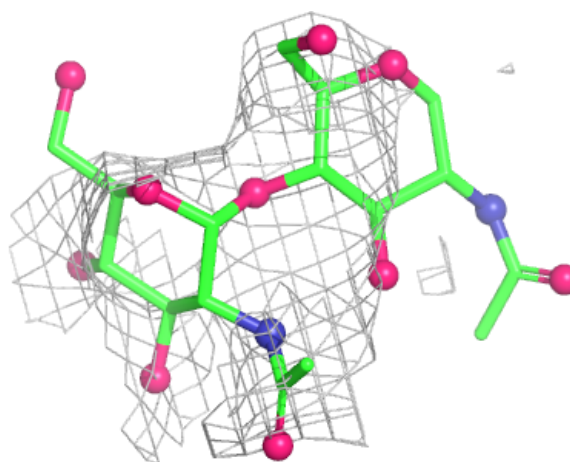
Electron density around Chain O:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



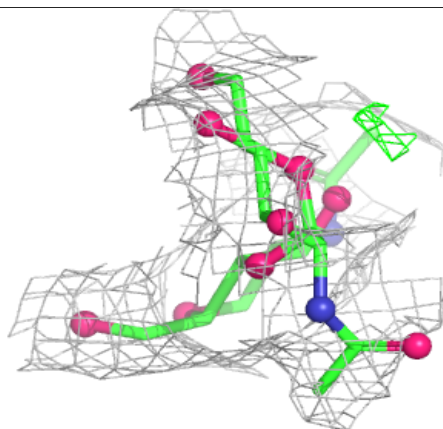
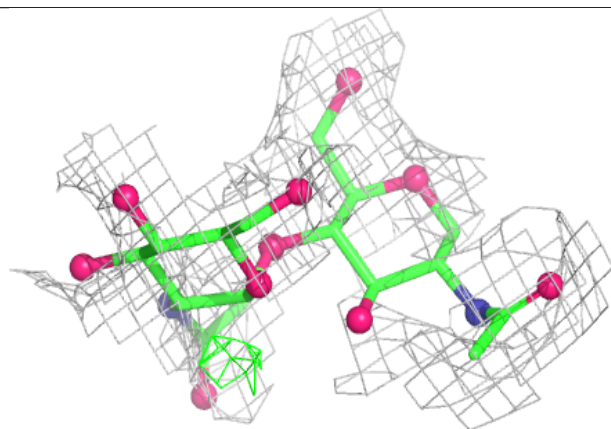
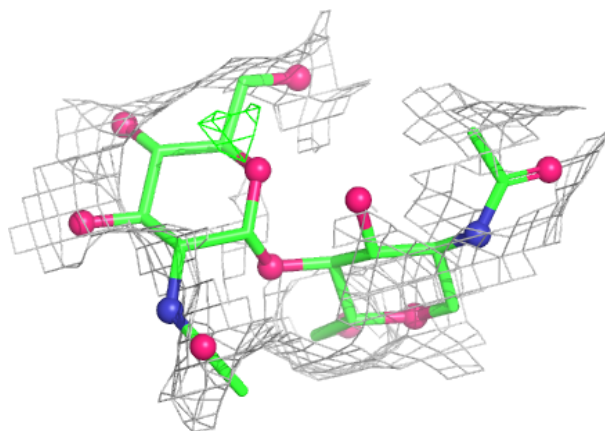
Electron density around Chain Q:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



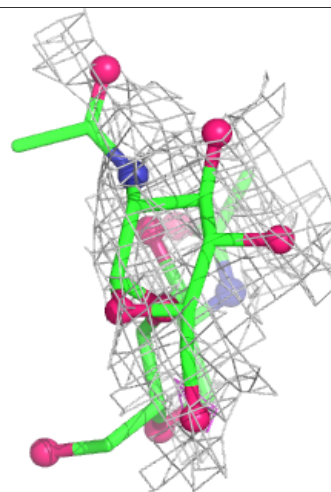
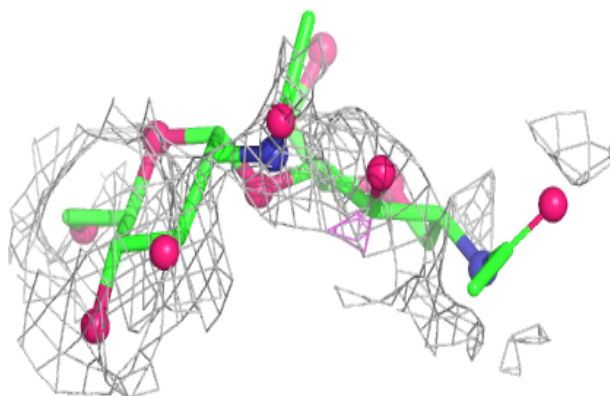
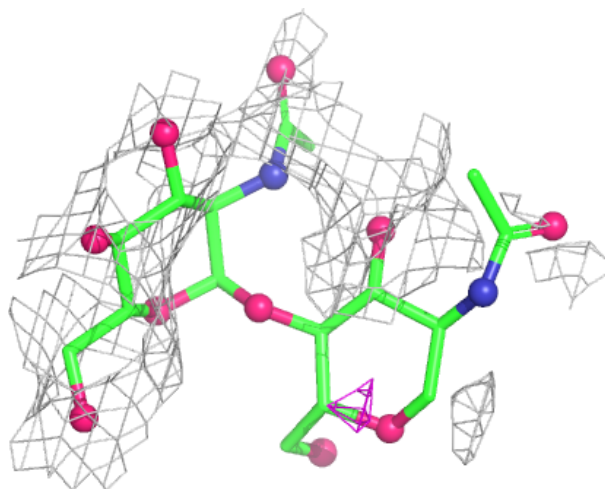
Electron density around Chain T:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



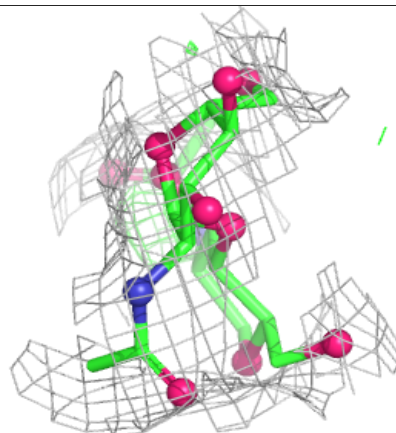
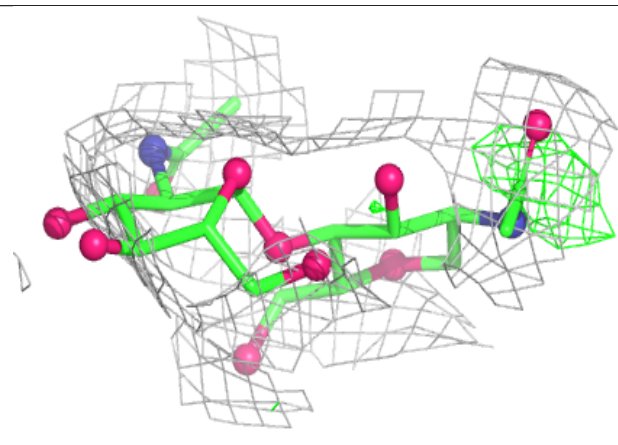
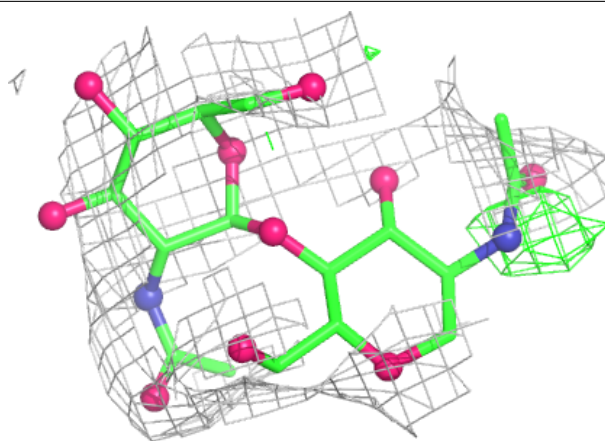
Electron density around Chain V:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



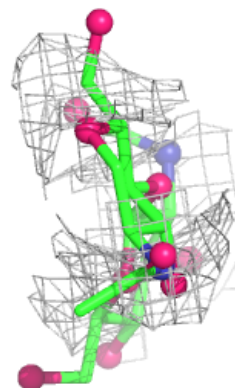
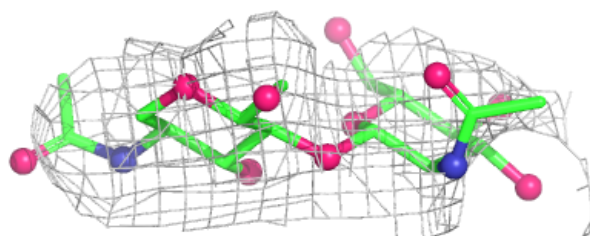
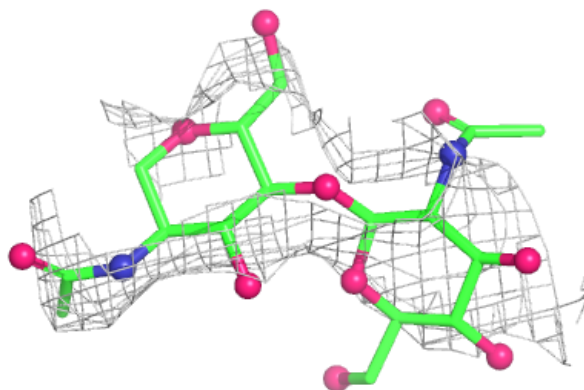
Electron density around Chain F:

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 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

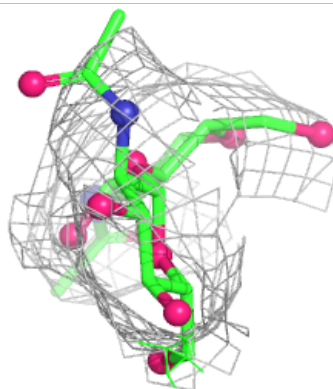
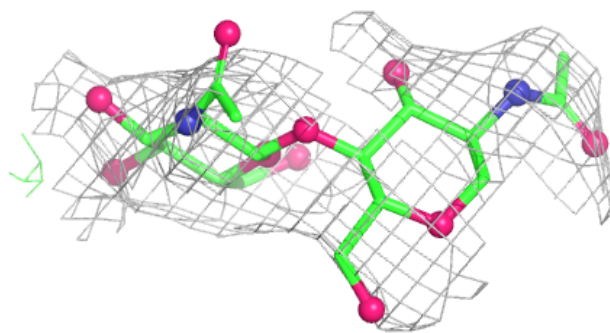
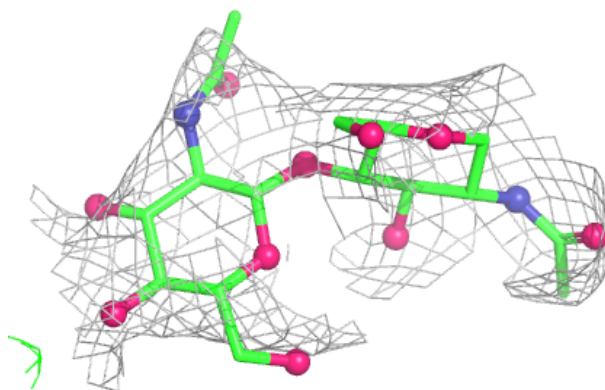


Electron density around Chain H:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

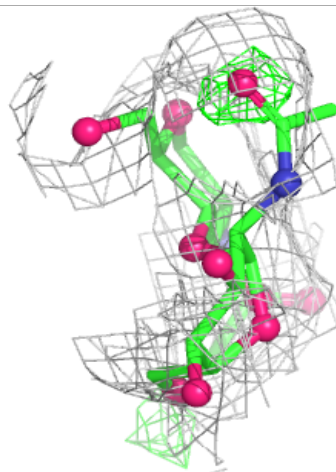
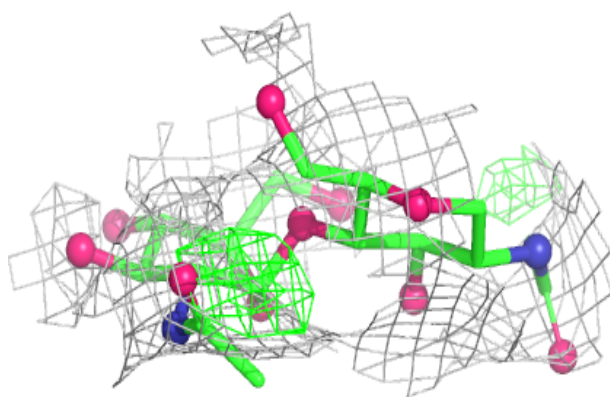
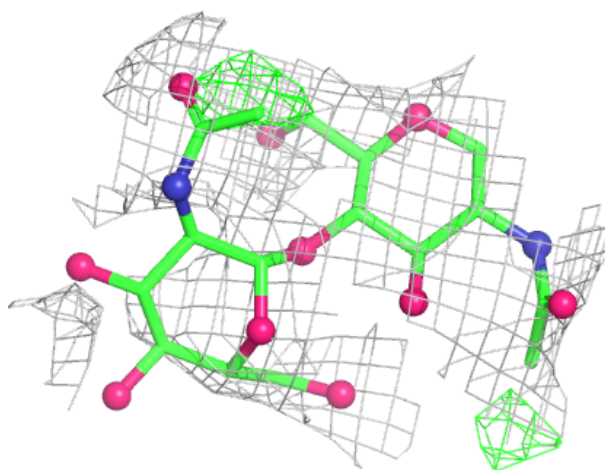
**Electron density around Chain I:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



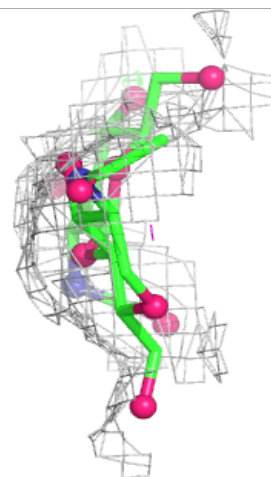
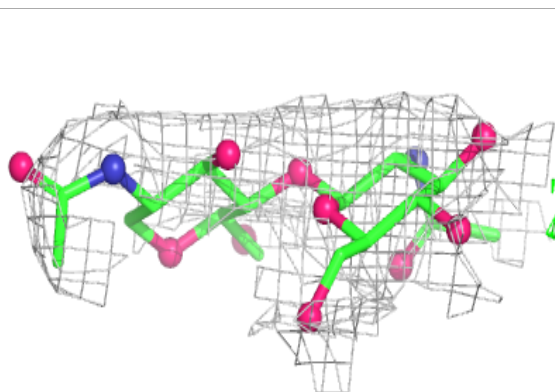
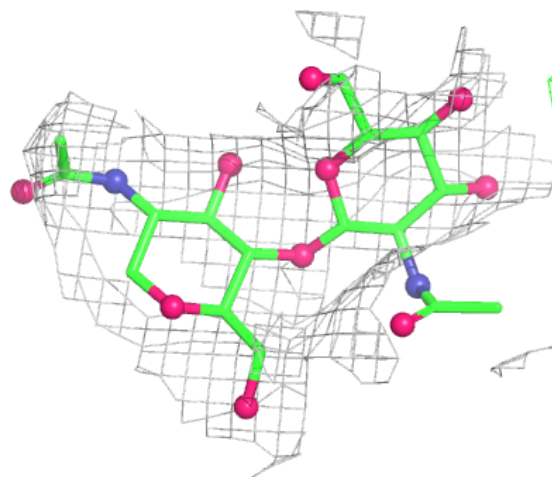
Electron density around Chain K:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



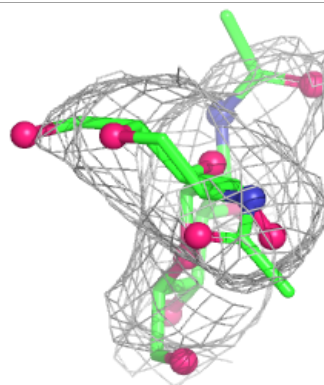
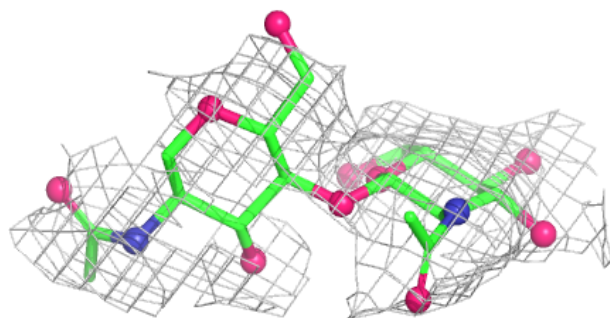
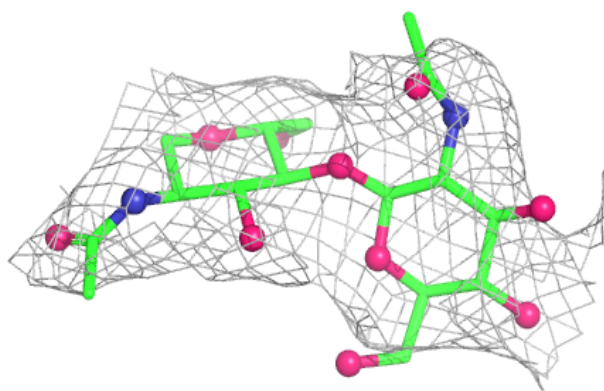
Electron density around Chain M:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

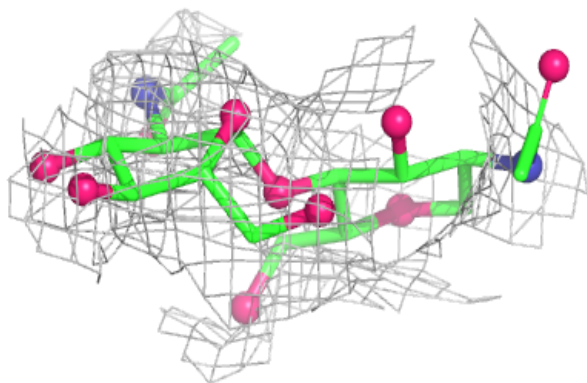
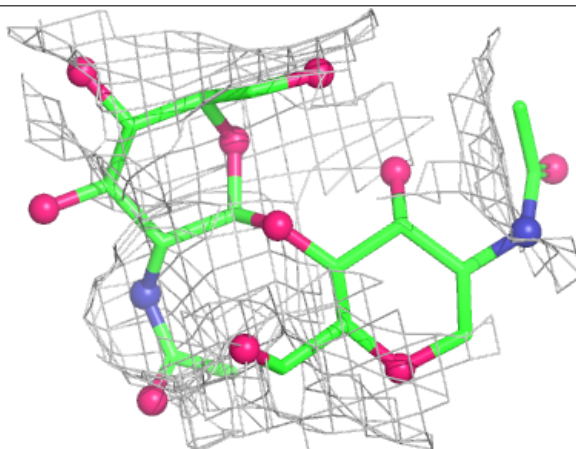


Electron density around Chain N:

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and green (positive)

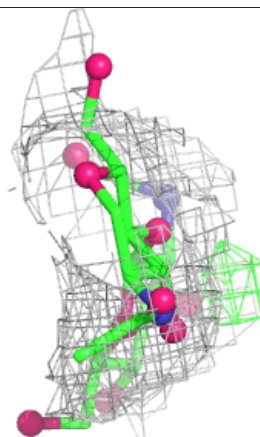
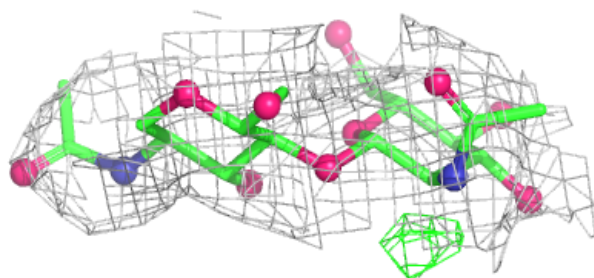
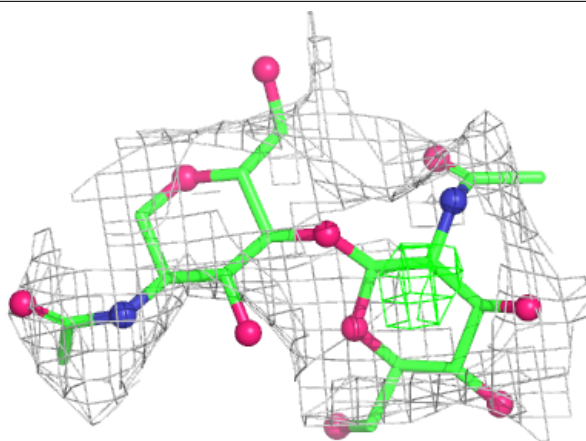
**Electron density around Chain P:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

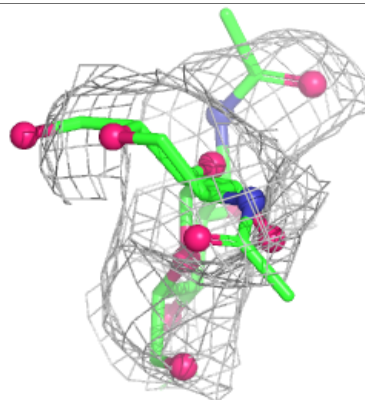
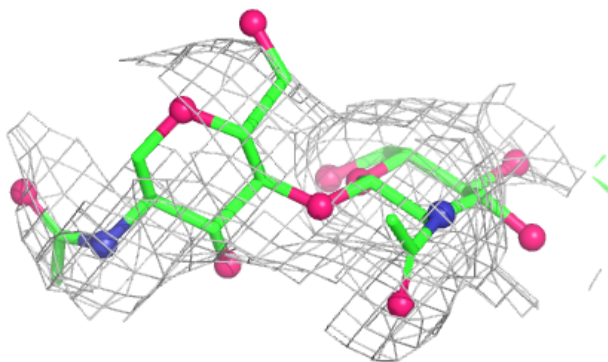
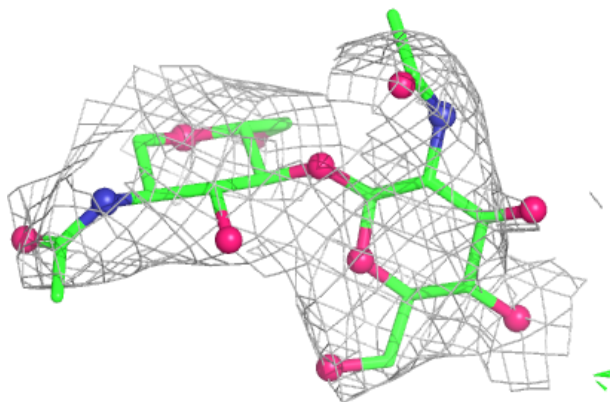


Electron density around Chain R:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

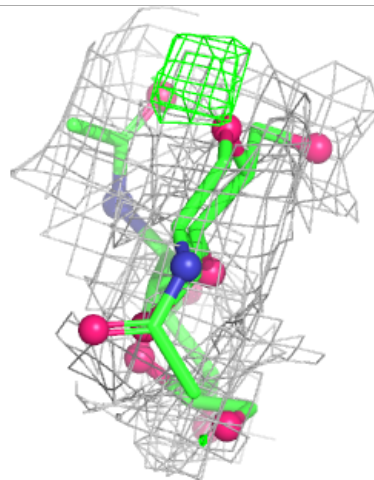
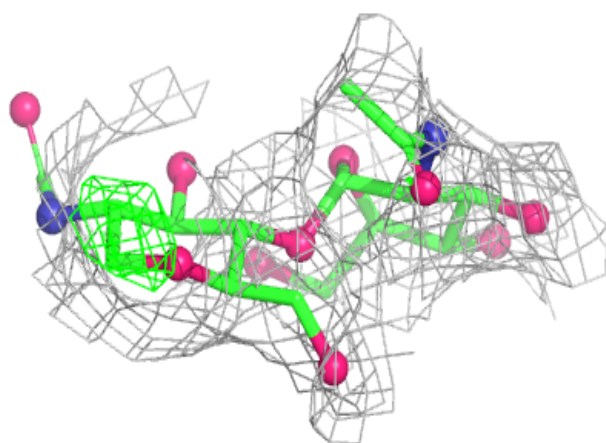
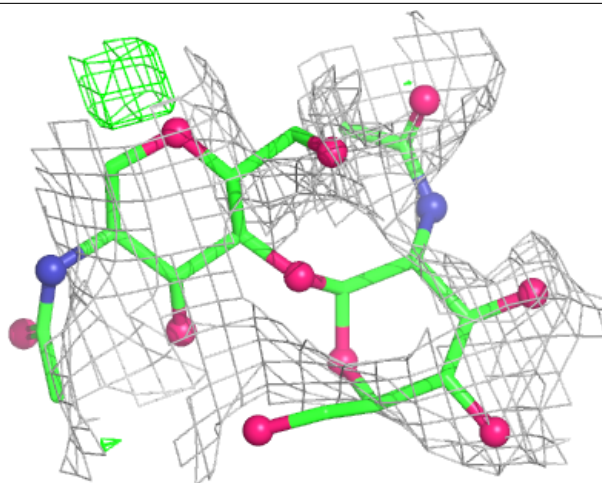
**Electron density around Chain S:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



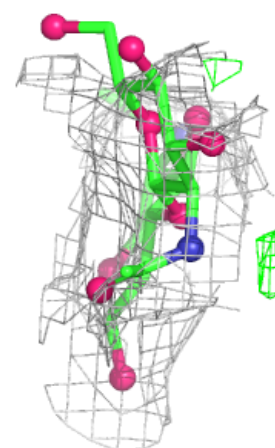
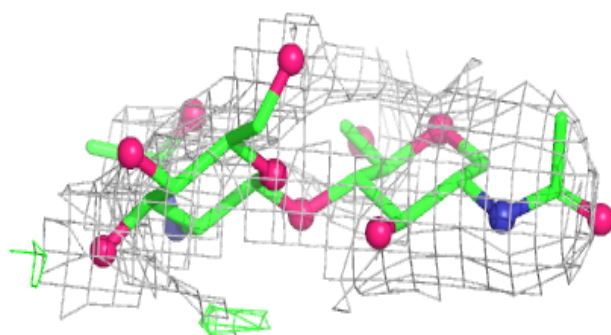
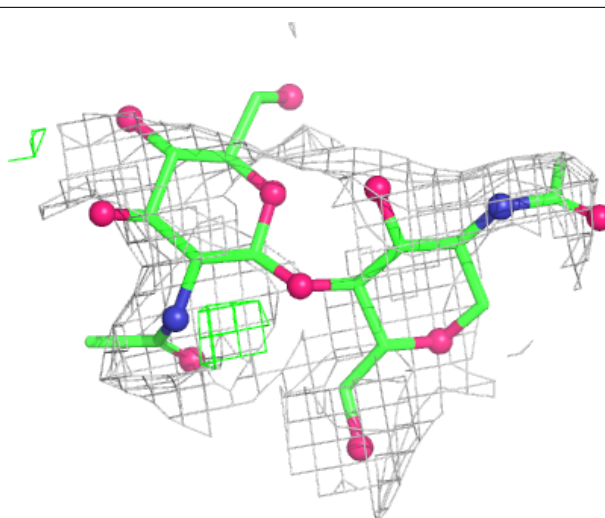
Electron density around Chain U:

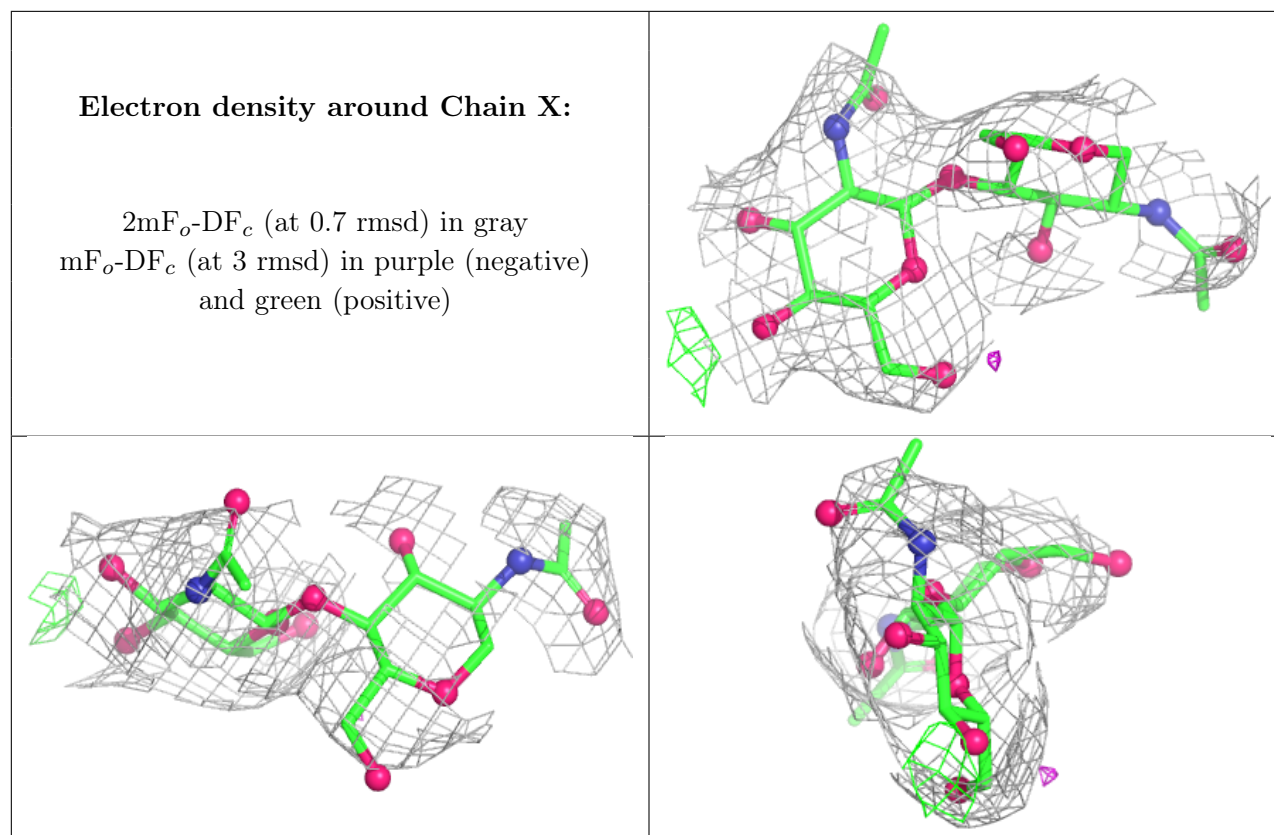
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain W:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	NAG	A	1760	14/15	0.15	0.21	155,155,155,155	0
4	NAG	B	2760	14/15	0.16	0.15	155,155,155,155	0
4	NAG	C	3760	14/15	0.29	0.19	155,155,155,155	0
4	NAG	D	4760	14/15	0.41	0.19	155,155,155,155	0
4	NAG	D	4759	14/15	0.73	0.13	57,57,57,57	0
4	NAG	B	2759	14/15	0.80	0.11	57,57,57,57	0
4	NAG	A	1759	14/15	0.83	0.11	57,57,57,57	0
4	NAG	C	3759	14/15	0.84	0.12	57,57,57,57	0
5	ZN	C	3752	1/1	0.93	0.15	52,52,52,52	0
5	ZN	B	2751	1/1	0.94	0.12	52,52,52,52	0
5	ZN	D	4752	1/1	0.94	0.08	52,52,52,52	0
5	ZN	D	4751	1/1	0.95	0.05	52,52,52,52	0
5	ZN	A	1752	1/1	0.96	0.08	52,52,52,52	0
5	ZN	B	2752	1/1	0.97	0.14	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	ZN	C	3751	1/1	0.98	0.06	52,52,52,52	0
5	ZN	A	1751	1/1	0.98	0.06	52,52,52,52	0

6.5 Other polymers [i](#)

There are no such residues in this entry.