



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 05:25 AM UTC

PDB ID : 8IOX / pdb_00008iox
Title : Escherichia coli OpgD mutant-D388N
Authors : Motouchi, S.; Nakajima, M.
Deposited on : 2023-03-13
Resolution : 2.95 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)
Xtrriage (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

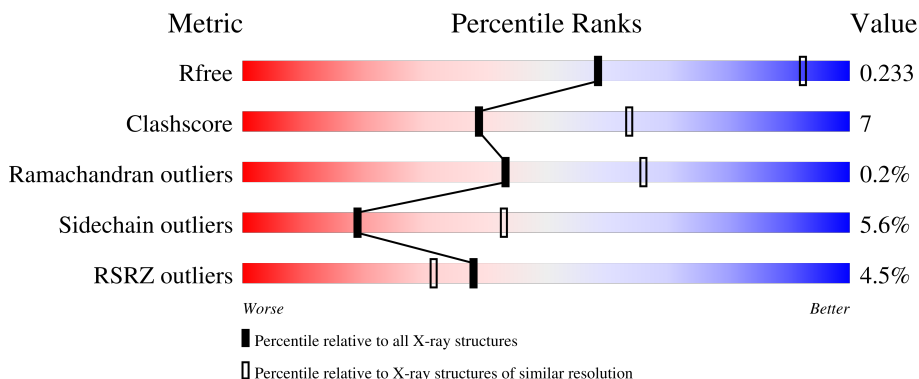
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.95 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.



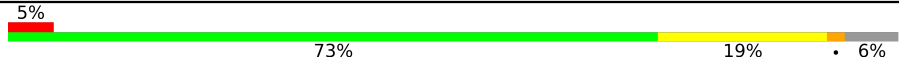

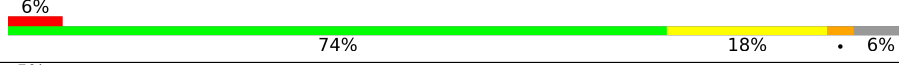



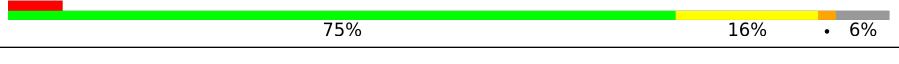
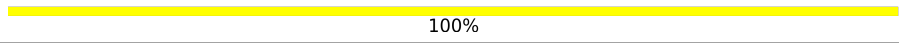
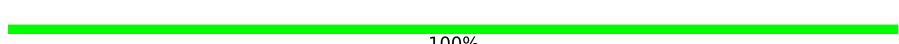
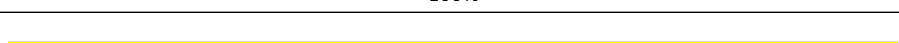
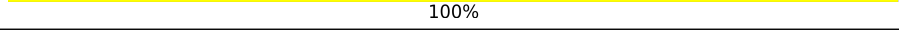
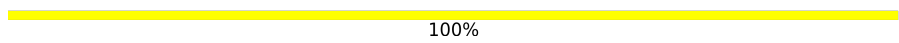

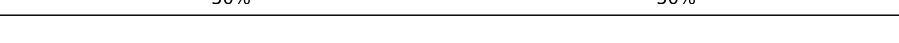
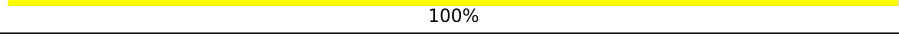
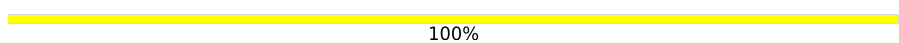
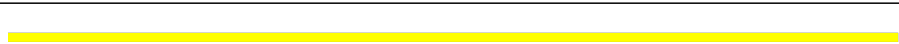
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1130 (2.98-2.94)
Clashscore	190562	1157 (2.98-2.94)
Ramachandran outliers	187476	1101 (2.98-2.94)
Sidechain outliers	187428	1101 (2.98-2.94)
RSRZ outliers	180081	1130 (2.98-2.94)

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	559	 3% 75% 18% • 6%
1	B	559	 6% 75% 17% • 6%
1	C	559	 4% 74% 18% • 6%
1	D	559	 3% 72% 20% • 6%
1	E	559	 3% 76% 16% • 6%

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Mol	Chain	Length	Quality of chain
1	F	559	 5% 73% 19% • 6%
1	G	559	 3% 76% 16% • 6%
1	H	559	 6% 74% 18% • 6%
1	I	559	 5% 72% 19% • 6%
1	J	559	 3% 75% 18% • 6%
1	K	559	 4% 74% 18% • 6%
1	L	559	 6% 75% 16% • 6%
2	M	2	 100%
2	N	2	 100%
2	O	2	 100%
2	P	2	 100%
2	Q	2	 50% 50%
2	R	2	 100%
2	S	2	 100%
2	T	2	 100%
2	U	2	 100%
2	V	2	 100%

2 Entry composition i

There are 3 unique types of molecules in this entry. The entry contains 51848 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 Glucans biosynthesis protein D.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	524	4246	2704	738	780	24	0	0	0
1	B	524	4246	2704	738	780	24	0	0	0
1	C	524	4246	2704	738	780	24	0	0	0
1	D	524	4246	2704	738	780	24	0	0	0
1	E	524	4246	2704	738	780	24	0	0	0
1	F	524	4246	2704	738	780	24	0	0	0
1	G	524	4246	2704	738	780	24	0	0	0
1	H	524	4246	2704	738	780	24	0	0	0
1	I	524	4246	2704	738	780	24	0	0	0
1	J	524	4246	2704	738	780	24	0	0	0
1	K	524	4246	2704	738	780	24	0	0	0
1	L	524	4246	2704	738	780	24	0	0	0

There are 108 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	388	ASN	ASP	engineered mutation	UNP P40120
A	552	LEU	-	expression tag	UNP P40120
A	553	GLU	-	expression tag	UNP P40120
A	554	HIS	-	expression tag	UNP P40120
A	555	HIS	-	expression tag	UNP P40120

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Chain	Residue	Modelled	Actual	Comment	Reference
A	556	HIS	-	expression tag	UNP P40120
A	557	HIS	-	expression tag	UNP P40120
A	558	HIS	-	expression tag	UNP P40120
A	559	HIS	-	expression tag	UNP P40120
B	388	ASN	ASP	engineered mutation	UNP P40120
B	552	LEU	-	expression tag	UNP P40120
B	553	GLU	-	expression tag	UNP P40120
B	554	HIS	-	expression tag	UNP P40120
B	555	HIS	-	expression tag	UNP P40120
B	556	HIS	-	expression tag	UNP P40120
B	557	HIS	-	expression tag	UNP P40120
B	558	HIS	-	expression tag	UNP P40120
B	559	HIS	-	expression tag	UNP P40120
C	388	ASN	ASP	engineered mutation	UNP P40120
C	552	LEU	-	expression tag	UNP P40120
C	553	GLU	-	expression tag	UNP P40120
C	554	HIS	-	expression tag	UNP P40120
C	555	HIS	-	expression tag	UNP P40120
C	556	HIS	-	expression tag	UNP P40120
C	557	HIS	-	expression tag	UNP P40120
C	558	HIS	-	expression tag	UNP P40120
C	559	HIS	-	expression tag	UNP P40120
D	388	ASN	ASP	engineered mutation	UNP P40120
D	552	LEU	-	expression tag	UNP P40120
D	553	GLU	-	expression tag	UNP P40120
D	554	HIS	-	expression tag	UNP P40120
D	555	HIS	-	expression tag	UNP P40120
D	556	HIS	-	expression tag	UNP P40120
D	557	HIS	-	expression tag	UNP P40120
D	558	HIS	-	expression tag	UNP P40120
D	559	HIS	-	expression tag	UNP P40120
E	388	ASN	ASP	engineered mutation	UNP P40120
E	552	LEU	-	expression tag	UNP P40120
E	553	GLU	-	expression tag	UNP P40120
E	554	HIS	-	expression tag	UNP P40120
E	555	HIS	-	expression tag	UNP P40120
E	556	HIS	-	expression tag	UNP P40120
E	557	HIS	-	expression tag	UNP P40120
E	558	HIS	-	expression tag	UNP P40120
E	559	HIS	-	expression tag	UNP P40120
F	388	ASN	ASP	engineered mutation	UNP P40120
F	552	LEU	-	expression tag	UNP P40120

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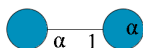
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F	554	HIS	-	expression tag	UNP P40120
F	555	HIS	-	expression tag	UNP P40120
F	556	HIS	-	expression tag	UNP P40120
F	557	HIS	-	expression tag	UNP P40120
F	558	HIS	-	expression tag	UNP P40120
F	559	HIS	-	expression tag	UNP P40120
G	388	ASN	ASP	engineered mutation	UNP P40120
G	552	LEU	-	expression tag	UNP P40120
G	553	GLU	-	expression tag	UNP P40120
G	554	HIS	-	expression tag	UNP P40120
G	555	HIS	-	expression tag	UNP P40120
G	556	HIS	-	expression tag	UNP P40120
G	557	HIS	-	expression tag	UNP P40120
G	558	HIS	-	expression tag	UNP P40120
G	559	HIS	-	expression tag	UNP P40120
H	388	ASN	ASP	engineered mutation	UNP P40120
H	552	LEU	-	expression tag	UNP P40120
H	553	GLU	-	expression tag	UNP P40120
H	554	HIS	-	expression tag	UNP P40120
H	555	HIS	-	expression tag	UNP P40120
H	556	HIS	-	expression tag	UNP P40120
H	557	HIS	-	expression tag	UNP P40120
H	558	HIS	-	expression tag	UNP P40120
H	559	HIS	-	expression tag	UNP P40120
I	388	ASN	ASP	engineered mutation	UNP P40120
I	552	LEU	-	expression tag	UNP P40120
I	553	GLU	-	expression tag	UNP P40120
I	554	HIS	-	expression tag	UNP P40120
I	555	HIS	-	expression tag	UNP P40120
I	556	HIS	-	expression tag	UNP P40120
I	557	HIS	-	expression tag	UNP P40120
I	558	HIS	-	expression tag	UNP P40120
I	559	HIS	-	expression tag	UNP P40120
J	388	ASN	ASP	engineered mutation	UNP P40120
J	552	LEU	-	expression tag	UNP P40120
J	553	GLU	-	expression tag	UNP P40120
J	554	HIS	-	expression tag	UNP P40120
J	555	HIS	-	expression tag	UNP P40120
J	556	HIS	-	expression tag	UNP P40120
J	557	HIS	-	expression tag	UNP P40120
J	558	HIS	-	expression tag	UNP P40120

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Chain	Residue	Modelled	Actual	Comment	Reference
J	559	HIS	-	expression tag	UNP P40120
K	388	ASN	ASP	engineered mutation	UNP P40120
K	552	LEU	-	expression tag	UNP P40120
K	553	GLU	-	expression tag	UNP P40120
K	554	HIS	-	expression tag	UNP P40120
K	555	HIS	-	expression tag	UNP P40120
K	556	HIS	-	expression tag	UNP P40120
K	557	HIS	-	expression tag	UNP P40120
K	558	HIS	-	expression tag	UNP P40120
K	559	HIS	-	expression tag	UNP P40120
L	388	ASN	ASP	engineered mutation	UNP P40120
L	552	LEU	-	expression tag	UNP P40120
L	553	GLU	-	expression tag	UNP P40120
L	554	HIS	-	expression tag	UNP P40120
L	555	HIS	-	expression tag	UNP P40120
L	556	HIS	-	expression tag	UNP P40120
L	557	HIS	-	expression tag	UNP P40120
L	558	HIS	-	expression tag	UNP P40120
L	559	HIS	-	expression tag	UNP P40120

- Molecule 2 is an oligosaccharide called alpha-D-glucopyranose-(1-1)-alpha-D-glucopyranose.



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	M	2	Total	C	O	0	0	0
			23	12	11			
2	N	2	Total	C	O	0	0	0
			23	12	11			
2	O	2	Total	C	O	0	0	0
			23	12	11			
2	P	2	Total	C	O	0	0	0
			23	12	11			
2	Q	2	Total	C	O	0	0	0
			23	12	11			
2	R	2	Total	C	O	0	0	0
			23	12	11			
2	S	2	Total	C	O	0	0	0
			23	12	11			

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	T	2	Total	C	O	0	0	0
			23	12	11			
2	U	2	Total	C	O	0	0	0
			23	12	11			
2	V	2	Total	C	O	0	0	0
			23	12	11			

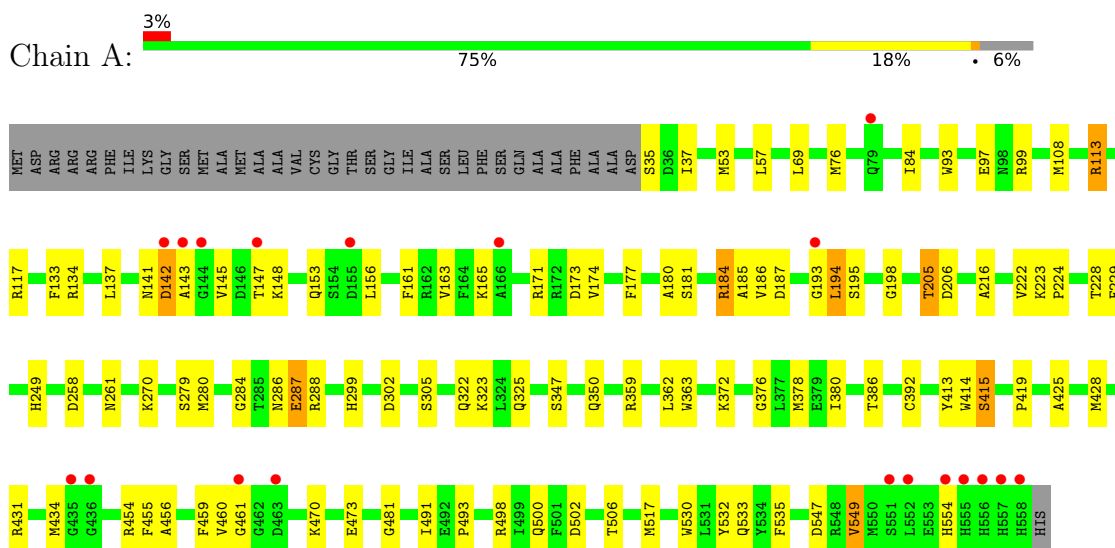
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	64	Total	O	0	0
			64	64		
3	B	43	Total	O	0	0
			43	43		
3	C	47	Total	O	0	0
			47	47		
3	D	71	Total	O	0	0
			71	71		
3	E	74	Total	O	0	0
			74	74		
3	F	52	Total	O	0	0
			52	52		
3	G	78	Total	O	0	0
			78	78		
3	H	42	Total	O	0	0
			42	42		
3	I	37	Total	O	0	0
			37	37		
3	J	66	Total	O	0	0
			66	66		
3	K	56	Total	O	0	0
			56	56		
3	L	36	Total	O	0	0
			36	36		

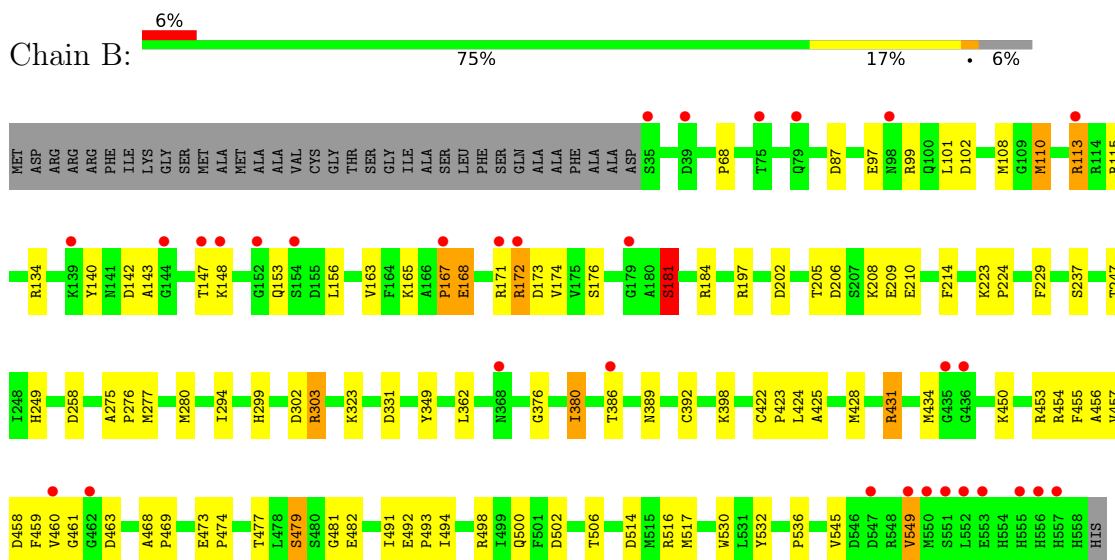
3 Residue-property plots

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.

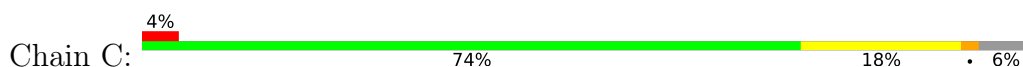
- Molecule 1: Glucans biosynthesis protein D

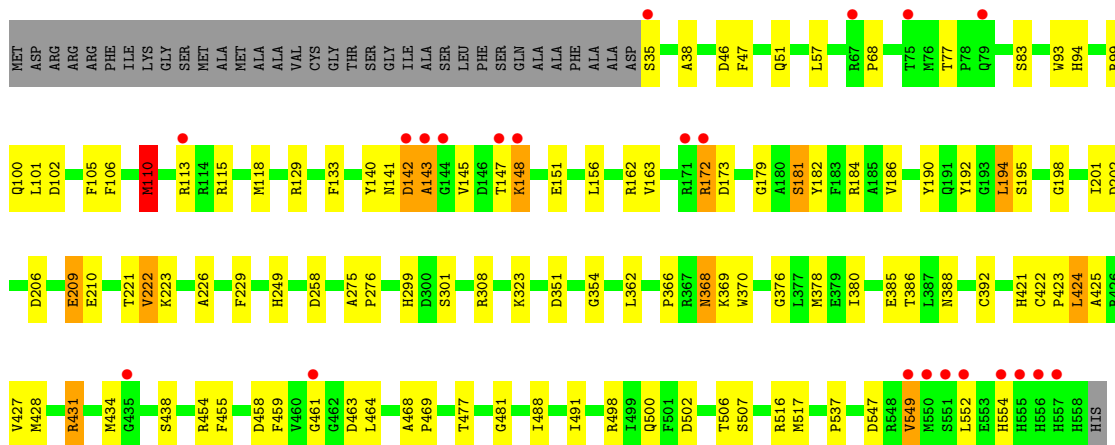


- Molecule 1: Glucans biosynthesis protein D

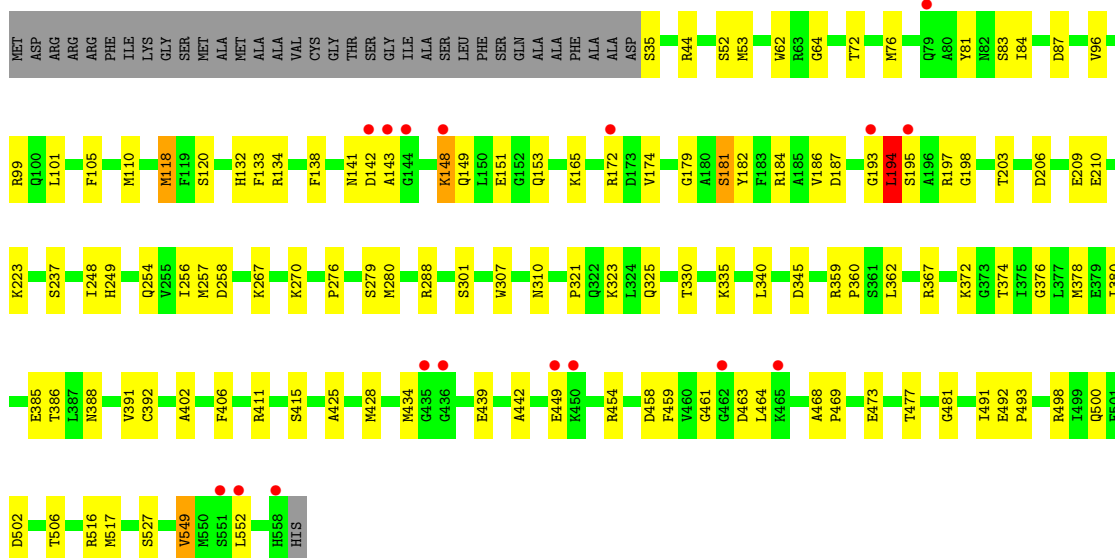
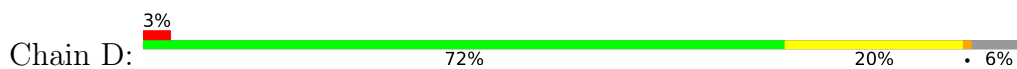


- Molecule 1: Glucans biosynthesis protein D

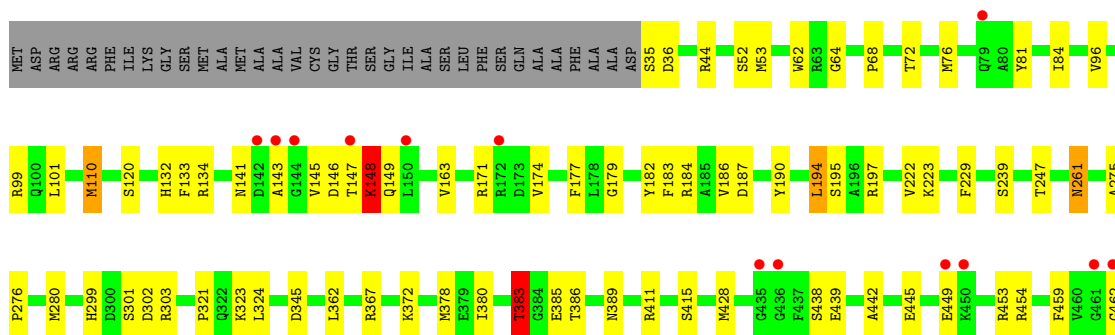
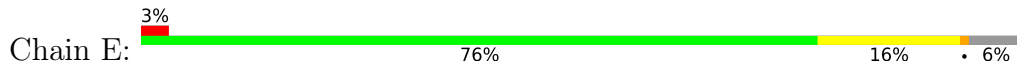




• Molecule 1: Glucans biosynthesis protein D

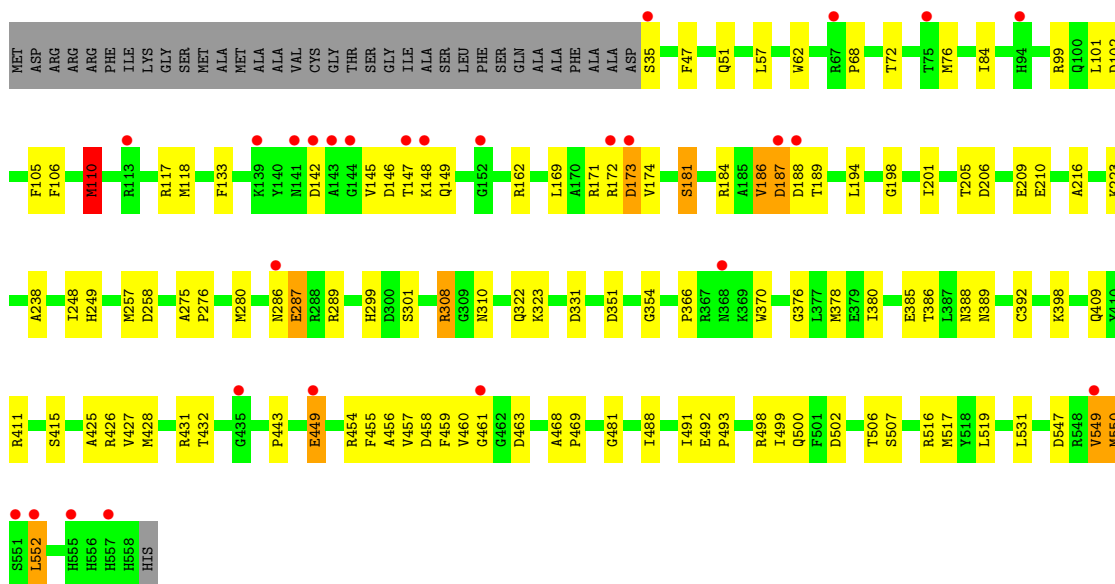


• Molecule 1: Glucans biosynthesis protein D

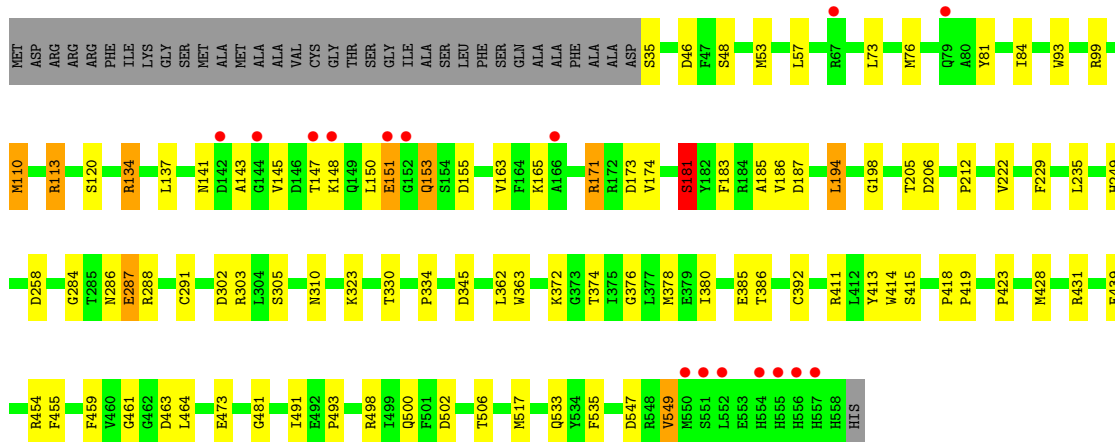
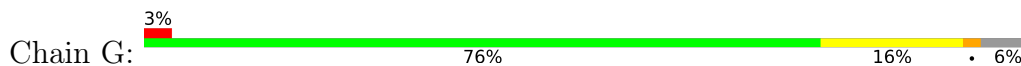




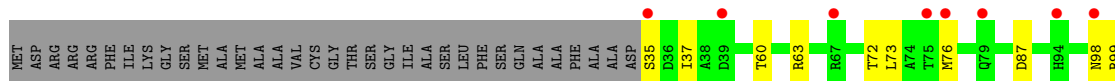
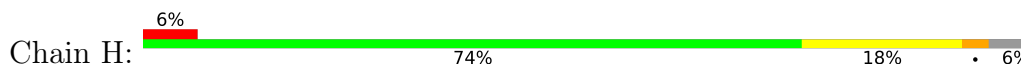
• Molecule 1: Glucans biosynthesis protein D

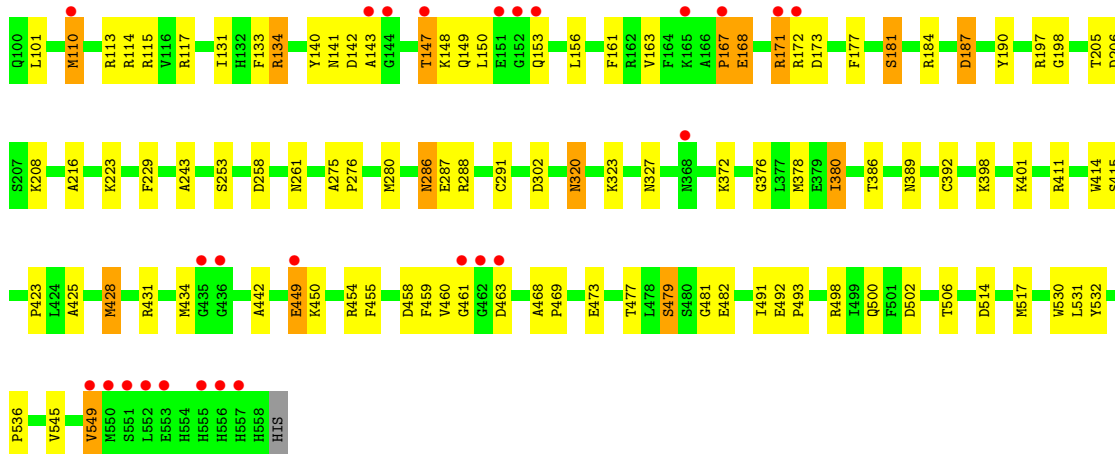


• Molecule 1: Glucans biosynthesis protein D

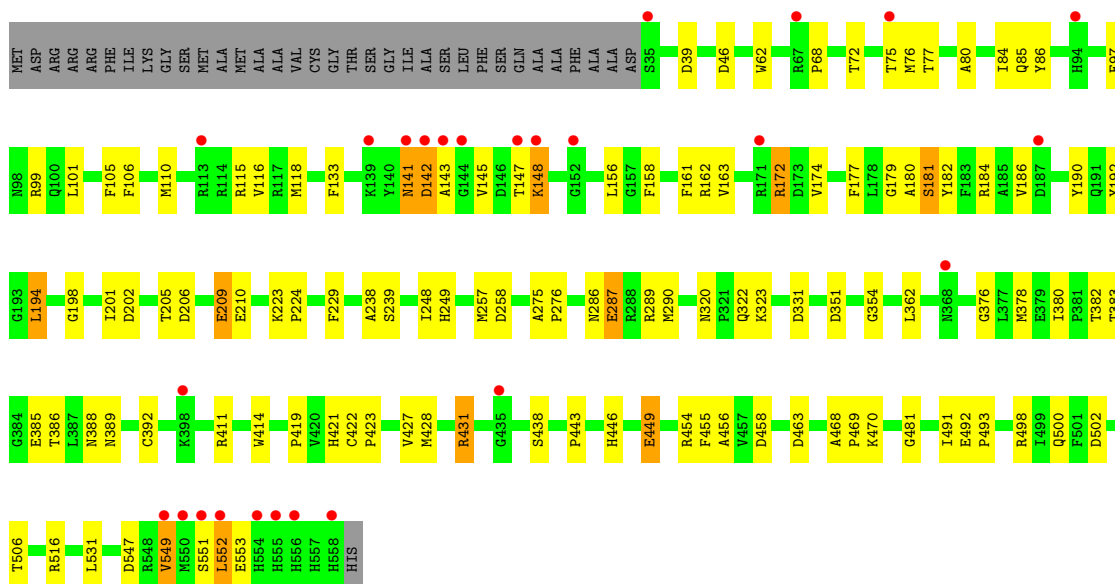


• Molecule 1: Glucans biosynthesis protein D

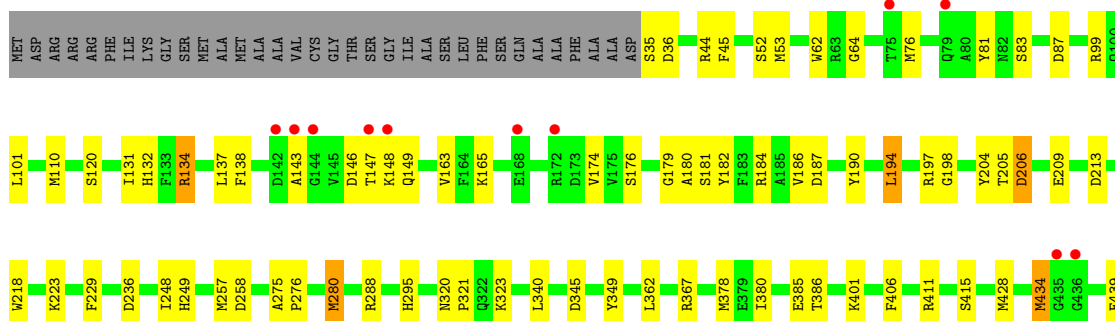
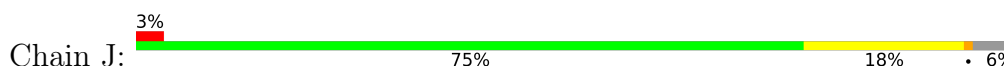




● Molecule 1: Glucans biosynthesis protein D



● Molecule 1: Glucans biosynthesis protein D



GLC1
GLC2

- Molecule 2: alpha-D-glucopyranose-(1-1)-alpha-D-glucopyranose

Chain N:  100%GLC1
GLC2

- Molecule 2: alpha-D-glucopyranose-(1-1)-alpha-D-glucopyranose

Chain O:  100%GLC1
GLC2

- Molecule 2: alpha-D-glucopyranose-(1-1)-alpha-D-glucopyranose

Chain P:  100%GLC1
GLC2

- Molecule 2: alpha-D-glucopyranose-(1-1)-alpha-D-glucopyranose

Chain Q:  50% 50%GLC1
GLC2

- Molecule 2: alpha-D-glucopyranose-(1-1)-alpha-D-glucopyranose

Chain R:  100%GLC1
GLC2


- Molecule 2: alpha-D-glucopyranose-(1-1)-alpha-D-glucopyranose

Chain S:  100%GLC1
GLC2

- Molecule 2: alpha-D-glucopyranose-(1-1)-alpha-D-glucopyranose

Chain T:  100%GLC1
GLC2

- Molecule 2: alpha-D-glucopyranose-(1-1)-alpha-D-glucopyranose

Chain U:  100%

GLC1
GLC2

- Molecule 2: alpha-D-glucopyranose-(1-1)-alpha-D-glucopyranose

Chain V:  100%

GLC1
GLC2

4 Data and refinement statistics i

Property	Value	Source
Space group	C 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	226.75Å 392.76Å 324.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.14 – 2.95 49.14 – 2.95	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.14-2.95) 99.9 (49.14-2.95)	Depositor EDS
R_{merge}	0.21	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.62 (at 2.96Å)	Xtrriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.194 , 0.232 0.198 , 0.233	Depositor DCC
R_{free} test set	14722 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å ²)	38.1	Xtrriage
Anisotropy	0.008	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 42.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	0.469 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.477 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtrriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	51848	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.76% 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 [i](#)

5.1 Standard geometry [i](#)

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

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	1.02	0/4375	1.31	7/5938 (0.1%)
1	B	1.01	0/4375	1.32	10/5938 (0.2%)
1	C	1.04	2/4375 (0.0%)	1.32	11/5938 (0.2%)
1	D	1.02	1/4375 (0.0%)	1.32	9/5938 (0.2%)
1	E	1.02	1/4375 (0.0%)	1.31	10/5938 (0.2%)
1	F	1.03	2/4375 (0.0%)	1.31	12/5938 (0.2%)
1	G	1.02	1/4375 (0.0%)	1.32	12/5938 (0.2%)
1	H	1.03	1/4375 (0.0%)	1.34	9/5938 (0.2%)
1	I	1.03	3/4375 (0.1%)	1.34	11/5938 (0.2%)
1	J	1.03	1/4375 (0.0%)	1.32	10/5938 (0.2%)
1	K	1.02	1/4375 (0.0%)	1.31	5/5938 (0.1%)
1	L	1.02	1/4375 (0.0%)	1.33	9/5938 (0.2%)
All	All	1.02	14/52500 (0.0%)	1.32	115/71256 (0.2%)

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	427	VAL	C-O	-5.61	1.18	1.24
1	F	68	PRO	C-O	-5.48	1.17	1.23
1	I	68	PRO	C-O	-5.46	1.17	1.23
1	C	427	VAL	C-O	-5.41	1.18	1.24
1	H	197	ARG	C-O	5.36	1.30	1.23
1	J	340	LEU	C-O	5.36	1.30	1.23
1	G	334	PRO	C-O	-5.27	1.17	1.23
1	I	427	VAL	C-O	-5.22	1.18	1.24
1	D	340	LEU	C-O	5.21	1.30	1.23
1	I	419	PRO	C-O	-5.18	1.18	1.24
1	K	334	PRO	C-O	-5.14	1.17	1.23
1	E	68	PRO	C-O	-5.09	1.17	1.23
1	L	334	PRO	C-O	-5.02	1.18	1.23
1	C	68	PRO	C-O	-5.00	1.18	1.23

All (115) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	141	ASN	CB-CA-C	-8.30	107.00	116.63
1	H	536	PRO	N-CA-CB	7.64	107.47	103.19
1	B	536	PRO	N-CA-CB	7.26	107.25	103.19
1	H	423	PRO	N-CA-C	-7.16	107.23	114.68
1	L	141	ASN	CB-CA-C	-7.12	108.37	116.63
1	L	536	PRO	N-CA-CB	7.06	107.14	103.19
1	I	547	ASP	CA-CB-CG	6.94	119.54	112.60
1	C	547	ASP	CA-CB-CG	6.89	119.49	112.60
1	G	181	SER	N-CA-C	-6.89	104.18	112.59
1	G	141	ASN	CB-CA-C	-6.86	106.73	116.34
1	L	423	PRO	N-CA-C	-6.78	107.63	114.68
1	K	302	ASP	CA-CB-CG	6.62	119.22	112.60
1	I	423	PRO	N-CA-C	-6.58	107.84	114.68
1	G	345	ASP	CA-CB-CG	6.55	119.15	112.60
1	I	209	GLU	CB-CG-CD	6.52	123.69	112.60
1	D	406	PHE	CA-C-O	-6.30	113.94	120.99
1	I	110	MET	CB-CA-C	-6.24	109.36	116.54
1	C	209	GLU	CB-CG-CD	6.12	123.01	112.60
1	L	110	MET	CB-CA-C	-6.12	109.51	116.54
1	E	171	ARG	CA-C-N	-6.07	114.16	123.14
1	E	171	ARG	C-N-CA	-6.07	114.16	123.14
1	B	110	MET	CB-CA-C	-5.98	109.66	116.54
1	H	223	LYS	CB-CA-C	5.97	118.89	109.27
1	A	547	ASP	CA-CB-CG	5.95	118.55	112.60
1	K	334	PRO	CA-C-O	-5.94	114.57	121.34
1	G	547	ASP	CA-CB-CG	5.94	118.54	112.60
1	E	36	ASP	CA-CB-CG	5.93	118.53	112.60
1	D	223	LYS	CB-CA-C	5.91	117.98	109.11
1	C	308	ARG	CA-C-N	5.90	126.49	119.94
1	C	308	ARG	C-N-CA	5.90	126.49	119.94
1	I	449	GLU	CB-CG-CD	5.88	122.59	112.60
1	F	547	ASP	CA-CB-CG	5.88	118.47	112.60
1	I	516	ARG	CB-CA-C	5.84	119.87	109.65
1	I	223	LYS	CB-CA-C	5.82	118.56	109.42
1	G	110	MET	CB-CA-C	-5.81	109.86	116.54
1	G	334	PRO	CA-C-O	-5.79	114.73	121.34
1	B	294	ILE	N-CA-C	-5.79	105.74	112.98
1	E	110	MET	CB-CA-C	-5.79	109.89	116.54
1	D	345	ASP	CA-CB-CG	5.78	118.38	112.60
1	F	110	MET	CB-CA-C	-5.77	109.93	116.63
1	L	331	ASP	CA-CB-CG	5.73	118.33	112.60
1	F	223	LYS	CB-CA-C	5.72	117.68	109.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	331	ASP	CA-CB-CG	5.69	118.29	112.60
1	C	516	ARG	CB-CA-C	5.69	120.00	109.70
1	C	388	ASN	CB-CA-C	5.67	119.29	110.67
1	K	110	MET	CB-CA-C	-5.67	110.06	116.63
1	D	458	ASP	CA-CB-CG	5.64	118.24	112.60
1	G	423	PRO	N-CA-C	-5.63	108.83	114.68
1	H	205	THR	CA-C-N	5.58	128.08	120.54
1	H	205	THR	C-N-CA	5.58	128.08	120.54
1	C	223	LYS	CB-CA-C	5.56	117.43	109.26
1	C	110	MET	CB-CA-C	-5.55	110.16	116.54
1	B	181	SER	N-CA-C	-5.54	106.40	112.72
1	F	516	ARG	CB-CA-C	5.53	119.33	109.65
1	A	180	ALA	CA-C-O	-5.49	115.78	119.68
1	D	181	SER	N-CA-C	-5.49	106.46	112.72
1	H	98	ASN	N-CA-C	-5.44	106.59	113.23
1	D	209	GLU	CB-CG-CD	5.42	121.82	112.60
1	I	331	ASP	CA-CB-CG	5.42	118.02	112.60
1	E	464	LEU	N-CA-C	-5.41	105.54	111.82
1	L	223	LYS	CB-CA-C	5.39	117.95	109.27
1	E	148	LYS	N-CA-C	-5.36	106.91	113.50
1	A	223	LYS	CB-CA-C	5.36	117.14	109.26
1	F	209	GLU	CB-CG-CD	5.35	121.70	112.60
1	K	236	ASP	CA-CB-CG	5.33	117.93	112.60
1	H	187	ASP	CA-CB-CG	5.33	117.93	112.60
1	A	261	ASN	CA-C-N	5.33	130.27	122.39
1	A	261	ASN	C-N-CA	5.33	130.27	122.39
1	A	460	VAL	CA-C-O	-5.32	115.10	121.28
1	J	209	GLU	CB-CG-CD	5.32	121.64	112.60
1	J	406	PHE	CA-C-O	-5.31	115.40	121.40
1	B	423	PRO	N-CA-C	-5.30	107.73	114.35
1	J	206	ASP	CA-CB-CG	5.29	117.89	112.60
1	G	171	ARG	CA-C-N	-5.27	115.35	123.14
1	G	171	ARG	C-N-CA	-5.27	115.35	123.14
1	G	155	ASP	N-CA-C	-5.26	106.86	113.28
1	D	321	PRO	CA-C-O	-5.26	115.60	122.12
1	E	345	ASP	CA-CB-CG	5.25	117.86	112.60
1	J	345	ASP	CA-CB-CG	5.25	117.85	112.60
1	B	223	LYS	CB-CA-C	5.25	117.72	109.27
1	J	223	LYS	CB-CA-C	5.24	116.97	109.11
1	E	321	PRO	CA-C-O	-5.24	115.62	122.12
1	B	474	PRO	N-CA-CB	5.23	106.73	103.23
1	I	388	ASN	CB-CA-C	5.22	119.48	110.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	147	THR	CA-CB-OG1	-5.21	101.78	109.60
1	F	331	ASP	CA-CB-CG	5.19	117.79	112.60
1	B	516	ARG	CB-CA-C	5.18	118.60	109.80
1	B	214	PHE	N-CA-C	-5.15	100.77	108.96
1	J	236	ASP	CA-CB-CG	5.14	117.75	112.60
1	J	321	PRO	CA-C-O	-5.14	115.74	122.12
1	J	288	ARG	CA-C-O	-5.14	116.21	122.64
1	I	39	ASP	CA-CB-CG	5.14	117.74	112.60
1	C	221	THR	CA-C-O	-5.14	115.06	120.92
1	L	205	THR	CA-C-N	5.13	127.41	120.38
1	L	205	THR	C-N-CA	5.13	127.41	120.38
1	K	228	THR	CA-CB-OG1	-5.12	101.92	109.60
1	C	537	PRO	CA-C-N	5.11	127.92	120.51
1	C	537	PRO	C-N-CA	5.11	127.92	120.51
1	F	460	VAL	CA-C-N	-5.11	115.19	121.83
1	F	460	VAL	C-N-CA	-5.11	115.19	121.83
1	J	36	ASP	CA-CB-CG	5.09	117.69	112.60
1	I	180	ALA	CB-CA-C	-5.09	110.69	116.54
1	L	221	THR	CA-C-O	-5.08	115.42	120.96
1	E	547	ASP	CA-CB-CG	5.07	117.67	112.60
1	G	461	GLY	CA-C-O	-5.07	117.32	122.59
1	J	131	ILE	CA-C-O	-5.06	115.12	121.04
1	G	183	PHE	CA-CB-CG	5.06	118.86	113.80
1	A	302	ASP	CA-CB-CG	5.05	117.65	112.60
1	E	383	THR	CB-CA-C	5.05	118.78	109.99
1	D	288	ARG	CA-C-O	-5.04	116.34	122.64
1	F	552	LEU	N-CA-C	-5.04	107.63	112.97
1	F	186	VAL	N-CA-CB	-5.04	106.81	112.45
1	D	388	ASN	CB-CA-C	5.03	118.31	110.67
1	F	308	ARG	CA-C-N	5.02	125.55	119.98
1	F	308	ARG	C-N-CA	5.02	125.55	119.98

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	4246	0	4037	55	0
1	B	4246	0	4037	53	0
1	C	4246	0	4037	66	0
1	D	4246	0	4037	66	0
1	E	4246	0	4037	60	0
1	F	4246	0	4037	64	0
1	G	4246	0	4037	52	0
1	H	4246	0	4037	53	0
1	I	4246	0	4037	62	0
1	J	4246	0	4037	53	0
1	K	4246	0	4037	65	0
1	L	4246	0	4037	62	0
2	M	23	0	21	0	0
2	N	23	0	21	0	0
2	O	23	0	21	0	0
2	P	23	0	21	0	0
2	Q	23	0	21	1	0
2	R	23	0	21	0	0
2	S	23	0	21	0	0
2	T	23	0	21	0	0
2	U	23	0	21	0	0
2	V	23	0	21	0	0
3	A	64	0	0	2	0
3	B	43	0	0	0	0
3	C	47	0	0	1	0
3	D	71	0	0	1	0
3	E	74	0	0	3	0
3	F	52	0	0	1	0
3	G	78	0	0	3	0
3	H	42	0	0	0	0
3	I	37	0	0	3	0
3	J	66	0	0	3	0
3	K	56	0	0	0	0
3	L	36	0	0	0	0
All	All	51848	0	48654	675	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (675) 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:H:491:ILE:HD11	1:H:498:ARG:HB2	1.44	1.00
1:B:425:ALA:HA	1:B:461:GLY:HA3	1.48	0.94
1:C:368:ASN:HD22	1:C:369:LYS:H	0.94	0.93
1:K:491:ILE:HD11	1:K:498:ARG:HB2	1.51	0.90
1:L:491:ILE:HD11	1:L:498:ARG:HB2	1.54	0.89
1:G:491:ILE:HD11	1:G:498:ARG:HB2	1.55	0.87
1:J:491:ILE:HD11	1:J:498:ARG:HB2	1.55	0.87
1:B:491:ILE:HD11	1:B:498:ARG:HB2	1.55	0.86
1:A:491:ILE:HD11	1:A:498:ARG:HB2	1.55	0.86
1:H:168:GLU:HG2	1:H:171:ARG:HG2	1.55	0.86
1:E:491:ILE:HD11	1:E:498:ARG:HB2	1.54	0.86
1:D:491:ILE:HD11	1:D:498:ARG:HB2	1.59	0.85
1:L:481:GLY:HA2	1:L:506:THR:HG23	1.60	0.82
1:I:75:THR:HA	3:I:626:HOH:O	1.79	0.81
1:B:481:GLY:HA2	1:B:506:THR:HG23	1.67	0.77
1:K:378:MET:HE3	1:K:380:ILE:HD11	1.65	0.77
1:D:481:GLY:HA2	1:D:506:THR:HG23	1.67	0.76
1:C:368:ASN:HD22	1:C:369:LYS:N	1.77	0.76
1:J:481:GLY:HA2	1:J:506:THR:HG23	1.68	0.76
1:A:141:ASN:C	1:A:143:ALA:H	1.94	0.75
1:D:81:TYR:HB2	1:D:110:MET:HE3	1.69	0.74
1:C:368:ASN:ND2	1:C:369:LYS:H	1.79	0.74
1:E:323:LYS:HG2	1:F:549:VAL:HG13	1.70	0.73
1:D:72:THR:H	1:D:149:GLN:HE22	1.35	0.73
1:E:132:HIS:HE1	3:E:626:HOH:O	1.71	0.72
1:B:68:PRO:HA	1:B:113:ARG:HH22	1.53	0.72
1:I:194:LEU:HD11	1:I:362:LEU:HB2	1.73	0.71
1:I:320:ASN:HD21	1:I:382:THR:H	1.38	0.70
1:D:194:LEU:HD21	1:D:362:LEU:HB2	1.72	0.70
1:H:481:GLY:HA2	1:H:506:THR:HG23	1.74	0.70
1:D:378:MET:HE3	1:D:380:ILE:HD11	1.74	0.69
1:K:134:ARG:HG3	1:K:137:LEU:HG	1.73	0.69
1:A:194:LEU:HD21	1:A:362:LEU:HB2	1.73	0.69
1:E:481:GLY:HA2	1:E:506:THR:HG23	1.74	0.68
1:H:425:ALA:HA	1:H:461:GLY:HA3	1.74	0.68
1:D:258:ASP:OD1	1:D:411:ARG:HG3	1.92	0.68
1:A:134:ARG:HG3	1:A:137:LEU:HG	1.75	0.68
1:D:132:HIS:HE1	3:D:617:HOH:O	1.77	0.68
1:L:425:ALA:HA	1:L:461:GLY:HA3	1.75	0.68
1:E:378:MET:HE3	1:E:380:ILE:HD11	1.74	0.67
1:D:439:GLU:HG3	1:D:500:GLN:HE22	1.59	0.67
1:C:94:HIS:HB3	3:C:644:HOH:O	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:378:MET:HE3	1:C:380:ILE:HD11	1.78	0.66
1:K:288:ARG:HB3	1:K:291:CYS:SG	2.36	0.65
1:J:190:TYR:CE2	3:J:649:HOH:O	2.48	0.65
1:I:249:HIS:HE1	1:I:258:ASP:OD2	1.79	0.65
1:K:249:HIS:HE1	1:K:258:ASP:OD2	1.79	0.65
1:K:323:LYS:HG2	1:L:549:VAL:HG13	1.78	0.65
1:D:179:GLY:O	1:D:182:TYR:HB2	1.97	0.65
1:G:378:MET:HE3	1:G:380:ILE:HD11	1.79	0.64
1:G:481:GLY:HA2	1:G:506:THR:HG23	1.79	0.64
1:C:249:HIS:HE1	1:C:258:ASP:OD2	1.81	0.64
1:B:168:GLU:HB2	1:B:172:ARG:HH21	1.63	0.64
1:L:140:TYR:O	1:L:143:ALA:HB2	1.98	0.64
1:A:323:LYS:HG2	1:B:549:VAL:HG13	1.79	0.64
1:J:258:ASP:OD1	1:J:411:ARG:HG3	1.96	0.64
1:K:194:LEU:HD11	1:K:362:LEU:CB	2.28	0.63
1:C:323:LYS:HG2	1:D:549:VAL:HG13	1.79	0.63
1:B:99:ARG:HG2	1:B:101:LEU:O	1.98	0.63
1:E:190:TYR:HE2	3:E:616:HOH:O	1.80	0.63
1:E:439:GLU:HG3	1:E:500:GLN:HE22	1.63	0.63
1:K:141:ASN:C	1:K:143:ALA:H	2.05	0.63
1:B:172:ARG:HG2	1:B:172:ARG:O	1.98	0.63
1:J:378:MET:HE3	1:J:380:ILE:HD11	1.79	0.63
1:K:459:PHE:HE2	1:K:517:MET:CE	2.11	0.63
1:E:549:VAL:HG13	1:F:323:LYS:HG2	1.81	0.63
1:I:549:VAL:HG13	1:J:323:LYS:HG2	1.81	0.62
1:J:194:LEU:HD11	1:J:362:LEU:CB	2.29	0.62
1:A:378:MET:HE3	1:A:380:ILE:HD11	1.80	0.62
1:B:458:ASP:OD1	1:B:498:ARG:HG3	1.99	0.62
1:D:249:HIS:HE1	1:D:258:ASP:OD2	1.82	0.62
1:I:194:LEU:HD11	1:I:362:LEU:CB	2.29	0.62
1:I:458:ASP:OD1	1:I:498:ARG:HG3	1.99	0.62
1:I:491:ILE:HD11	1:I:498:ARG:HB2	1.81	0.62
1:A:481:GLY:HA2	1:A:506:THR:HG23	1.80	0.62
1:F:249:HIS:HE1	1:F:258:ASP:OD2	1.82	0.62
1:H:449:GLU:H	1:H:449:GLU:CD	2.08	0.61
1:J:249:HIS:HE1	1:J:258:ASP:OD2	1.83	0.61
1:C:491:ILE:HD11	1:C:498:ARG:HB2	1.83	0.61
1:E:81:TYR:HB2	1:E:110:MET:HE3	1.83	0.61
1:G:194:LEU:HD11	1:G:362:LEU:CB	2.30	0.61
1:E:146:ASP:C	1:E:148:LYS:H	2.08	0.61
1:J:459:PHE:HE2	1:J:517:MET:CE	2.14	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:110:MET:HE2	1:F:110:MET:HA	1.81	0.60
1:G:143:ALA:HB1	1:G:145:VAL:HG23	1.83	0.60
1:I:431:ARG:NH2	3:I:601:HOH:O	2.34	0.60
1:L:194:LEU:HD21	1:L:362:LEU:HB2	1.81	0.60
1:C:142:ASP:O	1:C:143:ALA:C	2.44	0.60
1:F:378:MET:HE3	1:F:380:ILE:HD11	1.84	0.60
1:G:76:MET:HE1	1:G:84:ILE:HD11	1.82	0.60
1:L:449:GLU:CD	1:L:449:GLU:H	2.10	0.60
1:E:454:ARG:NH1	1:E:502:ASP:OD1	2.35	0.59
1:E:190:TYR:CE2	3:E:616:HOH:O	2.52	0.59
1:A:181:SER:HB2	1:A:198:GLY:H	1.67	0.59
1:C:172:ARG:O	1:C:172:ARG:HG2	2.02	0.59
1:H:99:ARG:HG2	1:H:101:LEU:O	2.03	0.59
1:E:179:GLY:O	1:E:182:TYR:HB2	2.02	0.59
1:L:280:MET:HE1	1:L:298:ILE:HG22	1.85	0.59
1:C:458:ASP:OD1	1:C:498:ARG:HG3	2.03	0.58
1:E:459:PHE:HE1	1:E:517:MET:CE	2.16	0.58
1:C:172:ARG:CZ	1:C:190:TYR:CE2	2.86	0.58
1:J:454:ARG:NH1	1:J:502:ASP:OD1	2.36	0.58
1:I:323:LYS:HG2	1:J:549:VAL:HG13	1.85	0.58
1:A:249:HIS:HE1	1:A:258:ASP:OD2	1.86	0.58
1:F:425:ALA:HA	1:F:461:GLY:HA3	1.85	0.58
1:E:323:LYS:HG2	1:F:549:VAL:CG1	2.34	0.58
1:D:194:LEU:HD11	1:D:362:LEU:CB	2.33	0.58
1:G:174:VAL:HA	1:G:186:VAL:HG22	1.86	0.58
1:F:146:ASP:HB3	1:F:149:GLN:HG3	1.86	0.57
1:F:72:THR:OG1	1:F:145:VAL:HA	2.04	0.57
1:K:174:VAL:HA	1:K:186:VAL:HG22	1.86	0.57
1:L:93:TRP:CD2	1:L:222:VAL:HG22	2.40	0.57
1:D:449:GLU:CD	1:D:449:GLU:H	2.12	0.57
1:F:105:PHE:CE1	1:F:118:MET:HG2	2.39	0.57
1:C:425:ALA:HA	1:C:461:GLY:HA3	1.85	0.57
1:F:481:GLY:HA2	1:F:506:THR:HG23	1.86	0.57
1:L:99:ARG:HG2	1:L:101:LEU:O	2.04	0.57
1:I:174:VAL:HA	1:I:186:VAL:HG22	1.87	0.57
1:I:551:SER:HB2	1:I:553:GLU:HG2	1.87	0.57
1:J:197:ARG:HB2	1:J:276:PRO:HG2	1.86	0.57
1:F:458:ASP:OD1	1:F:498:ARG:HG3	2.04	0.56
1:I:443:PRO:HB2	1:I:446:HIS:O	2.05	0.56
1:D:459:PHE:HE1	1:D:517:MET:CE	2.18	0.56
1:E:449:GLU:CD	1:E:449:GLU:H	2.13	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:449:GLU:H	1:F:449:GLU:CD	2.13	0.56
1:G:194:LEU:HD11	1:G:362:LEU:HB3	1.86	0.56
1:D:194:LEU:HD11	1:D:362:LEU:HB3	1.86	0.56
1:C:105:PHE:CE1	1:C:118:MET:HG2	2.40	0.56
1:G:249:HIS:HE1	1:G:258:ASP:OD2	1.89	0.56
1:A:174:VAL:HA	1:A:186:VAL:HG22	1.87	0.56
1:D:206:ASP:HB2	1:D:270:LYS:HZ3	1.70	0.56
1:H:63:ARG:HD2	1:H:114:ARG:NH1	2.20	0.56
1:C:423:PRO:HG2	1:C:424:LEU:HD13	1.87	0.56
1:E:459:PHE:CE1	1:E:517:MET:CE	2.89	0.56
1:G:46:ASP:OD1	1:G:48:SER:HB3	2.06	0.56
1:G:455:PHE:O	1:G:500:GLN:HA	2.06	0.56
1:H:458:ASP:OD1	1:H:498:ARG:HG3	2.06	0.56
1:L:458:ASP:OD1	1:L:498:ARG:HG3	2.05	0.56
1:H:140:TYR:O	1:H:143:ALA:HB3	2.06	0.55
1:C:455:PHE:O	1:C:500:GLN:HA	2.06	0.55
1:J:134:ARG:HG3	1:J:137:LEU:HG	1.89	0.55
1:E:302:ASP:OD1	1:E:303:ARG:HG2	2.07	0.55
1:E:72:THR:H	1:E:149:GLN:NE2	2.04	0.55
1:C:194:LEU:HD11	1:C:362:LEU:HB2	1.88	0.55
1:C:172:ARG:CG	1:C:190:TYR:CD2	2.90	0.54
1:E:442:ALA:HB3	1:F:385:GLU:HG2	1.89	0.54
1:F:491:ILE:HD11	1:F:498:ARG:HB2	1.89	0.54
1:I:248:ILE:HG12	1:I:257:MET:HG2	1.87	0.54
1:K:455:PHE:O	1:K:500:GLN:HA	2.08	0.54
1:D:454:ARG:NH1	1:D:502:ASP:OD1	2.40	0.54
1:B:140:TYR:O	1:B:143:ALA:HB2	2.07	0.54
1:E:99:ARG:HG2	1:E:101:LEU:O	2.06	0.54
1:E:194:LEU:HD11	1:E:362:LEU:CB	2.37	0.54
1:J:190:TYR:HE2	3:J:649:HOH:O	1.88	0.54
1:F:454:ARG:HG3	1:F:454:ARG:HH11	1.73	0.54
1:K:194:LEU:HD11	1:K:362:LEU:HB3	1.88	0.54
1:E:76:MET:HE1	1:E:84:ILE:HD11	1.88	0.54
1:A:455:PHE:O	1:A:500:GLN:HA	2.07	0.54
1:C:385:GLU:HG2	1:D:442:ALA:HB3	1.90	0.54
1:K:194:LEU:HD11	1:K:362:LEU:HB2	1.90	0.54
1:I:351:ASP:OD2	1:I:354:GLY:N	2.35	0.53
1:G:305:SER:HB3	1:G:363:TRP:HZ3	1.73	0.53
1:E:194:LEU:HD11	1:E:362:LEU:HB2	1.91	0.53
1:F:455:PHE:O	1:F:500:GLN:HA	2.09	0.53
1:G:81:TYR:HB2	1:G:110:MET:HE3	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:378:MET:HE3	1:I:380:ILE:HD11	1.91	0.53
1:C:194:LEU:HD11	1:C:362:LEU:CB	2.38	0.53
1:H:163:VAL:HG21	1:H:229:PHE:CZ	2.44	0.53
1:I:455:PHE:O	1:I:500:GLN:HA	2.08	0.53
1:B:299:HIS:CE1	1:B:349:TYR:HE2	2.27	0.53
1:C:83:SER:OG	1:C:143:ALA:HB2	2.09	0.53
1:E:197:ARG:HB2	1:E:276:PRO:HG2	1.90	0.53
1:C:549:VAL:HG13	1:D:323:LYS:HG2	1.90	0.53
1:D:99:ARG:HG2	1:D:101:LEU:O	2.08	0.53
1:D:367:ARG:NH1	1:D:411:ARG:NH2	2.56	0.53
1:I:133:PHE:CD2	1:I:133:PHE:C	2.85	0.53
1:E:383:THR:HG22	1:F:443:PRO:O	2.09	0.53
1:G:76:MET:HE3	1:G:145:VAL:HG22	1.91	0.53
1:K:148:LYS:O	1:K:151:GLU:HG2	2.09	0.53
1:K:163:VAL:HG21	1:K:229:PHE:CZ	2.44	0.53
1:L:431:ARG:HH11	1:L:431:ARG:HG2	1.73	0.53
1:A:530:TRP:CZ2	1:A:532:TYR:HB2	2.44	0.52
1:I:549:VAL:CG1	1:J:323:LYS:HG2	2.39	0.52
1:B:380:ILE:HD12	1:B:389:ASN:HA	1.90	0.52
1:C:181:SER:HB2	1:C:198:GLY:H	1.74	0.52
1:I:320:ASN:ND2	1:I:382:THR:H	2.05	0.52
1:J:194:LEU:HD11	1:J:362:LEU:HB2	1.89	0.52
1:C:93:TRP:CD2	1:C:222:VAL:HG22	2.45	0.52
1:I:454:ARG:NH1	1:I:502:ASP:OD1	2.42	0.52
1:K:187:ASP:HB3	1:K:415:SER:HA	1.91	0.52
1:A:76:MET:HE1	1:A:84:ILE:HD11	1.90	0.52
1:J:99:ARG:HG2	1:J:101:LEU:O	2.09	0.52
1:J:439:GLU:HG3	1:J:500:GLN:HE22	1.73	0.52
1:K:386:THR:HG22	1:L:444:GLY:H	1.74	0.52
1:C:148:LYS:O	1:C:151:GLU:HG2	2.10	0.52
1:C:422:CYS:SG	1:C:423:PRO:HD2	2.50	0.52
1:B:302:ASP:OD1	1:B:303:ARG:HG2	2.10	0.51
1:C:421:HIS:HD2	1:C:422:CYS:O	1.93	0.51
1:D:193:GLY:HA3	1:D:360:PRO:HD2	1.92	0.51
1:B:460:VAL:CG1	1:B:494:ILE:HD12	2.40	0.51
1:C:172:ARG:CG	1:C:190:TYR:HD2	2.23	0.51
1:D:148:LYS:HA	1:D:151:GLU:HG3	1.91	0.51
1:H:459:PHE:HE1	1:H:517:MET:CE	2.23	0.51
1:A:141:ASN:O	1:A:143:ALA:N	2.43	0.51
1:E:367:ARG:CZ	1:E:411:ARG:NH2	2.73	0.51
1:I:320:ASN:HD22	1:I:320:ASN:C	2.19	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:165:LYS:HD3	1:K:174:VAL:HG11	1.93	0.51
1:D:174:VAL:HA	1:D:186:VAL:HG22	1.92	0.51
1:D:367:ARG:CZ	1:D:411:ARG:NH2	2.74	0.51
1:H:286:ASN:OD1	1:H:286:ASN:N	2.44	0.51
1:J:187:ASP:HB3	1:J:415:SER:HA	1.93	0.51
1:G:134:ARG:HG2	1:G:137:LEU:HG	1.93	0.50
1:L:459:PHE:HE1	1:L:517:MET:CE	2.24	0.50
1:C:110:MET:HE2	1:C:110:MET:HA	1.92	0.50
1:K:454:ARG:NH1	1:K:502:ASP:OD1	2.44	0.50
1:A:459:PHE:HE1	1:A:517:MET:CE	2.24	0.50
1:J:174:VAL:HA	1:J:186:VAL:HG22	1.94	0.50
1:B:422:CYS:SG	1:B:424:LEU:HB2	2.51	0.50
1:D:138:PHE:O	1:K:171:ARG:NH1	2.45	0.50
1:F:248:ILE:HG12	1:F:257:MET:HG2	1.93	0.50
1:K:468:ALA:N	1:K:469:PRO:HD2	2.27	0.50
1:L:351:ASP:OD2	1:L:354:GLY:N	2.39	0.50
1:B:167:PRO:HD2	1:B:172:ARG:NH2	2.26	0.50
1:G:302:ASP:OD2	1:G:303:ARG:HG2	2.10	0.50
1:H:449:GLU:HG2	1:H:450:LYS:H	1.76	0.50
1:A:286:ASN:O	1:A:287:GLU:C	2.54	0.50
1:B:456:ALA:HB1	1:B:498:ARG:HD3	1.93	0.50
1:H:479:SER:HB3	1:H:514:ASP:H	1.76	0.50
1:F:47:PHE:O	1:F:51:GLN:HG3	2.11	0.50
1:G:330:THR:HA	1:G:374:THR:HG22	1.94	0.50
1:I:75:THR:HG22	3:I:626:HOH:O	2.12	0.50
1:F:454:ARG:NH1	1:F:502:ASP:OD1	2.45	0.49
1:J:76:MET:O	1:J:110:MET:HE1	2.12	0.49
1:L:289:ARG:HD3	1:L:320:ASN:O	2.12	0.49
1:L:320:ASN:HD21	1:L:382:THR:H	1.58	0.49
1:A:187:ASP:HB3	1:A:415:SER:HA	1.94	0.49
1:A:425:ALA:HA	1:A:461:GLY:HA3	1.94	0.49
1:A:549:VAL:HG13	1:B:323:LYS:HG2	1.94	0.49
1:E:184:ARG:HG2	1:E:195:SER:HA	1.93	0.49
1:F:459:PHE:HE1	1:F:517:MET:CE	2.25	0.49
1:C:275:ALA:N	1:C:276:PRO:CD	2.76	0.49
1:D:52:SER:O	1:D:53:MET:C	2.56	0.49
1:H:380:ILE:HD12	1:H:389:ASN:HA	1.95	0.49
1:L:459:PHE:CE1	1:L:517:MET:HE3	2.47	0.49
1:G:439:GLU:HG3	1:G:500:GLN:HE22	1.77	0.49
1:D:197:ARG:HB2	1:D:276:PRO:HG2	1.94	0.49
1:E:146:ASP:C	1:E:148:LYS:N	2.71	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:163:VAL:HG21	1:G:229:PHE:CZ	2.48	0.49
1:I:552:LEU:HG	1:J:204:TYR:CZ	2.47	0.49
1:L:459:PHE:CE1	1:L:517:MET:CE	2.95	0.49
1:G:181:SER:HB2	1:G:198:GLY:H	1.76	0.49
1:H:455:PHE:O	1:H:500:GLN:HA	2.13	0.49
1:C:140:TYR:O	1:C:143:ALA:HB3	2.13	0.49
1:E:380:ILE:O	1:E:389:ASN:HB2	2.12	0.49
1:H:454:ARG:NH1	1:H:502:ASP:OD1	2.45	0.49
1:I:141:ASN:O	1:I:142:ASP:C	2.56	0.49
1:J:52:SER:O	1:J:53:MET:C	2.55	0.49
1:K:530:TRP:CZ2	1:K:532:TYR:HB2	2.48	0.49
1:L:456:ALA:HB1	1:L:498:ARG:HD3	1.94	0.49
1:G:549:VAL:HG13	1:H:323:LYS:HG2	1.95	0.49
1:H:72:THR:HB	1:H:149:GLN:NE2	2.28	0.49
1:H:181:SER:HB2	1:H:198:GLY:H	1.78	0.49
1:B:454:ARG:NH1	1:B:502:ASP:OD1	2.46	0.49
1:D:76:MET:O	1:D:110:MET:HE1	2.13	0.49
1:D:425:ALA:HA	1:D:461:GLY:HA3	1.94	0.49
1:G:323:LYS:HG2	1:H:549:VAL:HG13	1.94	0.49
1:H:187:ASP:HB3	1:H:415:SER:HA	1.94	0.49
1:A:171:ARG:NH2	1:J:87:ASP:OD2	2.47	0.48
1:D:141:ASN:C	1:D:143:ALA:N	2.70	0.48
1:K:280:MET:HE1	1:K:298:ILE:HG22	1.95	0.48
1:C:431:ARG:HD2	1:C:498:ARG:HH12	1.78	0.48
1:E:141:ASN:C	1:E:143:ALA:N	2.71	0.48
1:I:105:PHE:CE1	1:I:118:MET:HG2	2.48	0.48
1:K:283:CYS:HB2	1:K:290:MET:O	2.13	0.48
1:G:165:LYS:HD2	3:G:640:HOH:O	2.13	0.48
1:C:47:PHE:O	1:C:51:GLN:HG3	2.13	0.48
1:H:115:ARG:HG2	1:H:156:LEU:O	2.14	0.48
1:H:140:TYR:O	1:H:143:ALA:CB	2.62	0.48
1:H:258:ASP:OD1	1:H:411:ARG:HG3	2.13	0.48
1:K:549:VAL:HG13	1:L:323:LYS:HG2	1.96	0.48
1:E:96:VAL:O	1:E:99:ARG:HB2	2.13	0.48
1:J:367:ARG:NH1	1:J:411:ARG:NH2	2.62	0.48
1:K:228:THR:OG1	1:K:249:HIS:HD2	1.97	0.48
1:F:76:MET:HE1	1:F:84:ILE:HD11	1.95	0.48
1:F:275:ALA:N	1:F:276:PRO:CD	2.76	0.48
1:G:113:ARG:NH1	1:G:113:ARG:HG2	2.28	0.48
1:E:462:GLY:O	1:E:464:LEU:N	2.47	0.47
1:G:491:ILE:HG22	1:G:493:PRO:HD2	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:194:LEU:HD11	1:J:362:LEU:HB3	1.95	0.47
1:K:53:MET:O	1:K:57:LEU:HB2	2.14	0.47
1:F:468:ALA:HB3	1:F:469:PRO:CD	2.44	0.47
1:L:530:TRP:CZ2	1:L:532:TYR:HB2	2.49	0.47
1:E:367:ARG:NH1	1:E:411:ARG:NH2	2.63	0.47
1:F:187:ASP:OD1	1:F:415:SER:HA	2.13	0.47
1:K:141:ASN:C	1:K:143:ALA:N	2.71	0.47
1:L:193:GLY:HA3	1:L:360:PRO:HD2	1.95	0.47
1:C:148:LYS:HD2	1:C:148:LYS:HA	1.71	0.47
1:F:388:ASN:ND2	3:F:603:HOH:O	2.48	0.47
1:G:454:ARG:NH1	1:G:502:ASP:OD1	2.47	0.47
1:J:81:TYR:HB2	1:J:110:MET:HE3	1.97	0.47
1:J:367:ARG:CZ	1:J:411:ARG:NH2	2.77	0.47
1:D:105:PHE:CE1	1:D:118:MET:CG	2.97	0.47
1:F:187:ASP:C	1:F:189:THR:H	2.22	0.47
1:I:184:ARG:HG3	1:I:192:TYR:CD1	2.49	0.47
1:L:193:GLY:HA3	1:L:359:ARG:HB3	1.97	0.47
1:L:454:ARG:NH1	1:L:502:ASP:OD1	2.47	0.47
1:D:193:GLY:HA2	1:D:359:ARG:HD3	1.97	0.47
1:G:148:LYS:O	1:G:151:GLU:HG2	2.14	0.47
1:D:307:TRP:CE2	1:D:335:LYS:HD2	2.50	0.47
1:F:457:VAL:HB	1:F:517:MET:HE1	1.97	0.47
1:G:194:LEU:HD11	1:G:362:LEU:HB2	1.95	0.47
1:G:323:LYS:HG2	1:H:549:VAL:HG22	1.97	0.47
1:J:280:MET:HE3	1:J:280:MET:HB3	1.77	0.47
1:K:351:ASP:OD1	1:K:354:GLY:N	2.34	0.47
1:A:53:MET:O	1:A:57:LEU:HB2	2.15	0.47
1:D:367:ARG:NH1	1:D:411:ARG:HH21	2.13	0.47
1:I:172:ARG:CZ	1:I:190:TYR:CE2	2.98	0.47
1:L:380:ILE:HD12	1:L:389:ASN:HA	1.97	0.47
1:B:459:PHE:HE1	1:B:517:MET:CE	2.27	0.47
1:C:366:PRO:HB3	1:C:370:TRP:CE2	2.50	0.47
1:L:168:GLU:HG2	1:L:171:ARG:HG3	1.97	0.47
1:B:163:VAL:HG21	1:B:229:PHE:CZ	2.50	0.47
1:H:530:TRP:CZ2	1:H:532:TYR:HB2	2.50	0.47
1:I:143:ALA:HB1	1:I:145:VAL:HG23	1.97	0.47
1:L:288:ARG:HB3	1:L:291:CYS:SG	2.55	0.47
1:A:163:VAL:HG21	1:A:229:PHE:CZ	2.51	0.46
1:I:481:GLY:HA2	1:I:506:THR:HG23	1.97	0.46
1:J:248:ILE:HG12	1:J:257:MET:HG2	1.97	0.46
1:L:457:VAL:HB	1:L:517:MET:HE1	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:533:GLN:HG2	1:A:535:PHE:CZ	2.50	0.46
1:C:143:ALA:HB1	1:C:145:VAL:HG23	1.96	0.46
1:E:133:PHE:CG	1:E:134:ARG:N	2.83	0.46
1:F:117:ARG:O	1:F:216:ALA:HA	2.14	0.46
1:B:299:HIS:CE1	1:B:349:TYR:CE2	3.03	0.46
1:H:492:GLU:N	1:H:493:PRO:CD	2.78	0.46
1:I:456:ALA:HB1	1:I:498:ARG:HD3	1.98	0.46
1:E:145:VAL:O	1:E:147:THR:HG23	2.16	0.46
1:G:113:ARG:HG2	1:G:113:ARG:HH11	1.79	0.46
1:K:459:PHE:HE2	1:K:517:MET:HE2	1.79	0.46
1:A:376:GLY:O	1:A:392:CYS:HA	2.16	0.46
1:D:210:GLU:OE2	1:D:237:SER:OG	2.31	0.46
1:D:385:GLU:H	1:D:385:GLU:HG2	1.57	0.46
1:F:187:ASP:C	1:F:189:THR:N	2.73	0.46
1:F:187:ASP:CG	1:F:415:SER:HA	2.40	0.46
1:J:146:ASP:HB3	1:J:149:GLN:HG2	1.97	0.46
1:C:179:GLY:O	1:C:182:TYR:HB2	2.16	0.46
1:D:142:ASP:O	1:D:143:ALA:C	2.56	0.46
1:D:194:LEU:HG	1:D:195:SER:N	2.30	0.46
1:F:181:SER:HB2	1:F:198:GLY:H	1.81	0.46
1:H:133:PHE:CD2	1:H:133:PHE:C	2.94	0.46
1:K:305:SER:HB3	1:K:363:TRP:HZ3	1.81	0.46
1:C:133:PHE:CD2	1:C:133:PHE:C	2.93	0.46
1:D:105:PHE:CE1	1:D:118:MET:HG2	2.51	0.46
1:F:366:PRO:HB3	1:F:370:TRP:CE2	2.51	0.46
1:I:201:ILE:HB	1:I:210:GLU:HB3	1.97	0.46
1:K:422:CYS:C	1:K:424:LEU:H	2.24	0.46
1:D:72:THR:H	1:D:149:GLN:NE2	2.09	0.46
1:G:459:PHE:HE1	1:G:517:MET:CE	2.29	0.46
1:J:530:TRP:CZ2	1:J:532:TYR:HB2	2.51	0.46
1:A:323:LYS:O	1:A:325:GLN:HG2	2.15	0.46
1:F:409:GLN:HG2	2:Q:1:GLC:H2	1.97	0.46
1:K:184:ARG:HG2	1:K:195:SER:HA	1.97	0.46
1:F:286:ASN:O	1:F:287:GLU:C	2.60	0.45
1:G:286:ASN:O	1:G:287:GLU:C	2.58	0.45
1:I:97:GLU:O	1:I:224:PRO:HB3	2.16	0.45
1:B:459:PHE:CE1	1:B:517:MET:CE	2.99	0.45
1:D:76:MET:HE1	1:D:84:ILE:HD11	1.98	0.45
1:D:181:SER:HB2	1:D:198:GLY:H	1.81	0.45
1:G:229:PHE:HA	3:G:608:HOH:O	2.15	0.45
1:I:320:ASN:ND2	1:I:320:ASN:C	2.73	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:106:PHE:CD2	1:K:178:LEU:HD13	2.51	0.45
1:B:167:PRO:HD2	1:B:172:ARG:HH22	1.80	0.45
1:D:187:ASP:HB3	1:D:415:SER:HA	1.97	0.45
1:E:177:PHE:CD2	1:E:183:PHE:HB3	2.51	0.45
1:I:116:VAL:HB	1:I:158:PHE:O	2.16	0.45
1:K:133:PHE:CD2	1:K:133:PHE:C	2.94	0.45
1:B:530:TRP:CZ2	1:B:532:TYR:HB2	2.51	0.45
1:E:141:ASN:C	1:E:143:ALA:H	2.24	0.45
1:F:376:GLY:O	1:F:392:CYS:HA	2.17	0.45
1:A:193:GLY:HA3	1:A:359:ARG:HB3	1.98	0.45
1:J:385:GLU:H	1:J:385:GLU:HG2	1.60	0.45
1:K:181:SER:HB2	1:K:198:GLY:H	1.82	0.45
1:C:172:ARG:HG3	1:C:190:TYR:CD2	2.52	0.45
1:E:299:HIS:HB2	1:E:301:SER:O	2.17	0.45
1:I:376:GLY:O	1:I:392:CYS:HA	2.16	0.45
1:C:202:ASP:O	1:C:209:GLU:HA	2.17	0.45
1:E:143:ALA:HB1	1:E:145:VAL:HG23	1.99	0.45
1:F:351:ASP:OD2	1:F:354:GLY:N	2.40	0.45
1:K:376:GLY:O	1:K:392:CYS:HA	2.17	0.45
1:C:376:GLY:O	1:C:392:CYS:HA	2.15	0.45
1:E:552:LEU:HD21	1:F:205:THR:C	2.41	0.45
1:H:288:ARG:HB3	1:H:291:CYS:SG	2.57	0.45
1:I:275:ALA:N	1:I:276:PRO:CD	2.79	0.45
1:J:519:LEU:HB2	1:J:527:SER:HB3	1.99	0.45
1:B:181:SER:O	1:B:197:ARG:HA	2.17	0.45
1:E:324:LEU:HD22	1:F:550:MET:HG3	1.99	0.45
1:G:464:LEU:HD23	1:G:464:LEU:HA	1.82	0.45
1:I:421:HIS:O	1:I:422:CYS:C	2.60	0.45
1:I:468:ALA:HB3	1:I:469:PRO:CD	2.46	0.45
1:L:148:LYS:HD2	1:L:148:LYS:HA	1.76	0.45
1:L:468:ALA:N	1:L:469:PRO:HD2	2.31	0.45
1:H:184:ARG:HA	1:H:414:TRP:CH2	2.52	0.45
1:B:210:GLU:OE2	1:B:237:SER:OG	2.25	0.44
1:I:454:ARG:HH11	1:I:454:ARG:HG3	1.81	0.44
1:J:275:ALA:N	1:J:276:PRO:CD	2.80	0.44
1:F:380:ILE:HD12	1:F:389:ASN:HA	2.00	0.44
1:H:73:LEU:HD21	1:H:150:LEU:HD11	1.98	0.44
1:J:179:GLY:O	1:J:182:TYR:HB2	2.18	0.44
1:K:46:ASP:OD1	1:K:48:SER:HB3	2.18	0.44
1:L:305:SER:O	1:L:337:PHE:HA	2.17	0.44
1:D:96:VAL:O	1:D:99:ARG:HB2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:376:GLY:O	1:D:392:CYS:HA	2.17	0.44
1:G:212:PRO:HB3	1:G:235:LEU:HD21	1.99	0.44
1:D:468:ALA:HB3	1:D:469:PRO:CD	2.47	0.44
1:E:492:GLU:N	1:E:493:PRO:CD	2.80	0.44
1:G:73:LEU:HD21	1:G:150:LEU:HD11	1.98	0.44
1:J:83:SER:OG	1:J:143:ALA:HB2	2.16	0.44
1:L:115:ARG:HG2	1:L:156:LEU:O	2.17	0.44
1:A:284:GLY:O	1:A:288:ARG:HG2	2.17	0.44
1:B:108:MET:HE3	1:B:108:MET:HB3	1.87	0.44
1:G:113:ARG:HH11	1:G:113:ARG:CG	2.30	0.44
1:A:133:PHE:CD2	1:A:133:PHE:C	2.96	0.44
1:G:53:MET:O	1:G:57:LEU:HB2	2.17	0.44
1:G:533:GLN:HG2	1:G:535:PHE:CZ	2.52	0.44
1:A:143:ALA:HB1	1:A:145:VAL:HG23	1.99	0.44
1:A:299:HIS:HE1	3:A:602:HOH:O	2.00	0.44
1:C:46:ASP:OD1	1:C:46:ASP:C	2.61	0.44
1:F:106:PHE:CZ	1:F:162:ARG:HD3	2.53	0.44
1:G:284:GLY:O	1:G:288:ARG:HG2	2.18	0.44
1:K:491:ILE:HG22	1:K:493:PRO:HD2	2.00	0.44
1:D:280:MET:HE3	1:D:280:MET:HB3	1.94	0.44
1:E:52:SER:O	1:E:53:MET:C	2.61	0.44
1:E:76:MET:HE1	1:E:84:ILE:CD1	2.48	0.44
1:E:76:MET:O	1:E:110:MET:HE1	2.17	0.44
1:E:280:MET:HE3	1:E:280:MET:HB3	1.89	0.44
1:F:456:ALA:HB1	1:F:498:ARG:HD3	1.99	0.44
1:K:330:THR:HA	1:K:374:THR:HG22	2.00	0.44
1:A:37:ILE:O	1:A:134:ARG:NH2	2.47	0.44
1:B:376:GLY:O	1:B:392:CYS:HA	2.18	0.44
1:D:203:THR:HG21	1:D:391:VAL:HG11	1.99	0.44
1:G:418:PRO:CG	3:G:605:HOH:O	2.66	0.44
1:H:153:GLN:HE21	1:H:153:GLN:HB3	1.57	0.44
1:H:380:ILE:O	1:H:389:ASN:HB2	2.18	0.44
1:I:385:GLU:HG2	1:J:442:ALA:HB3	1.99	0.44
1:K:491:ILE:HD11	1:K:498:ARG:CB	2.37	0.44
1:L:184:ARG:HG3	1:L:192:TYR:CD1	2.53	0.44
1:L:295:HIS:HD2	1:L:349:TYR:O	2.00	0.44
1:A:185:ALA:HB3	1:A:414:TRP:CG	2.53	0.43
1:A:193:GLY:HA2	1:A:359:ARG:HD3	1.99	0.43
1:B:455:PHE:O	1:B:500:GLN:HA	2.16	0.43
1:C:140:TYR:O	1:C:141:ASN:C	2.61	0.43
1:F:258:ASP:OD1	1:F:411:ARG:HG3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:151:GLU:C	1:G:153:GLN:H	2.25	0.43
1:I:181:SER:HB2	1:I:198:GLY:H	1.84	0.43
1:A:205:THR:HG21	1:A:270:LYS:HB3	1.99	0.43
1:C:99:ARG:NH2	1:C:102:ASP:OD2	2.51	0.43
1:E:530:TRP:CZ2	1:E:532:TYR:HB2	2.53	0.43
1:J:62:TRP:CE3	1:J:64:GLY:HA2	2.53	0.43
1:K:481:GLY:HA2	1:K:506:THR:HG23	1.98	0.43
1:K:533:GLN:HG2	1:K:535:PHE:CZ	2.53	0.43
1:B:431:ARG:HG3	1:B:456:ALA:O	2.18	0.43
1:D:133:PHE:CG	1:D:134:ARG:N	2.85	0.43
1:H:280:MET:HE3	1:H:280:MET:HB3	1.91	0.43
1:I:46:ASP:OD1	1:I:46:ASP:C	2.61	0.43
1:L:431:ARG:HH11	1:L:431:ARG:CG	2.31	0.43
1:L:492:GLU:N	1:L:493:PRO:CD	2.81	0.43
1:A:69:LEU:HD12	1:A:113:ARG:HH12	1.83	0.43
1:A:305:SER:HB3	1:A:363:TRP:HZ3	1.83	0.43
1:A:347:SER:HA	1:A:350:GLN:NE2	2.34	0.43
1:B:277:MET:HG2	1:B:362:LEU:HD23	1.99	0.43
1:B:380:ILE:O	1:B:389:ASN:HB2	2.19	0.43
1:C:454:ARG:HG3	1:C:454:ARG:HH11	1.83	0.43
1:I:249:HIS:CE1	1:I:258:ASP:OD2	2.67	0.43
1:K:76:MET:HE1	1:K:84:ILE:HD11	2.00	0.43
1:K:323:LYS:HG2	1:L:549:VAL:CG1	2.47	0.43
1:K:413:TYR:CD1	1:K:419:PRO:HG3	2.54	0.43
1:A:97:GLU:O	1:A:224:PRO:HB3	2.18	0.43
1:F:173:ASP:OD1	1:F:173:ASP:N	2.50	0.43
1:F:380:ILE:O	1:F:389:ASN:HB2	2.19	0.43
1:H:468:ALA:N	1:H:469:PRO:HD2	2.34	0.43
1:I:106:PHE:CZ	1:I:162:ARG:HD3	2.53	0.43
1:K:76:MET:HE1	1:K:84:ILE:CD1	2.49	0.43
1:L:258:ASP:OD1	1:L:411:ARG:HG3	2.19	0.43
1:A:171:ARG:NH1	1:J:138:PHE:O	2.52	0.43
1:A:459:PHE:CE1	1:A:517:MET:CE	3.02	0.43
1:B:275:ALA:N	1:B:276:PRO:CD	2.82	0.43
1:C:38:ALA:HB1	1:C:129:ARG:HB2	2.00	0.43
1:C:105:PHE:CE1	1:C:118:MET:CG	3.01	0.43
1:H:37:ILE:HA	1:H:134:ARG:HH22	1.84	0.43
1:I:179:GLY:O	1:I:182:TYR:HB2	2.19	0.43
1:K:143:ALA:HB1	1:K:145:VAL:HG23	1.99	0.43
1:K:349:TYR:O	1:K:350:GLN:HB2	2.19	0.43
1:B:479:SER:HB3	1:B:514:ASP:H	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:492:GLU:N	1:B:493:PRO:CD	2.82	0.43
1:F:249:HIS:CE1	1:F:258:ASP:OD2	2.68	0.43
1:A:161:PHE:CE2	1:A:177:PHE:HB2	2.53	0.43
1:F:110:MET:HA	1:F:110:MET:CE	2.48	0.43
1:F:201:ILE:HB	1:F:210:GLU:HB3	2.01	0.43
1:G:376:GLY:O	1:G:392:CYS:HA	2.18	0.43
1:B:168:GLU:HB2	1:B:172:ARG:NH2	2.32	0.43
1:C:351:ASP:OD1	1:C:354:GLY:N	2.36	0.43
1:F:299:HIS:HB2	1:F:301:SER:O	2.18	0.43
1:K:474:PRO:HG3	1:K:499:ILE:HD12	2.01	0.43
1:L:179:GLY:O	1:L:182:TYR:HB2	2.19	0.43
1:A:413:TYR:CD1	1:A:419:PRO:HG3	2.54	0.42
1:A:532:TYR:CD1	1:A:533:GLN:N	2.87	0.42
1:C:549:VAL:HG22	1:D:323:LYS:HG2	2.01	0.42
1:D:464:LEU:HD23	1:D:464:LEU:HA	1.86	0.42
1:D:492:GLU:N	1:D:493:PRO:CD	2.82	0.42
1:E:62:TRP:CE3	1:E:64:GLY:HA2	2.54	0.42
1:L:93:TRP:CG	1:L:222:VAL:HG22	2.54	0.42
1:L:143:ALA:HB1	1:L:145:VAL:HG23	2.01	0.42
1:L:193:GLY:HA2	1:L:359:ARG:HD3	2.01	0.42
1:A:554:HIS:CE1	1:B:323:LYS:HD2	2.54	0.42
1:H:76:MET:HG3	1:H:110:MET:HE3	2.01	0.42
1:I:85:GLN:O	1:I:86:TYR:C	2.62	0.42
1:J:45:PHE:CE2	1:J:218:TRP:CD2	3.08	0.42
1:J:45:PHE:CE2	1:J:218:TRP:CE2	3.06	0.42
1:J:295:HIS:HD2	1:J:349:TYR:O	2.01	0.42
1:J:464:LEU:HD23	1:J:464:LEU:HA	1.84	0.42
1:K:37:ILE:O	1:K:134:ARG:NH2	2.50	0.42
1:K:161:PHE:CE2	1:K:177:PHE:HB2	2.54	0.42
1:K:549:VAL:CG1	1:L:323:LYS:HG2	2.49	0.42
1:G:288:ARG:HB3	1:G:291:CYS:SG	2.59	0.42
1:A:280:MET:HE3	1:A:280:MET:HB3	1.85	0.42
1:B:457:VAL:HB	1:B:517:MET:HE1	2.00	0.42
1:C:464:LEU:HD23	1:C:464:LEU:HA	1.86	0.42
1:E:261:ASN:OD1	1:E:261:ASN:C	2.62	0.42
1:F:174:VAL:HA	1:F:186:VAL:HG22	2.01	0.42
1:F:308:ARG:HB2	1:F:310:ASN:OD1	2.19	0.42
1:K:320:ASN:HD21	1:K:382:THR:H	1.66	0.42
1:L:108:MET:HE3	1:L:108:MET:HB3	1.96	0.42
1:B:459:PHE:CE1	1:B:517:MET:HE3	2.54	0.42
1:C:106:PHE:CZ	1:C:162:ARG:HD3	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:115:ARG:HG2	1:C:156:LEU:O	2.20	0.42
1:D:310:ASN:OD1	1:D:310:ASN:C	2.62	0.42
1:E:275:ALA:N	1:E:276:PRO:CD	2.82	0.42
1:H:172:ARG:CZ	1:H:190:TYR:CE2	3.02	0.42
1:C:172:ARG:NE	1:C:190:TYR:CE2	2.88	0.42
1:C:459:PHE:HE1	1:C:517:MET:CE	2.32	0.42
1:D:279:SER:OG	1:D:301:SER:HB2	2.19	0.42
1:G:310:ASN:OD1	1:G:310:ASN:C	2.63	0.42
1:A:76:MET:HE1	1:A:84:ILE:CD1	2.49	0.42
1:A:454:ARG:NH1	1:A:502:ASP:OD1	2.52	0.42
1:B:208:LYS:HE2	1:B:208:LYS:HB3	1.88	0.42
1:D:87:ASP:OD2	1:K:171:ARG:NH2	2.53	0.42
1:E:174:VAL:HA	1:E:186:VAL:HG22	2.02	0.42
1:G:413:TYR:CD1	1:G:419:PRO:HG3	2.55	0.42
1:I:286:ASN:O	1:I:287:GLU:C	2.62	0.42
1:J:194:LEU:HD21	1:J:362:LEU:HB2	2.00	0.42
1:E:187:ASP:HB3	1:E:415:SER:HA	2.02	0.42
1:J:132:HIS:HE1	3:J:624:HOH:O	2.02	0.42
1:J:181:SER:HB2	1:J:198:GLY:H	1.85	0.42
1:K:110:MET:O	1:K:113:ARG:NE	2.51	0.42
1:L:498:ARG:HD2	1:L:500:GLN:HE21	1.85	0.42
1:B:454:ARG:HG3	1:B:454:ARG:HH11	1.85	0.42
1:B:468:ALA:N	1:B:469:PRO:HD2	2.35	0.42
1:E:519:LEU:HB2	1:E:527:SER:HB3	2.02	0.42
1:B:202:ASP:O	1:B:209:GLU:HA	2.20	0.42
1:C:186:VAL:HG12	1:C:192:TYR:HA	2.02	0.42
1:H:37:ILE:HD12	1:H:131:ILE:HG21	2.02	0.42
1:H:275:ALA:N	1:H:276:PRO:CD	2.83	0.42
1:L:380:ILE:O	1:L:389:ASN:HB2	2.20	0.42
1:A:117:ARG:O	1:A:216:ALA:HA	2.20	0.41
1:D:62:TRP:CE3	1:D:64:GLY:HA2	2.54	0.41
1:F:105:PHE:CE1	1:F:118:MET:CG	3.03	0.41
1:K:550:MET:HE1	1:L:380:ILE:HG23	2.01	0.41
1:L:37:ILE:O	1:L:134:ARG:NH2	2.53	0.41
1:L:286:ASN:O	1:L:287:GLU:C	2.62	0.41
1:B:249:HIS:HE1	1:B:258:ASP:OD2	2.03	0.41
1:B:303:ARG:HG2	1:B:303:ARG:HH11	1.85	0.41
1:C:481:GLY:HA2	1:C:506:THR:HG23	2.02	0.41
1:D:254:GLN:NE2	1:D:256:ILE:HD11	2.35	0.41
1:F:99:ARG:NH2	1:F:102:ASP:OD2	2.53	0.41
1:G:76:MET:HE1	1:G:84:ILE:CD1	2.48	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:163:VAL:HG21	1:J:229:PHE:CZ	2.55	0.41
1:L:454:ARG:HG3	1:L:454:ARG:HH11	1.85	0.41
1:L:455:PHE:O	1:L:500:GLN:HA	2.19	0.41
1:A:322:GLN:HG3	1:A:323:LYS:HG3	2.00	0.41
1:J:180:ALA:HA	1:J:213:ASP:OD1	2.20	0.41
1:K:150:LEU:O	1:K:151:GLU:C	2.63	0.41
1:K:554:HIS:CE1	1:L:323:LYS:HD2	2.56	0.41
1:L:378:MET:HE3	1:L:380:ILE:HD11	2.03	0.41
1:C:100:GLN:HB2	1:C:226:ALA:O	2.20	0.41
1:C:299:HIS:HB2	1:C:301:SER:O	2.21	0.41
1:G:258:ASP:OD1	1:G:411:ARG:HG3	2.20	0.41
1:I:76:MET:HE1	1:I:84:ILE:HD11	2.02	0.41
1:I:148:LYS:HD2	1:I:148:LYS:HA	1.65	0.41
1:J:492:GLU:N	1:J:493:PRO:CD	2.83	0.41
1:L:228:THR:OG1	1:L:249:HIS:HD2	2.03	0.41
1:B:87:ASP:OD1	1:B:87:ASP:C	2.64	0.41
1:B:453:ARG:HD2	1:B:453:ARG:HA	1.89	0.41
1:G:185:ALA:HB3	1:G:414:TRP:CG	2.56	0.41
1:G:385:GLU:HG2	1:H:442:ALA:HB3	2.01	0.41
1:A:228:THR:OG1	1:A:249:HIS:HD2	2.04	0.41
1:C:99:ARG:HG2	1:C:101:LEU:O	2.21	0.41
1:D:330:THR:HA	1:D:374:THR:HG22	2.02	0.41
1:F:492:GLU:N	1:F:493:PRO:CD	2.83	0.41
1:H:378:MET:HE2	1:H:378:MET:HB3	1.85	0.41
1:D:425:ALA:HB3	1:D:527:SER:CB	2.51	0.41
1:F:133:PHE:CD2	1:F:133:PHE:C	2.97	0.41
1:H:208:LYS:HE2	1:H:208:LYS:HB3	1.90	0.41
1:H:243:ALA:O	1:H:261:ASN:HA	2.21	0.41
1:H:428:MET:HB3	1:H:460:VAL:HG22	2.02	0.41
1:K:119:PHE:HB2	1:K:218:TRP:CD1	2.55	0.41
1:K:442:ALA:HB3	1:L:385:GLU:HG2	2.03	0.41
1:E:146:ASP:OD1	1:E:148:LYS:HG2	2.21	0.41
1:A:108:MET:HG3	1:A:156:LEU:HG	2.03	0.41
1:B:97:GLU:O	1:B:224:PRO:HB3	2.21	0.41
1:B:115:ARG:HG2	1:B:156:LEU:O	2.20	0.41
1:C:454:ARG:NH1	1:C:502:ASP:OD1	2.54	0.41
1:C:468:ALA:HB3	1:C:469:PRO:CD	2.49	0.41
1:D:477:THR:HB	1:D:516:ARG:HB3	2.03	0.41
1:F:57:LEU:HD12	1:F:57:LEU:HA	1.91	0.41
1:F:62:TRP:CG	1:F:238:ALA:HA	2.56	0.41
1:F:99:ARG:HG2	1:F:101:LEU:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:206:ASP:OD1	1:F:206:ASP:N	2.43	0.41
1:F:280:MET:HE3	1:F:280:MET:HB3	1.82	0.41
1:H:161:PHE:CE2	1:H:177:PHE:HB2	2.55	0.41
1:I:99:ARG:HG2	1:I:101:LEU:O	2.21	0.41
1:I:202:ASP:O	1:I:209:GLU:HA	2.20	0.41
1:I:380:ILE:O	1:I:389:ASN:HB2	2.21	0.41
1:K:550:MET:HE3	1:K:550:MET:HB3	1.91	0.41
1:L:295:HIS:CD2	1:L:349:TYR:O	2.74	0.41
1:L:299:HIS:CE1	1:L:349:TYR:HE2	2.38	0.41
1:A:93:TRP:CH2	1:A:222:VAL:HG13	2.55	0.41
1:C:172:ARG:CZ	1:C:190:TYR:HE2	2.34	0.41
1:E:148:LYS:HB2	1:E:148:LYS:HE2	1.45	0.41
1:F:385:GLU:HG2	1:F:385:GLU:H	1.67	0.41
1:J:320:ASN:HD22	1:J:320:ASN:C	2.29	0.41
1:J:434:MET:HE1	1:J:447:TYR:HE1	1.86	0.41
1:A:491:ILE:HG22	1:A:493:PRO:HD2	2.02	0.40
1:C:201:ILE:HB	1:C:210:GLU:HB3	2.02	0.40
1:F:169:LEU:HD23	1:F:169:LEU:HA	1.90	0.40
1:G:93:TRP:CH2	1:G:222:VAL:HG13	2.57	0.40
1:G:187:ASP:HB3	1:G:415:SER:HA	2.03	0.40
1:H:87:ASP:OD1	1:H:87:ASP:C	2.64	0.40
1:H:167:PRO:HD2	1:H:172:ARG:HH22	1.86	0.40
1:I:62:TRP:CG	1:I:238:ALA:HA	2.56	0.40
1:I:184:ARG:HA	1:I:414:TRP:CH2	2.57	0.40
1:K:453:ARG:HD2	1:K:453:ARG:HA	1.89	0.40
1:L:93:TRP:CH2	1:L:222:VAL:HG13	2.56	0.40
1:D:248:ILE:HG12	1:D:257:MET:HG2	2.01	0.40
1:E:163:VAL:HG21	1:E:229:PHE:CZ	2.56	0.40
1:E:453:ARG:HD2	1:E:453:ARG:HA	1.92	0.40
1:I:72:THR:OG1	1:I:145:VAL:HA	2.21	0.40
1:I:163:VAL:HG21	1:I:229:PHE:CZ	2.56	0.40
1:J:295:HIS:CD2	1:J:349:TYR:O	2.74	0.40
1:C:554:HIS:HB3	1:D:325:GLN:NE2	2.36	0.40
1:F:499:ILE:HG13	1:F:519:LEU:HD21	2.02	0.40
1:H:286:ASN:O	1:H:287:GLU:C	2.65	0.40
1:H:376:GLY:O	1:H:392:CYS:HA	2.21	0.40
1:I:492:GLU:N	1:I:493:PRO:CD	2.83	0.40
1:L:249:HIS:HE1	1:L:258:ASP:OD2	2.04	0.40
1:A:456:ALA:HB1	1:A:498:ARG:HD3	2.03	0.40
1:B:99:ARG:NH2	1:B:102:ASP:OD2	2.54	0.40
1:B:280:MET:HE3	1:B:280:MET:HB3	1.88	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:481:GLY:CA	1:B:506:THR:HG23	2.45	0.40
1:D:83:SER:OG	1:D:143:ALA:HB2	2.22	0.40
1:E:438:SER:O	1:E:439:GLU:C	2.63	0.40
1:H:117:ARG:O	1:H:216:ALA:HA	2.21	0.40
1:I:77:THR:O	1:I:80:ALA:HB3	2.21	0.40
1:I:115:ARG:HG2	1:I:156:LEU:O	2.21	0.40
1:I:161:PHE:CZ	1:I:177:PHE:CD1	3.10	0.40
1:K:290:MET:HG2	1:K:383:THR:HA	2.02	0.40
1:L:187:ASP:HB3	1:L:415:SER:HA	2.02	0.40
1:L:308:ARG:HD2	1:L:314:ILE:HD12	2.04	0.40
1:A:184:ARG:HG2	3:A:632:HOH:O	2.21	0.40
1:C:57:LEU:HD12	1:C:57:LEU:HA	1.88	0.40
1:C:163:VAL:HG21	1:C:229:PHE:CZ	2.56	0.40
1:D:267:LYS:C	1:D:402:ALA:HB2	2.46	0.40
1:E:197:ARG:HB2	1:E:276:PRO:CG	2.51	0.40
1:H:320:ASN:C	1:H:320:ASN:HD22	2.30	0.40
1:I:290:MET:HG2	1:I:383:THR:HA	2.02	0.40
1:K:422:CYS:SG	1:K:424:LEU:HB2	2.61	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	522/559 (93%)	494 (95%)	26 (5%)	2 (0%)	30	53
1	B	522/559 (93%)	497 (95%)	25 (5%)	0	100	100
1	C	522/559 (93%)	495 (95%)	26 (5%)	1 (0%)	43	66
1	D	522/559 (93%)	496 (95%)	25 (5%)	1 (0%)	43	66
1	E	522/559 (93%)	497 (95%)	24 (5%)	1 (0%)	43	66
1	F	522/559 (93%)	489 (94%)	31 (6%)	2 (0%)	30	53

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	G	522/559 (93%)	488 (94%)	32 (6%)	2 (0%)	30	53
1	H	522/559 (93%)	493 (94%)	29 (6%)	0	100	100
1	I	522/559 (93%)	496 (95%)	24 (5%)	2 (0%)	30	53
1	J	522/559 (93%)	498 (95%)	24 (5%)	0	100	100
1	K	522/559 (93%)	490 (94%)	29 (6%)	3 (1%)	21	45
1	L	522/559 (93%)	490 (94%)	31 (6%)	1 (0%)	43	66
All	All	6264/6708 (93%)	5923 (95%)	326 (5%)	15 (0%)	43	66

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	463	ASP
1	A	142	ASP
1	A	287	GLU
1	G	151	GLU
1	K	287	GLU
1	F	287	GLU
1	G	287	GLU
1	K	142	ASP
1	K	151	GLU
1	L	287	GLU
1	C	143	ALA
1	D	194	LEU
1	F	142	ASP
1	I	142	ASP
1	I	287	GLU

5.3.2 Protein sidechains [i](#)

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	446/470 (95%)	422 (95%)	24 (5%)	20	44
1	B	446/470 (95%)	411 (92%)	35 (8%)	11	30

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	446/470 (95%)	418 (94%)	28 (6%)	16	38
1	D	446/470 (95%)	428 (96%)	18 (4%)	28	53
1	E	446/470 (95%)	427 (96%)	19 (4%)	26	52
1	F	446/470 (95%)	418 (94%)	28 (6%)	16	38
1	G	446/470 (95%)	426 (96%)	20 (4%)	24	50
1	H	446/470 (95%)	410 (92%)	36 (8%)	11	28
1	I	446/470 (95%)	424 (95%)	22 (5%)	22	48
1	J	446/470 (95%)	421 (94%)	25 (6%)	19	43
1	K	446/470 (95%)	427 (96%)	19 (4%)	26	52
1	L	446/470 (95%)	422 (95%)	24 (5%)	20	44
All	All	5352/5640 (95%)	5054 (94%)	298 (6%)	19	43

All (298) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	SER
1	A	99	ARG
1	A	113	ARG
1	A	142	ASP
1	A	147	THR
1	A	148	LYS
1	A	153	GLN
1	A	165	LYS
1	A	173	ASP
1	A	184	ARG
1	A	194	LEU
1	A	195	SER
1	A	205	THR
1	A	206	ASP
1	A	279	SER
1	A	372	LYS
1	A	386	THR
1	A	415	SER
1	A	428	MET
1	A	431	ARG
1	A	434	MET
1	A	470	LYS
1	A	473	GLU

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Mol	Chain	Res	Type
1	A	549	VAL
1	B	110	MET
1	B	113	ARG
1	B	134	ARG
1	B	142	ASP
1	B	147	THR
1	B	148	LYS
1	B	153	GLN
1	B	165	LYS
1	B	167	PRO
1	B	168	GLU
1	B	171	ARG
1	B	172	ARG
1	B	173	ASP
1	B	174	VAL
1	B	176	SER
1	B	181	SER
1	B	184	ARG
1	B	205	THR
1	B	206	ASP
1	B	247	THR
1	B	303	ARG
1	B	380	ILE
1	B	386	THR
1	B	398	LYS
1	B	428	MET
1	B	431	ARG
1	B	434	MET
1	B	450	LYS
1	B	463	ASP
1	B	473	GLU
1	B	477	THR
1	B	479	SER
1	B	482	GLU
1	B	545	VAL
1	B	549	VAL
1	C	35	SER
1	C	77	THR
1	C	110	MET
1	C	113	ARG
1	C	142	ASP
1	C	147	THR

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Mol	Chain	Res	Type
1	C	148	LYS
1	C	172	ARG
1	C	173	ASP
1	C	181	SER
1	C	184	ARG
1	C	194	LEU
1	C	195	SER
1	C	206	ASP
1	C	222	VAL
1	C	368	ASN
1	C	386	THR
1	C	424	LEU
1	C	428	MET
1	C	431	ARG
1	C	434	MET
1	C	438	SER
1	C	463	ASP
1	C	477	THR
1	C	488	ILE
1	C	507	SER
1	C	549	VAL
1	C	552	LEU
1	D	35	SER
1	D	44	ARG
1	D	118	MET
1	D	120	SER
1	D	148	LYS
1	D	153	GLN
1	D	165	LYS
1	D	172	ARG
1	D	184	ARG
1	D	194	LEU
1	D	372	LYS
1	D	386	THR
1	D	428	MET
1	D	434	MET
1	D	463	ASP
1	D	473	GLU
1	D	549	VAL
1	D	552	LEU
1	E	35	SER
1	E	44	ARG

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Mol	Chain	Res	Type
1	E	120	SER
1	E	148	LYS
1	E	194	LEU
1	E	222	VAL
1	E	223	LYS
1	E	239	SER
1	E	247	THR
1	E	261	ASN
1	E	372	LYS
1	E	383	THR
1	E	385	GLU
1	E	386	THR
1	E	428	MET
1	E	445	GLU
1	E	463	ASP
1	E	473	GLU
1	E	549	VAL
1	F	35	SER
1	F	110	MET
1	F	147	THR
1	F	148	LYS
1	F	171	ARG
1	F	172	ARG
1	F	173	ASP
1	F	181	SER
1	F	184	ARG
1	F	187	ASP
1	F	188	ASP
1	F	194	LEU
1	F	289	ARG
1	F	322	GLN
1	F	386	THR
1	F	398	LYS
1	F	426	ARG
1	F	428	MET
1	F	431	ARG
1	F	432	THR
1	F	449	GLU
1	F	463	ASP
1	F	488	ILE
1	F	507	SER
1	F	531	LEU

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Mol	Chain	Res	Type
1	F	549	VAL
1	F	550	MET
1	F	552	LEU
1	G	35	SER
1	G	99	ARG
1	G	113	ARG
1	G	120	SER
1	G	134	ARG
1	G	147	THR
1	G	153	GLN
1	G	171	ARG
1	G	173	ASP
1	G	181	SER
1	G	194	LEU
1	G	205	THR
1	G	206	ASP
1	G	372	LYS
1	G	386	THR
1	G	428	MET
1	G	431	ARG
1	G	463	ASP
1	G	473	GLU
1	G	549	VAL
1	H	35	SER
1	H	60	THR
1	H	110	MET
1	H	113	ARG
1	H	134	ARG
1	H	142	ASP
1	H	147	THR
1	H	148	LYS
1	H	167	PRO
1	H	168	GLU
1	H	171	ARG
1	H	173	ASP
1	H	181	SER
1	H	206	ASP
1	H	253	SER
1	H	286	ASN
1	H	302	ASP
1	H	320	ASN
1	H	327	ASN

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Mol	Chain	Res	Type
1	H	372	LYS
1	H	380	ILE
1	H	386	THR
1	H	398	LYS
1	H	401	LYS
1	H	428	MET
1	H	431	ARG
1	H	434	MET
1	H	449	GLU
1	H	463	ASP
1	H	473	GLU
1	H	477	THR
1	H	479	SER
1	H	482	GLU
1	H	531	LEU
1	H	545	VAL
1	H	549	VAL
1	I	141	ASN
1	I	147	THR
1	I	148	LYS
1	I	172	ARG
1	I	181	SER
1	I	194	LEU
1	I	205	THR
1	I	206	ASP
1	I	239	SER
1	I	289	ARG
1	I	322	GLN
1	I	386	THR
1	I	411	ARG
1	I	428	MET
1	I	431	ARG
1	I	438	SER
1	I	449	GLU
1	I	463	ASP
1	I	470	LYS
1	I	531	LEU
1	I	549	VAL
1	I	552	LEU
1	J	35	SER
1	J	44	ARG
1	J	120	SER

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Mol	Chain	Res	Type
1	J	134	ARG
1	J	147	THR
1	J	148	LYS
1	J	165	LYS
1	J	176	SER
1	J	184	ARG
1	J	194	LEU
1	J	205	THR
1	J	206	ASP
1	J	280	MET
1	J	386	THR
1	J	401	LYS
1	J	428	MET
1	J	434	MET
1	J	449	GLU
1	J	463	ASP
1	J	465	LYS
1	J	473	GLU
1	J	531	LEU
1	J	549	VAL
1	J	550	MET
1	J	552	LEU
1	K	35	SER
1	K	44	ARG
1	K	113	ARG
1	K	120	SER
1	K	142	ASP
1	K	148	LYS
1	K	173	ASP
1	K	194	LEU
1	K	205	THR
1	K	206	ASP
1	K	322	GLN
1	K	372	LYS
1	K	386	THR
1	K	401	LYS
1	K	428	MET
1	K	431	ARG
1	K	473	GLU
1	K	549	VAL
1	K	552	LEU
1	L	110	MET

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Mol	Chain	Res	Type
1	L	139	LYS
1	L	142	ASP
1	L	147	THR
1	L	167	PRO
1	L	168	GLU
1	L	171	ARG
1	L	176	SER
1	L	194	LEU
1	L	205	THR
1	L	206	ASP
1	L	247	THR
1	L	280	MET
1	L	386	THR
1	L	387	LEU
1	L	398	LYS
1	L	401	LYS
1	L	431	ARG
1	L	434	MET
1	L	449	GLU
1	L	463	ASP
1	L	473	GLU
1	L	545	VAL
1	L	549	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (162) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	41	GLN
1	A	100	GLN
1	A	126	HIS
1	A	249	HIS
1	A	254	GLN
1	A	262	HIS
1	A	295	HIS
1	A	325	GLN
1	A	327	ASN
1	A	350	GLN
1	A	533	GLN
1	A	554	HIS
1	A	557	HIS
1	B	41	GLN
1	B	132	HIS

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Mol	Chain	Res	Type
1	B	149	GLN
1	B	249	HIS
1	B	254	GLN
1	B	295	HIS
1	B	325	GLN
1	B	368	ASN
1	B	417	GLN
1	B	421	HIS
1	B	554	HIS
1	B	558	HIS
1	C	41	GLN
1	C	79	GLN
1	C	85	GLN
1	C	100	GLN
1	C	149	GLN
1	C	249	HIS
1	C	254	GLN
1	C	295	HIS
1	C	325	GLN
1	C	327	ASN
1	C	368	ASN
1	C	421	HIS
1	C	533	GLN
1	C	558	HIS
1	D	85	GLN
1	D	100	GLN
1	D	132	HIS
1	D	149	GLN
1	D	249	HIS
1	D	254	GLN
1	D	295	HIS
1	D	320	ASN
1	D	325	GLN
1	D	555	HIS
1	D	557	HIS
1	D	558	HIS
1	E	85	GLN
1	E	94	HIS
1	E	100	GLN
1	E	132	HIS
1	E	149	GLN
1	E	254	GLN

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Mol	Chain	Res	Type
1	E	295	HIS
1	E	325	GLN
1	E	327	ASN
1	E	388	ASN
1	E	522	GLN
1	E	533	GLN
1	E	554	HIS
1	E	555	HIS
1	E	557	HIS
1	E	558	HIS
1	F	41	GLN
1	F	43	GLN
1	F	85	GLN
1	F	100	GLN
1	F	249	HIS
1	F	295	HIS
1	F	325	GLN
1	F	327	ASN
1	F	388	ASN
1	F	421	HIS
1	F	533	GLN
1	F	558	HIS
1	G	41	GLN
1	G	85	GLN
1	G	126	HIS
1	G	249	HIS
1	G	254	GLN
1	G	295	HIS
1	G	325	GLN
1	G	327	ASN
1	G	333	ASN
1	G	533	GLN
1	G	554	HIS
1	G	558	HIS
1	H	41	GLN
1	H	149	GLN
1	H	153	GLN
1	H	249	HIS
1	H	254	GLN
1	H	295	HIS
1	H	320	ASN
1	H	325	GLN

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Mol	Chain	Res	Type
1	H	327	ASN
1	H	368	ASN
1	H	421	HIS
1	H	533	GLN
1	H	554	HIS
1	H	557	HIS
1	H	558	HIS
1	I	41	GLN
1	I	95	ASN
1	I	100	GLN
1	I	149	GLN
1	I	249	HIS
1	I	320	ASN
1	I	325	GLN
1	I	327	ASN
1	I	368	ASN
1	I	421	HIS
1	I	533	GLN
1	J	41	GLN
1	J	94	HIS
1	J	100	GLN
1	J	126	HIS
1	J	132	HIS
1	J	153	GLN
1	J	249	HIS
1	J	254	GLN
1	J	295	HIS
1	J	320	ASN
1	J	322	GLN
1	J	325	GLN
1	J	421	HIS
1	J	554	HIS
1	J	555	HIS
1	J	557	HIS
1	J	558	HIS
1	K	41	GLN
1	K	79	GLN
1	K	100	GLN
1	K	249	HIS
1	K	254	GLN
1	K	320	ASN
1	K	325	GLN

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Mol	Chain	Res	Type
1	K	327	ASN
1	K	350	GLN
1	K	533	GLN
1	K	554	HIS
1	K	557	HIS
1	L	41	GLN
1	L	43	GLN
1	L	100	GLN
1	L	149	GLN
1	L	249	HIS
1	L	254	GLN
1	L	295	HIS
1	L	320	ASN
1	L	325	GLN
1	L	332	ASN
1	L	368	ASN
1	L	417	GLN
1	L	421	HIS
1	L	554	HIS
1	L	557	HIS
1	L	558	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

20 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	GLC	M	1	2	11,11,12	1.06	1 (9%)	15,15,17	1.93	3 (20%)
2	GLC	M	2	2	12,12,12	0.68	0	17,17,17	1.29	3 (17%)
2	GLC	N	1	2	11,11,12	0.36	0	15,15,17	0.55	0
2	GLC	N	2	2	12,12,12	0.42	0	17,17,17	1.00	0
2	GLC	O	1	2	11,11,12	1.05	0	15,15,17	1.41	3 (20%)
2	GLC	O	2	2	12,12,12	0.53	0	17,17,17	1.25	3 (17%)
2	GLC	P	1	2	11,11,12	0.58	0	15,15,17	1.29	2 (13%)
2	GLC	P	2	2	12,12,12	0.92	0	17,17,17	1.67	4 (23%)
2	GLC	Q	1	2	11,11,12	0.38	0	15,15,17	0.92	0
2	GLC	Q	2	2	12,12,12	0.39	0	17,17,17	0.53	0
2	GLC	R	1	2	11,11,12	1.12	1 (9%)	15,15,17	1.92	4 (26%)
2	GLC	R	2	2	12,12,12	0.65	0	17,17,17	1.34	3 (17%)
2	GLC	S	1	2	11,11,12	0.58	0	15,15,17	1.55	2 (13%)
2	GLC	S	2	2	12,12,12	1.04	0	17,17,17	1.49	6 (35%)
2	GLC	T	1	2	11,11,12	1.39	1 (9%)	15,15,17	1.19	1 (6%)
2	GLC	T	2	2	12,12,12	1.57	1 (8%)	17,17,17	1.22	1 (5%)
2	GLC	U	1	2	11,11,12	0.53	0	15,15,17	1.45	2 (13%)
2	GLC	U	2	2	12,12,12	1.00	1 (8%)	17,17,17	1.56	4 (23%)
2	GLC	V	1	2	11,11,12	1.16	1 (9%)	15,15,17	2.07	6 (40%)
2	GLC	V	2	2	12,12,12	0.69	0	17,17,17	1.26	2 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GLC	M	1	2	-	0/2/19/22	0/1/1/1
2	GLC	M	2	2	-	2/2/22/22	0/1/1/1
2	GLC	N	1	2	-	0/2/19/22	0/1/1/1
2	GLC	N	2	2	-	0/2/22/22	0/1/1/1
2	GLC	O	1	2	-	0/2/19/22	0/1/1/1
2	GLC	O	2	2	-	0/2/22/22	0/1/1/1
2	GLC	P	1	2	-	2/2/19/22	0/1/1/1
2	GLC	P	2	2	-	0/2/22/22	0/1/1/1
2	GLC	Q	1	2	-	0/2/19/22	0/1/1/1
2	GLC	Q	2	2	-	0/2/22/22	0/1/1/1
2	GLC	R	1	2	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GLC	R	2	2	-	2/2/22/22	0/1/1/1
2	GLC	S	1	2	-	0/2/19/22	0/1/1/1
2	GLC	S	2	2	-	2/2/22/22	0/1/1/1
2	GLC	T	1	2	-	2/2/19/22	0/1/1/1
2	GLC	T	2	2	-	0/2/22/22	0/1/1/1
2	GLC	U	1	2	-	0/2/19/22	0/1/1/1
2	GLC	U	2	2	-	0/2/22/22	0/1/1/1
2	GLC	V	1	2	-	0/2/19/22	0/1/1/1
2	GLC	V	2	2	-	0/2/22/22	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	T	2	GLC	C4-C5	2.81	1.59	1.53
2	T	1	GLC	O4-C4	2.48	1.49	1.43
2	R	1	GLC	C4-C3	2.36	1.58	1.52
2	V	1	GLC	C4-C3	2.33	1.58	1.52
2	M	1	GLC	C4-C3	2.22	1.58	1.52
2	U	2	GLC	C4-C5	2.21	1.57	1.53

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	1	GLC	O3-C3-C4	4.78	121.64	110.38
2	V	1	GLC	O3-C3-C4	4.21	120.30	110.38
2	R	1	GLC	O3-C3-C4	4.16	120.19	110.38
2	S	1	GLC	C1-O5-C5	3.77	117.24	112.19
2	V	1	GLC	C2-C3-C4	-3.59	104.55	110.86
2	U	1	GLC	O5-C5-C6	3.30	114.09	107.66
2	R	1	GLC	O2-C2-C1	3.16	116.45	109.22
2	P	2	GLC	O5-C1-C2	3.14	115.82	110.30
2	M	1	GLC	C2-C3-C4	-3.13	105.36	110.86
2	O	1	GLC	C3-C4-C5	3.12	115.89	110.23
2	T	2	GLC	O4-C4-C5	3.03	116.78	109.32
2	U	2	GLC	C3-C4-C5	3.02	115.71	110.23
2	U	2	GLC	O5-C1-C2	3.01	115.60	110.30
2	P	2	GLC	C4-C3-C2	-2.94	105.66	110.83
2	V	1	GLC	O2-C2-C1	2.93	115.92	109.22
2	S	1	GLC	O5-C5-C6	2.84	113.19	107.66
2	V	2	GLC	O3-C3-C2	2.83	117.04	110.38
2	U	2	GLC	C4-C3-C2	-2.71	106.07	110.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	2	GLC	O3-C3-C4	2.71	116.76	110.38
2	R	1	GLC	O3-C3-C2	-2.67	104.61	110.05
2	M	2	GLC	O3-C3-C2	2.66	116.64	110.38
2	V	1	GLC	O4-C4-C3	2.62	116.54	110.38
2	S	2	GLC	C4-C3-C2	-2.61	106.25	110.83
2	U	1	GLC	O5-C5-C4	-2.60	104.51	110.83
2	V	2	GLC	O5-C5-C6	2.52	112.67	106.44
2	O	2	GLC	O5-C5-C6	2.46	112.55	106.44
2	S	2	GLC	O2-C2-C1	2.46	114.92	109.25
2	R	2	GLC	O3-C3-C2	2.46	116.17	110.38
2	R	1	GLC	C2-C3-C4	-2.43	106.59	110.86
2	R	2	GLC	O2-C2-C1	-2.42	103.67	109.25
2	T	1	GLC	O5-C1-C2	2.41	116.55	110.79
2	P	1	GLC	O5-C5-C4	-2.37	105.07	110.83
2	S	2	GLC	C3-C4-C5	2.31	114.43	110.23
2	S	2	GLC	C1-C2-C3	-2.31	105.64	110.36
2	O	1	GLC	C1-O5-C5	2.31	115.28	112.19
2	O	2	GLC	O5-C5-C4	-2.27	105.61	109.70
2	R	2	GLC	O5-C5-C6	2.26	112.03	106.44
2	S	2	GLC	O2-C2-C3	2.26	115.69	110.38
2	M	1	GLC	O2-C2-C1	2.23	114.32	109.22
2	O	1	GLC	C2-C3-C4	-2.18	107.02	110.86
2	M	2	GLC	O2-C2-C1	-2.18	104.22	109.25
2	P	1	GLC	O5-C5-C6	2.16	111.86	107.66
2	O	2	GLC	O5-C1-C2	2.15	114.09	110.30
2	V	1	GLC	C3-C4-C5	2.08	114.00	110.23
2	M	2	GLC	O5-C5-C6	2.07	111.56	106.44
2	P	2	GLC	C3-C4-C5	2.06	113.96	110.23
2	S	2	GLC	O5-C1-C2	2.05	113.91	110.30
2	V	1	GLC	O3-C3-C2	-2.05	105.87	110.05
2	U	2	GLC	O1-C1-C2	-2.05	103.05	108.98

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	T	1	GLC	O5-C5-C6-O6
2	M	2	GLC	C4-C5-C6-O6
2	T	1	GLC	C4-C5-C6-O6
2	M	2	GLC	O5-C5-C6-O6
2	P	1	GLC	C4-C5-C6-O6
2	P	1	GLC	O5-C5-C6-O6

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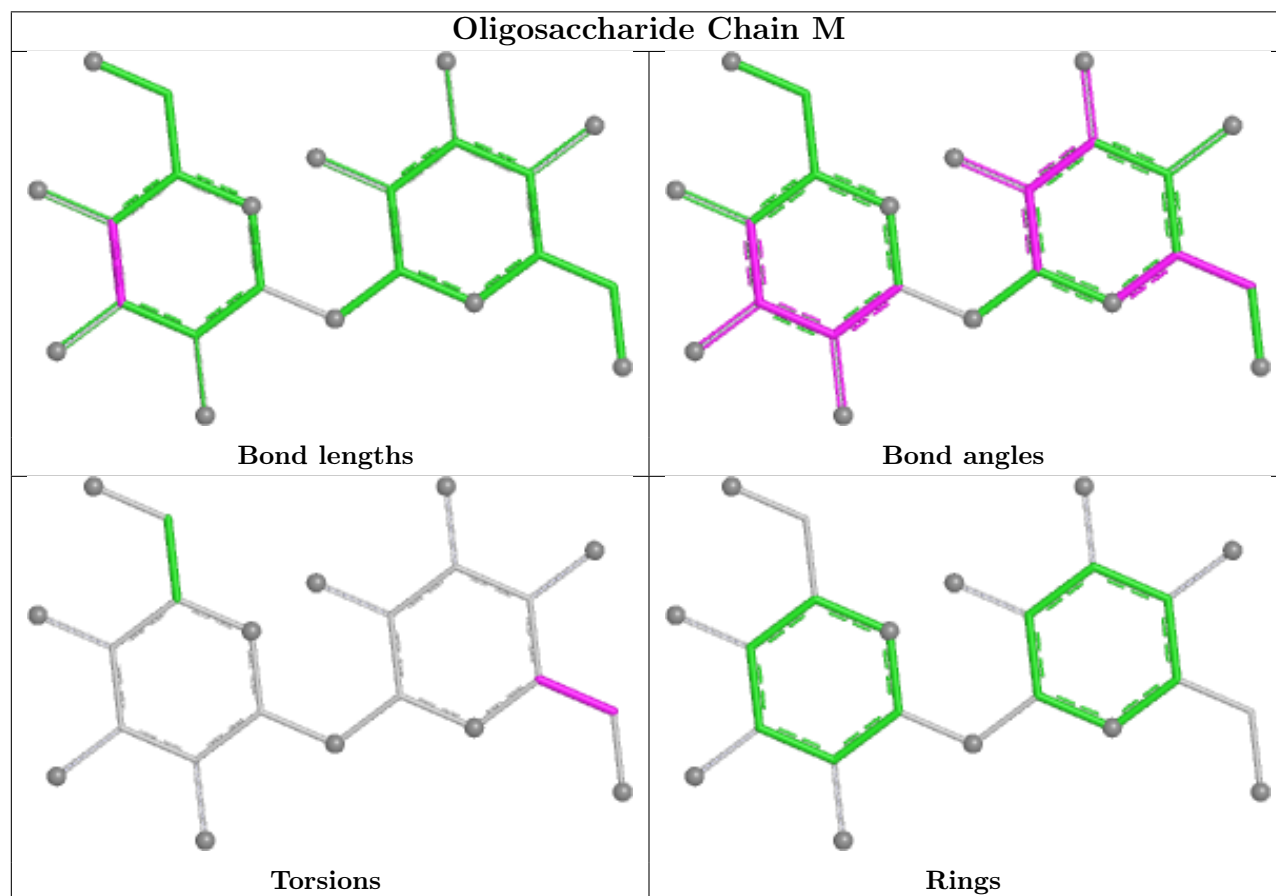
Mol	Chain	Res	Type	Atoms
2	R	2	GLC	C4-C5-C6-O6
2	S	2	GLC	C4-C5-C6-O6
2	S	2	GLC	O5-C5-C6-O6
2	R	2	GLC	O5-C5-C6-O6

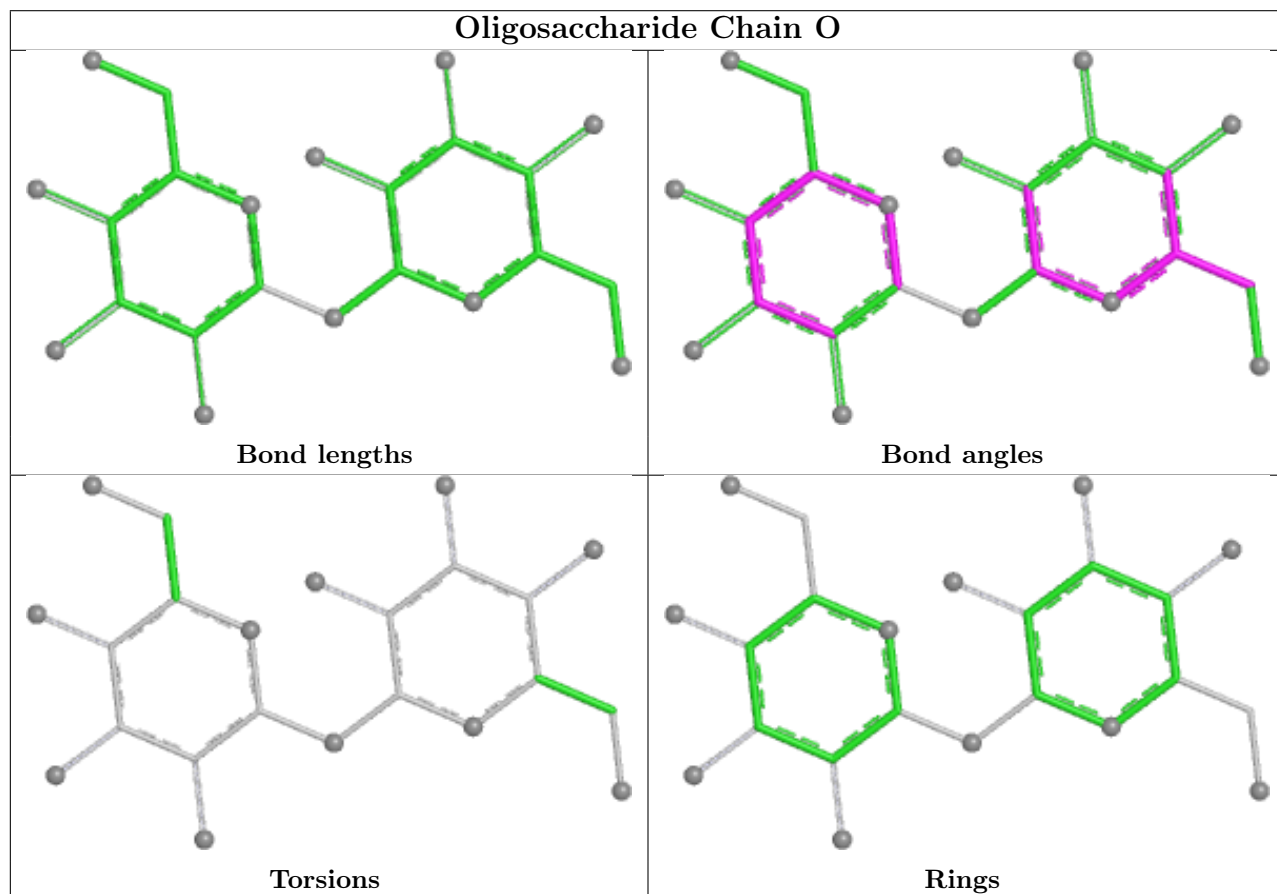
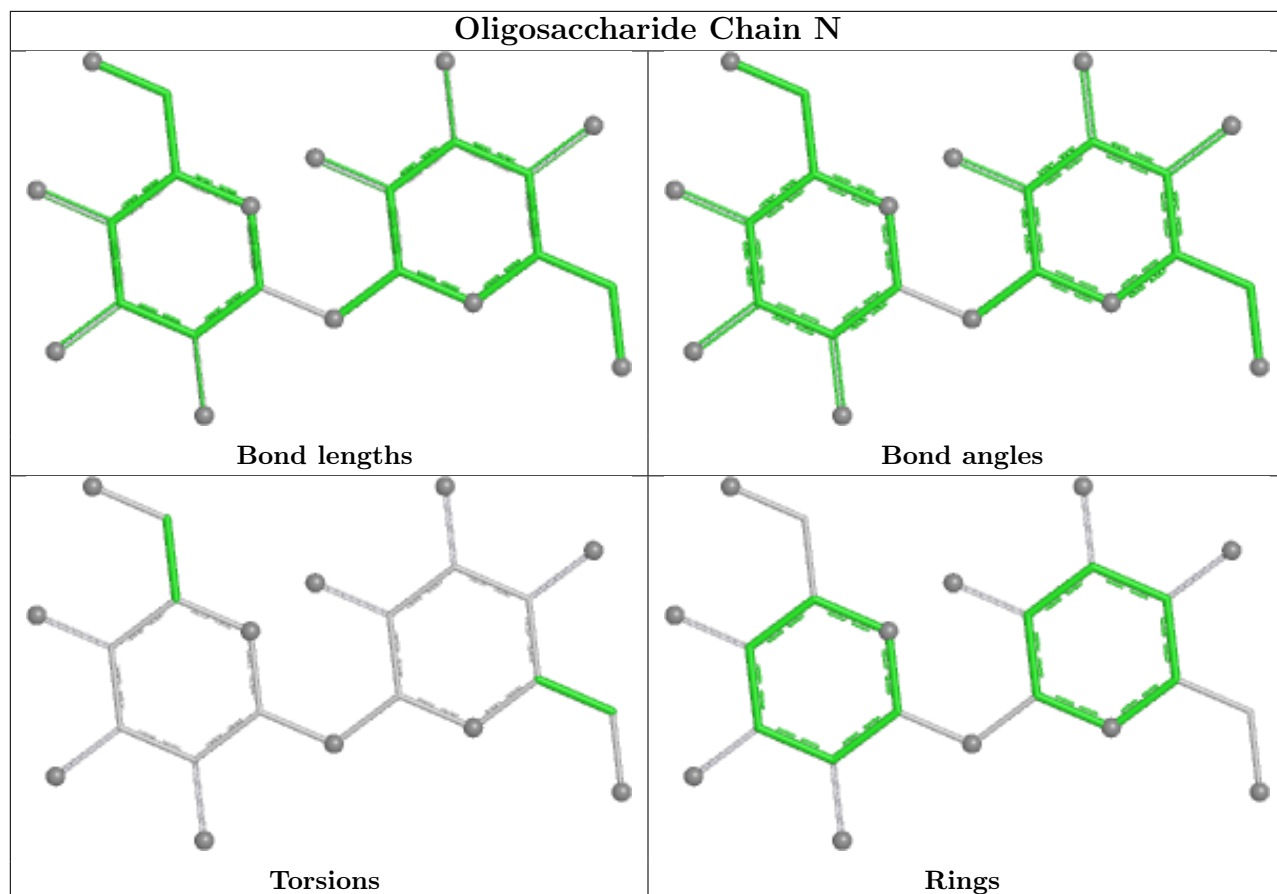
There are no ring outliers.

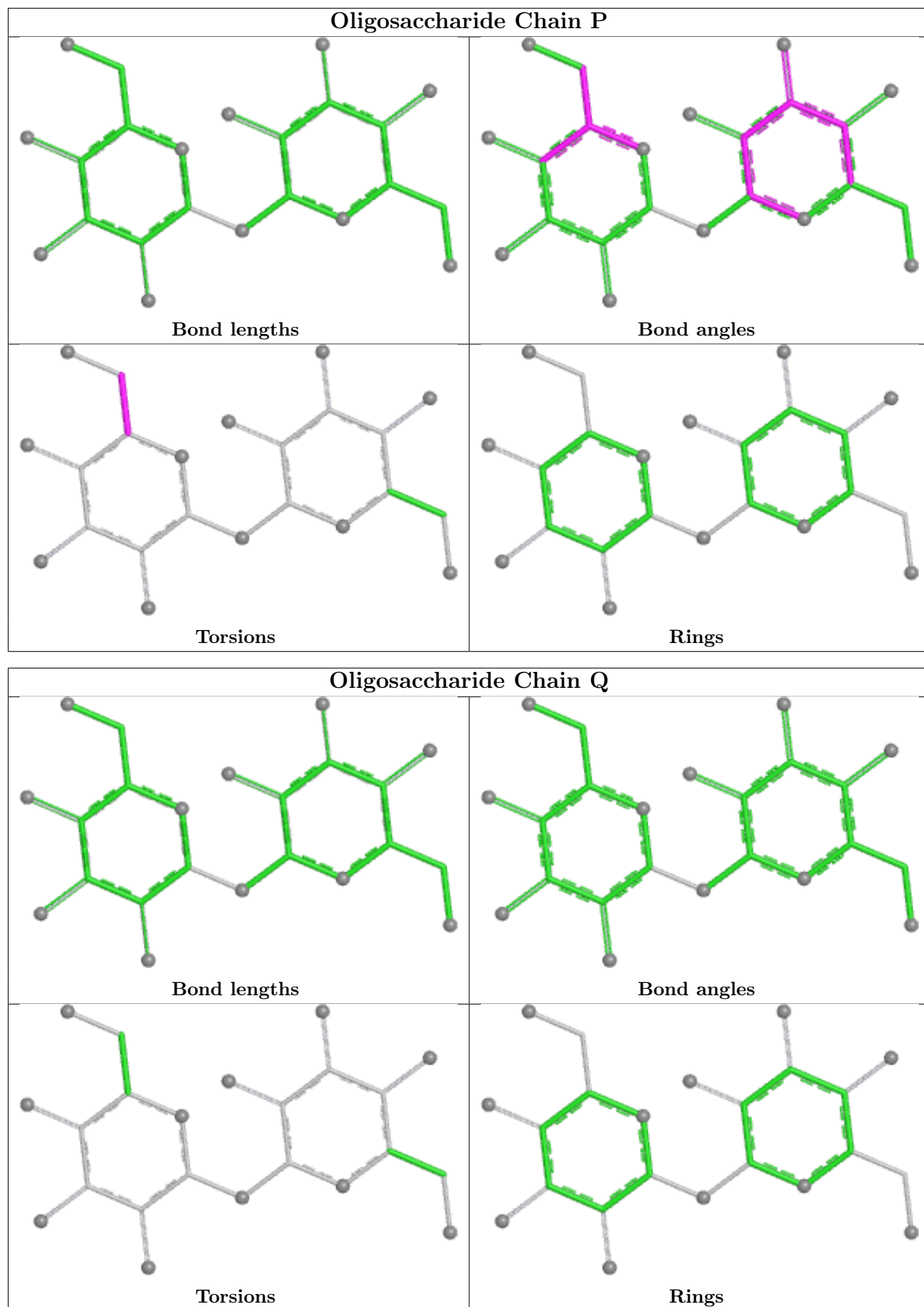
1 monomer is involved in 1 short contact:

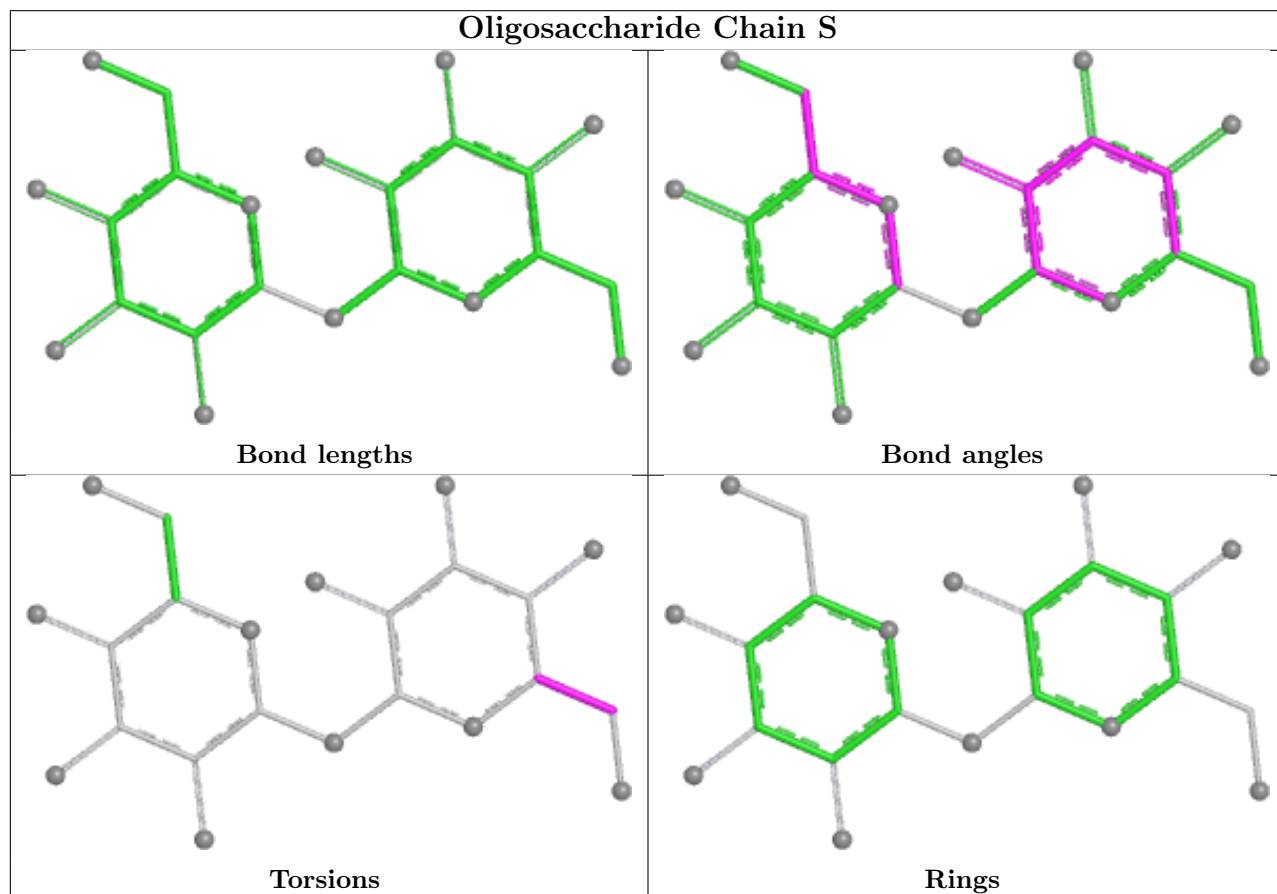
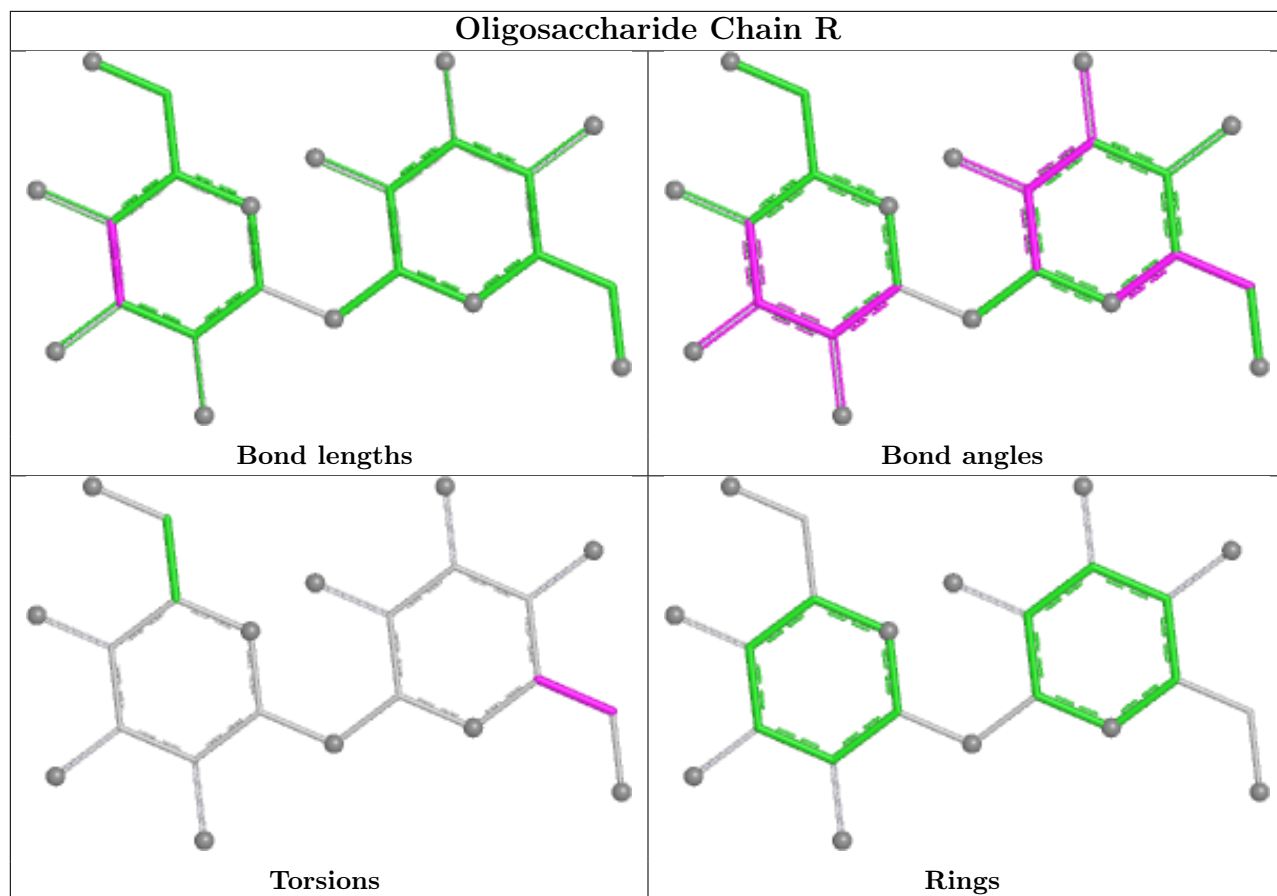
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	Q	1	GLC	1	0

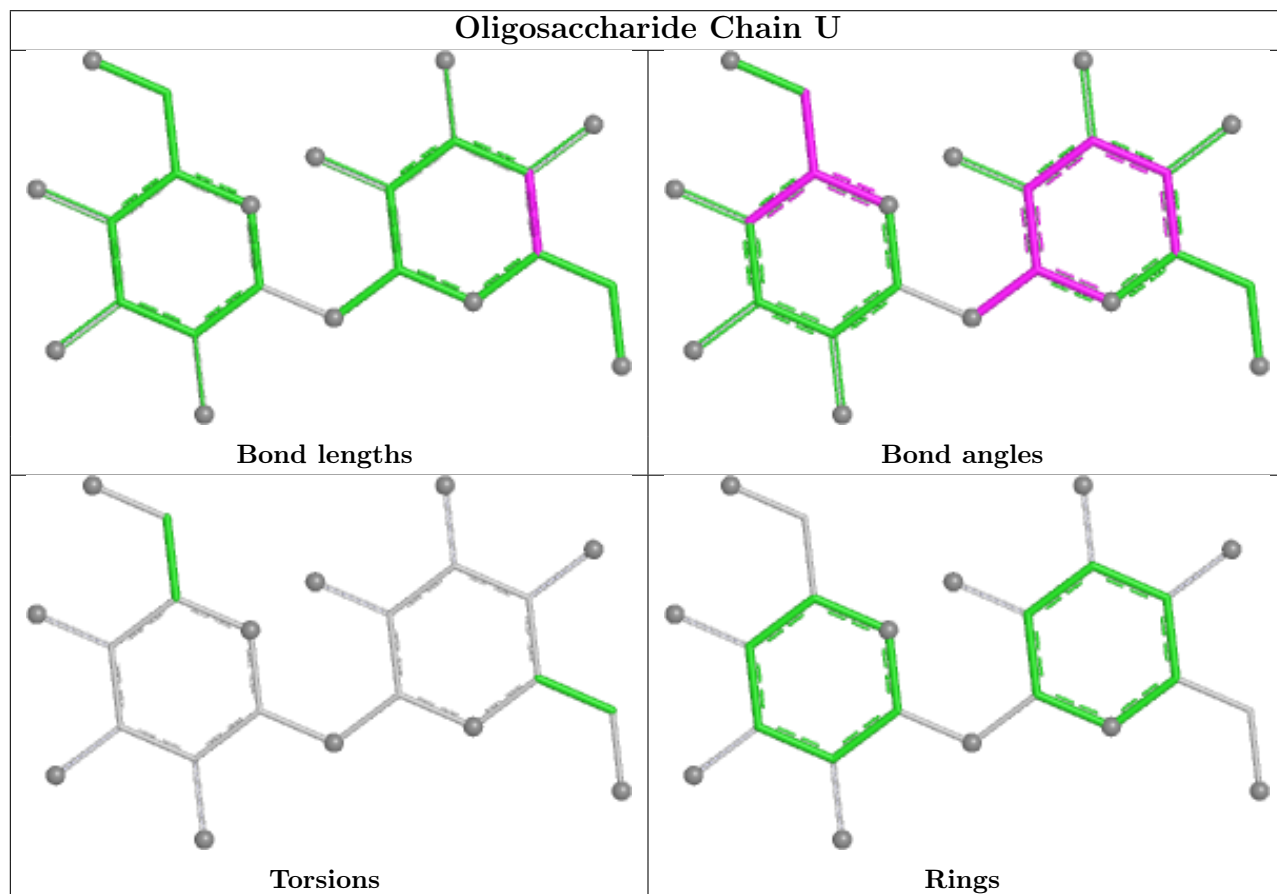
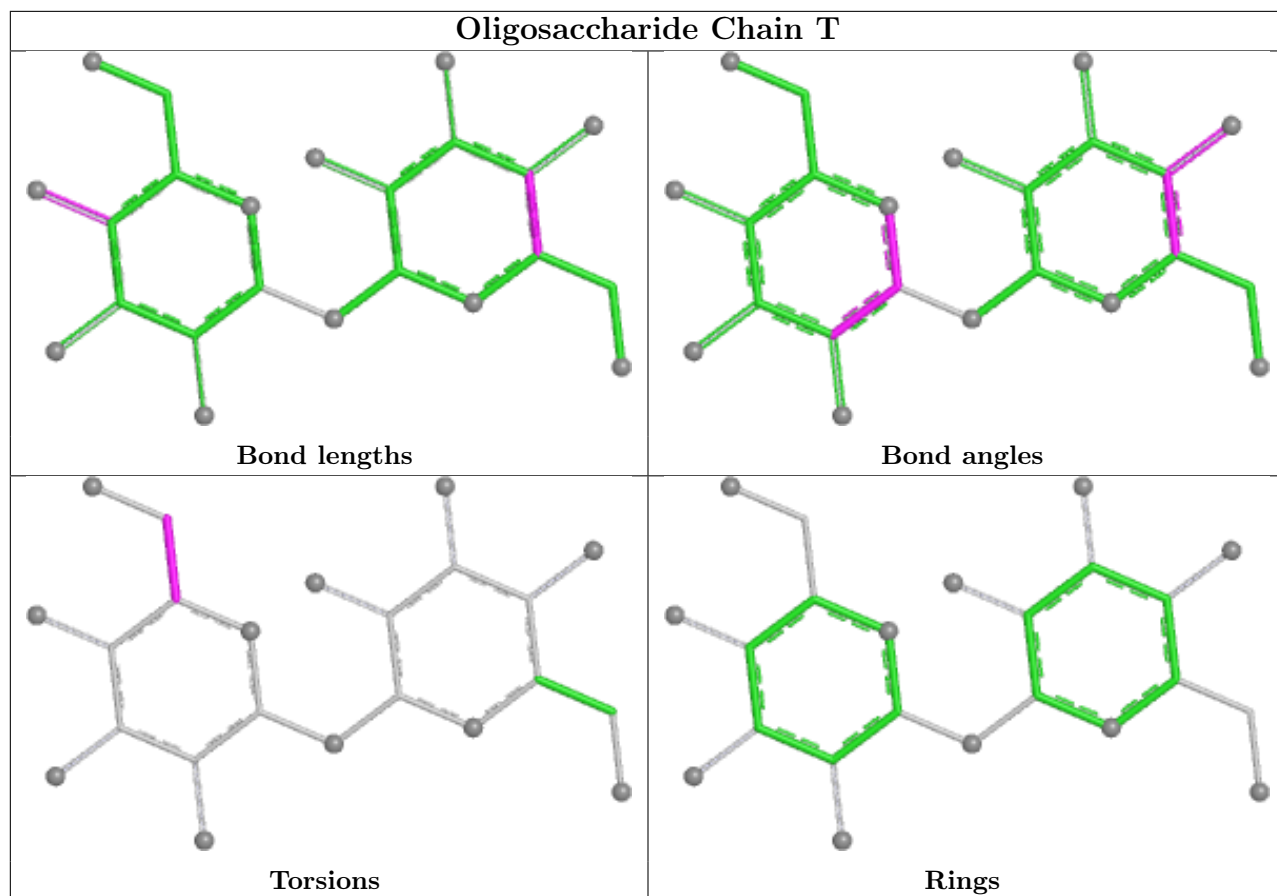
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

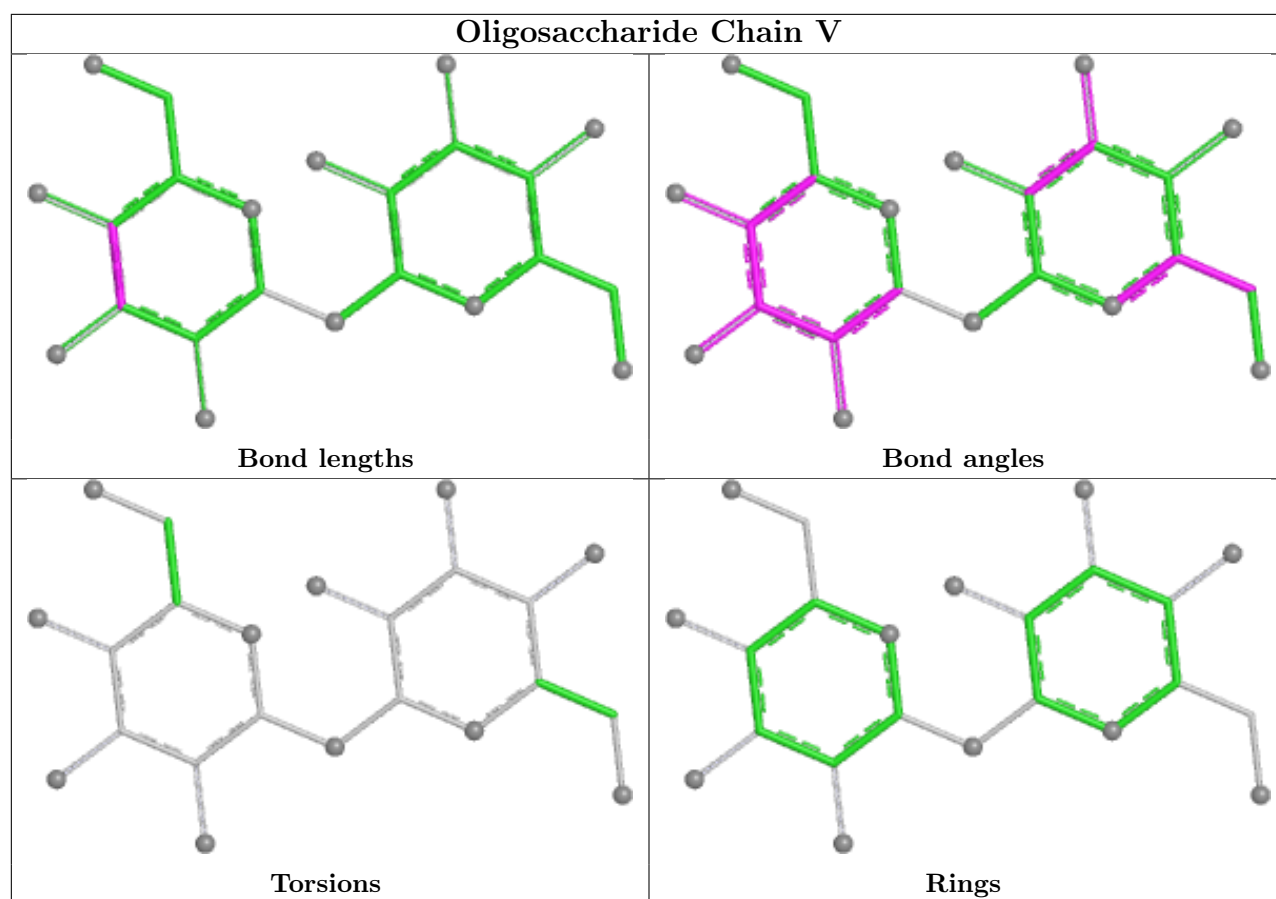












5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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	524/559 (93%)	-0.07	19 (3%) 46 38	20, 31, 57, 86	0
1	B	524/559 (93%)	0.12	31 (5%) 28 23	22, 36, 69, 92	0
1	C	524/559 (93%)	-0.00	22 (4%) 40 33	20, 33, 66, 94	0
1	D	524/559 (93%)	-0.05	17 (3%) 50 43	20, 32, 57, 82	0
1	E	524/559 (93%)	-0.03	17 (3%) 50 43	21, 32, 58, 92	0
1	F	524/559 (93%)	0.03	27 (5%) 33 28	20, 34, 66, 98	0
1	G	524/559 (93%)	-0.11	16 (3%) 51 44	20, 31, 58, 89	0
1	H	524/559 (93%)	0.13	34 (6%) 25 21	24, 36, 68, 94	0
1	I	524/559 (93%)	0.01	26 (4%) 34 28	20, 33, 65, 104	0
1	J	524/559 (93%)	-0.05	19 (3%) 46 38	20, 32, 59, 84	0
1	K	524/559 (93%)	-0.11	20 (3%) 44 36	20, 31, 59, 89	0
1	L	524/559 (93%)	0.13	33 (6%) 26 22	24, 37, 68, 96	0
All	All	6288/6708 (93%)	0.00	281 (4%) 38 31	20, 33, 64, 104	0

All (281) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	436	GLY	6.8
1	F	187	ASP	6.8
1	I	35	SER	5.6
1	L	193	GLY	5.2
1	J	142	ASP	5.0
1	B	35	SER	5.0
1	I	551	SER	4.9
1	J	147	THR	4.8
1	I	142	ASP	4.6
1	J	148	LYS	4.6
1	F	75	THR	4.5

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Mol	Chain	Res	Type	RSRZ
1	F	142	ASP	4.5
1	B	556	HIS	4.5
1	C	35	SER	4.5
1	I	75	THR	4.4
1	G	552	LEU	4.4
1	G	148	LYS	4.4
1	E	142	ASP	4.3
1	K	552	LEU	4.3
1	L	556	HIS	4.2
1	A	142	ASP	4.2
1	D	435	GLY	4.2
1	C	171	ARG	4.1
1	F	35	SER	4.1
1	H	435	GLY	4.0
1	H	35	SER	4.0
1	H	556	HIS	4.0
1	C	142	ASP	4.0
1	J	435	GLY	4.0
1	D	148	LYS	3.9
1	I	554	HIS	3.9
1	A	557	HIS	3.9
1	I	143	ALA	3.9
1	F	143	ALA	3.9
1	B	436	GLY	3.8
1	H	436	GLY	3.8
1	H	39	ASP	3.8
1	I	171	ARG	3.8
1	L	555	HIS	3.8
1	L	449	GLU	3.8
1	C	148	LYS	3.8
1	B	147	THR	3.8
1	C	554	HIS	3.7
1	G	557	HIS	3.7
1	B	435	GLY	3.7
1	H	555	HIS	3.7
1	F	551	SER	3.7
1	L	35	SER	3.7
1	K	435	GLY	3.7
1	F	67	ARG	3.7
1	F	113	ARG	3.7
1	B	39	ASP	3.7
1	D	436	GLY	3.7

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Mol	Chain	Res	Type	RSRZ
1	I	141	ASN	3.7
1	K	168	GLU	3.6
1	K	557	HIS	3.6
1	K	144	GLY	3.6
1	I	113	ARG	3.6
1	E	462	GLY	3.6
1	I	552	LEU	3.6
1	F	148	LYS	3.5
1	A	552	LEU	3.5
1	L	75	THR	3.5
1	H	172	ARG	3.5
1	C	144	GLY	3.5
1	L	552	LEU	3.5
1	C	147	THR	3.5
1	F	555	HIS	3.4
1	A	551	SER	3.4
1	H	75	THR	3.4
1	L	111	GLY	3.4
1	H	153	GLN	3.4
1	J	144	GLY	3.4
1	D	142	ASP	3.4
1	H	151	GLU	3.3
1	I	555	HIS	3.3
1	K	142	ASP	3.3
1	B	75	THR	3.3
1	D	195	SER	3.3
1	A	193	GLY	3.3
1	I	368	ASN	3.3
1	A	144	GLY	3.3
1	H	152	GLY	3.3
1	E	463	ASP	3.3
1	E	435	GLY	3.3
1	I	144	GLY	3.3
1	K	551	SER	3.3
1	H	449	GLU	3.2
1	A	147	THR	3.2
1	A	461	GLY	3.2
1	H	144	GLY	3.2
1	G	551	SER	3.2
1	B	148	LYS	3.2
1	D	552	LEU	3.2
1	F	144	GLY	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	435	GLY	3.2
1	J	462	GLY	3.2
1	G	151	GLU	3.1
1	C	555	HIS	3.1
1	I	558	HIS	3.1
1	B	171	ARG	3.1
1	C	67	ARG	3.1
1	I	67	ARG	3.1
1	I	148	LYS	3.1
1	F	188	ASP	3.1
1	J	551	SER	3.1
1	F	147	THR	3.1
1	F	172	ARG	3.1
1	L	147	THR	3.1
1	C	551	SER	3.1
1	E	551	SER	3.1
1	E	144	GLY	3.1
1	B	555	HIS	3.0
1	L	79	GLN	3.0
1	E	143	ALA	3.0
1	H	551	SER	3.0
1	F	435	GLY	3.0
1	K	558	HIS	3.0
1	I	187	ASP	3.0
1	F	549	VAL	3.0
1	E	79	GLN	3.0
1	K	79	GLN	3.0
1	B	368	ASN	2.9
1	G	147	THR	2.9
1	A	558	HIS	2.9
1	C	113	ARG	2.9
1	L	152	GLY	2.9
1	K	554	HIS	2.9
1	E	436	GLY	2.9
1	L	550	MET	2.9
1	L	39	ASP	2.9
1	B	98	ASN	2.9
1	H	98	ASN	2.9
1	B	113	ARG	2.9
1	C	172	ARG	2.8
1	I	435	GLY	2.8
1	B	167	PRO	2.8

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Mol	Chain	Res	Type	RSRZ
1	H	463	ASP	2.8
1	G	144	GLY	2.8
1	L	462	GLY	2.8
1	C	435	GLY	2.8
1	J	436	GLY	2.8
1	B	79	GLN	2.8
1	I	147	THR	2.8
1	A	79	GLN	2.7
1	A	556	HIS	2.7
1	F	139	LYS	2.7
1	I	550	MET	2.7
1	C	75	THR	2.7
1	J	552	LEU	2.7
1	E	557	HIS	2.7
1	D	172	ARG	2.7
1	H	79	GLN	2.7
1	L	151	GLU	2.7
1	L	148	LYS	2.7
1	B	462	GLY	2.7
1	H	549	VAL	2.7
1	D	144	GLY	2.7
1	B	551	SER	2.7
1	D	143	ALA	2.6
1	B	172	ARG	2.6
1	F	368	ASN	2.6
1	L	551	SER	2.6
1	A	436	GLY	2.6
1	B	549	VAL	2.6
1	J	463	ASP	2.6
1	K	143	ALA	2.6
1	E	461	GLY	2.6
1	B	550	MET	2.6
1	J	79	GLN	2.6
1	D	465	LYS	2.5
1	B	144	GLY	2.5
1	B	552	LEU	2.5
1	E	147	THR	2.5
1	L	153	GLN	2.5
1	G	142	ASP	2.5
1	A	143	ALA	2.5
1	F	557	HIS	2.5
1	E	552	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	F	552	LEU	2.5
1	D	449	GLU	2.5
1	G	555	HIS	2.5
1	H	550	MET	2.5
1	H	147	THR	2.5
1	B	557	HIS	2.4
1	L	223	LYS	2.4
1	J	554	HIS	2.4
1	L	557	HIS	2.4
1	B	179	GLY	2.4
1	B	460	VAL	2.4
1	F	152	GLY	2.4
1	L	463	ASP	2.4
1	L	549	VAL	2.4
1	J	465	LYS	2.4
1	A	554	HIS	2.4
1	F	286	ASN	2.4
1	D	193	GLY	2.4
1	H	462	GLY	2.4
1	L	435	GLY	2.4
1	F	173	ASP	2.4
1	B	386	THR	2.4
1	B	152	GLY	2.3
1	E	172	ARG	2.3
1	G	152	GLY	2.3
1	H	461	GLY	2.3
1	J	168	GLU	2.3
1	H	552	LEU	2.3
1	D	462	GLY	2.3
1	H	143	ALA	2.3
1	L	368	ASN	2.3
1	L	85	GLN	2.3
1	J	75	THR	2.3
1	I	152	GLY	2.3
1	D	79	GLN	2.3
1	L	558	HIS	2.3
1	H	167	PRO	2.3
1	C	461	GLY	2.3
1	I	139	LYS	2.2
1	A	155	ASP	2.2
1	B	547	ASP	2.2
1	G	554	HIS	2.2

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Mol	Chain	Res	Type	RSRZ
1	K	555	HIS	2.2
1	C	552	LEU	2.2
1	E	449	GLU	2.2
1	L	398	LYS	2.2
1	F	94	HIS	2.2
1	D	551	SER	2.2
1	F	461	GLY	2.2
1	H	110	MET	2.2
1	A	166	ALA	2.2
1	F	449	GLU	2.2
1	H	553	GLU	2.2
1	G	67	ARG	2.2
1	G	79	GLN	2.2
1	C	549	VAL	2.2
1	K	436	GLY	2.2
1	L	139	LYS	2.2
1	L	450	LYS	2.2
1	K	449	GLU	2.2
1	C	79	GLN	2.2
1	H	368	ASN	2.2
1	L	144	GLY	2.2
1	K	151	GLU	2.2
1	K	113	ARG	2.1
1	B	139	LYS	2.1
1	K	75	THR	2.1
1	B	553	GLU	2.1
1	D	558	HIS	2.1
1	H	76	MET	2.1
1	K	547	ASP	2.1
1	C	143	ALA	2.1
1	G	556	HIS	2.1
1	J	557	HIS	2.1
1	K	556	HIS	2.1
1	C	550	MET	2.1
1	H	165	LYS	2.1
1	H	67	ARG	2.1
1	J	172	ARG	2.1
1	A	555	HIS	2.1
1	D	450	LYS	2.1
1	G	550	MET	2.1
1	H	94	HIS	2.1
1	I	398	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	I	556	HIS	2.1
1	J	461	GLY	2.1
1	K	152	GLY	2.1
1	L	113	ARG	2.1
1	J	143	ALA	2.1
1	B	154	SER	2.0
1	C	557	HIS	2.0
1	H	171	ARG	2.0
1	E	450	LYS	2.0
1	C	556	HIS	2.0
1	H	557	HIS	2.0
1	I	94	HIS	2.0
1	I	549	VAL	2.0
1	E	150	LEU	2.0
1	L	169	LEU	2.0
1	F	141	ASN	2.0
1	G	166	ALA	2.0
1	A	463	ASP	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.

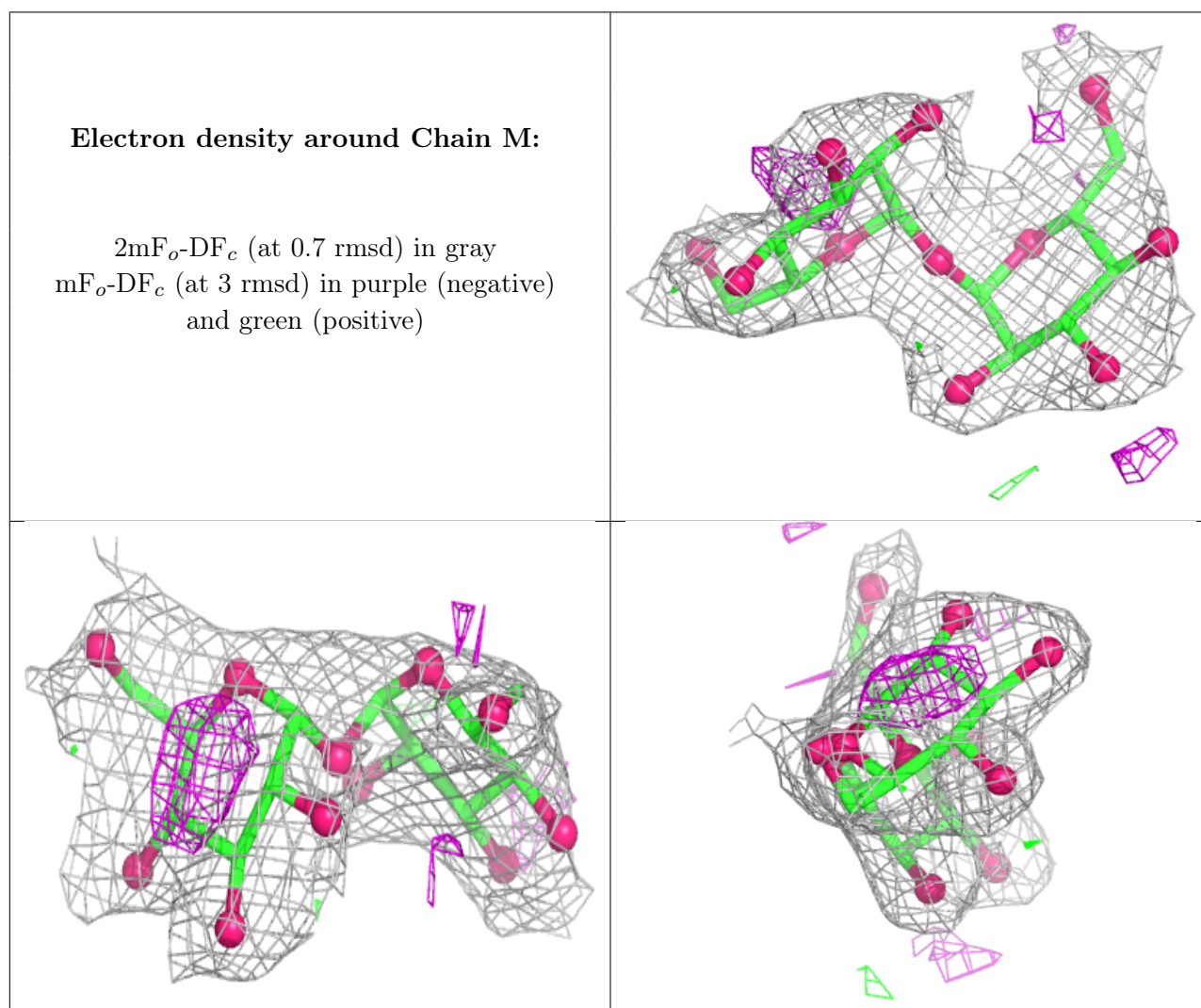
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	GLC	N	2	12/12	0.70	0.17	20,20,20,20	0
2	GLC	Q	1	11/12	0.73	0.16	20,20,20,20	0
2	GLC	N	1	11/12	0.77	0.15	20,20,20,20	0
2	GLC	Q	2	12/12	0.82	0.14	20,20,20,20	0
2	GLC	T	1	11/12	0.82	0.14	36,43,48,57	0
2	GLC	P	2	12/12	0.87	0.15	58,67,73,74	0
2	GLC	O	1	11/12	0.87	0.15	53,67,73,75	0
2	GLC	S	1	11/12	0.90	0.14	63,74,77,78	0
2	GLC	M	1	11/12	0.90	0.14	44,53,58,58	0
2	GLC	T	2	12/12	0.90	0.11	37,42,45,47	0

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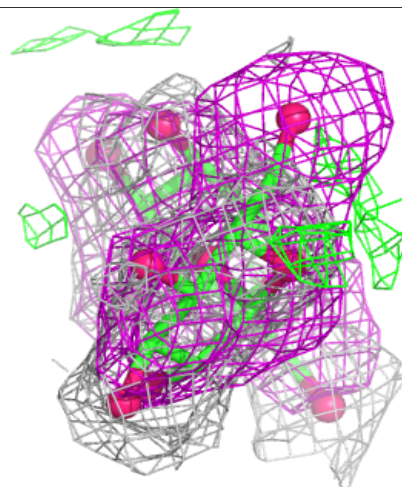
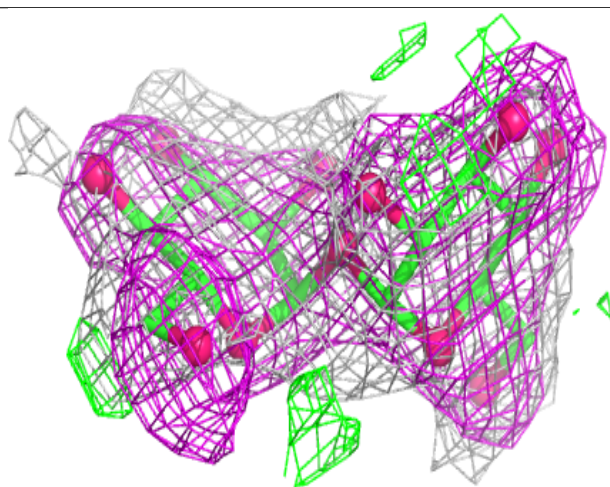
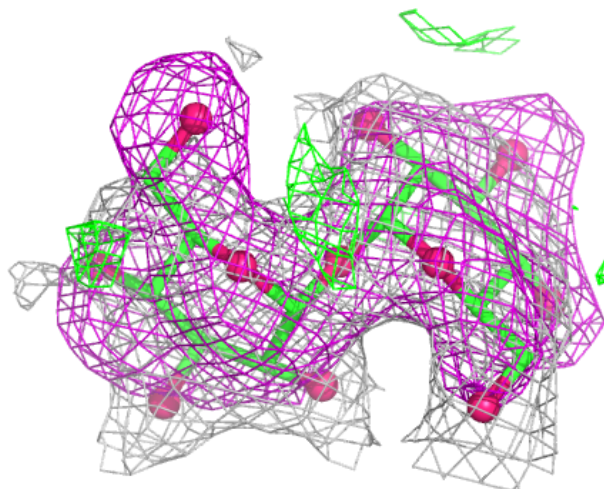
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	GLC	U	2	12/12	0.90	0.12	52,64,68,70	0
2	GLC	S	2	12/12	0.91	0.13	58,68,72,73	0
2	GLC	V	1	11/12	0.91	0.13	42,51,55,56	0
2	GLC	R	1	11/12	0.92	0.13	44,51,53,54	0
2	GLC	O	2	12/12	0.93	0.11	53,70,77,79	0
2	GLC	U	1	11/12	0.93	0.11	50,64,71,73	0
2	GLC	P	1	11/12	0.93	0.11	51,61,74,77	0
2	GLC	R	2	12/12	0.93	0.10	46,54,57,62	0
2	GLC	V	2	12/12	0.93	0.10	47,57,61,64	0
2	GLC	M	2	12/12	0.95	0.10	45,56,62,62	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.



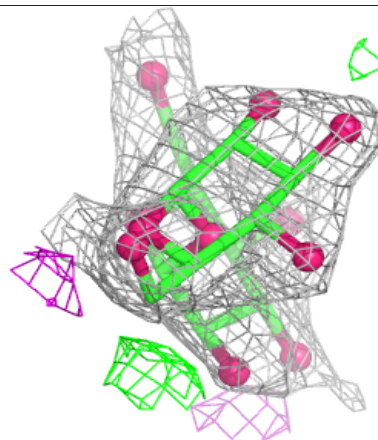
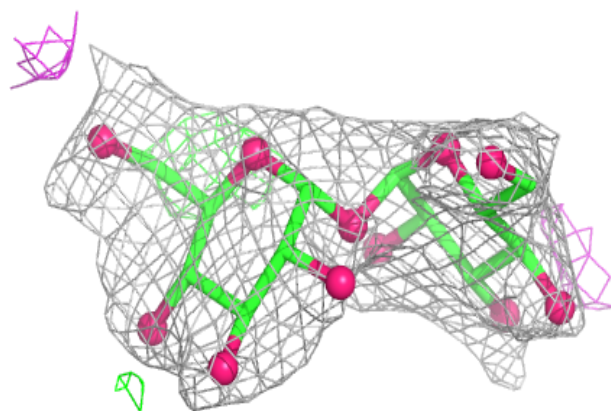
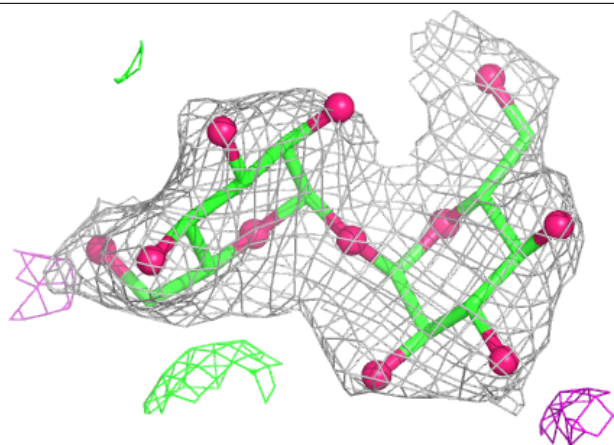
Electron density around Chain N:

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



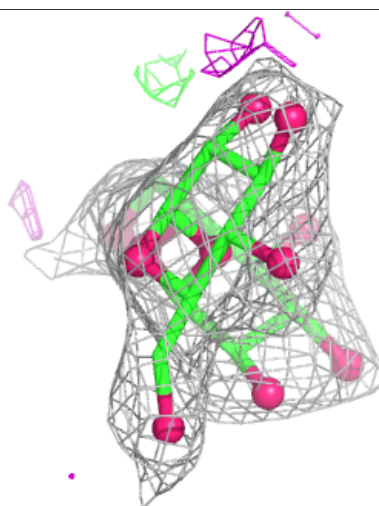
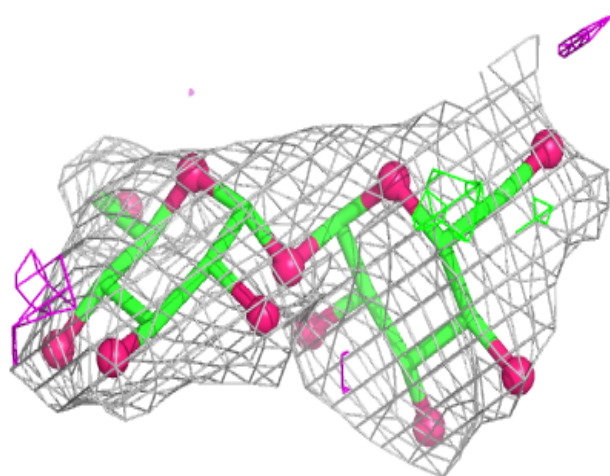
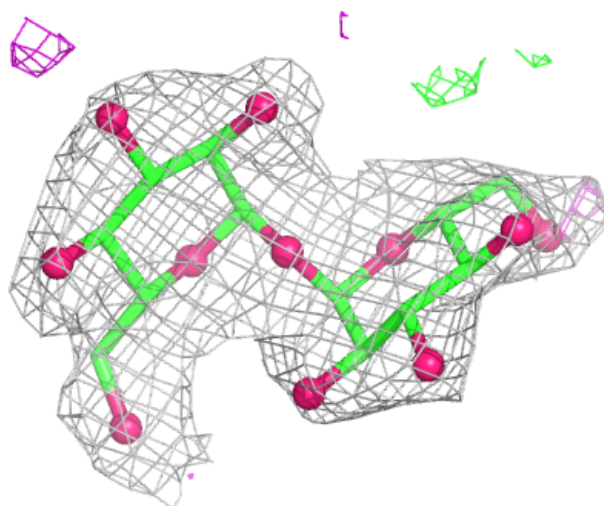
Electron density around Chain O:

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



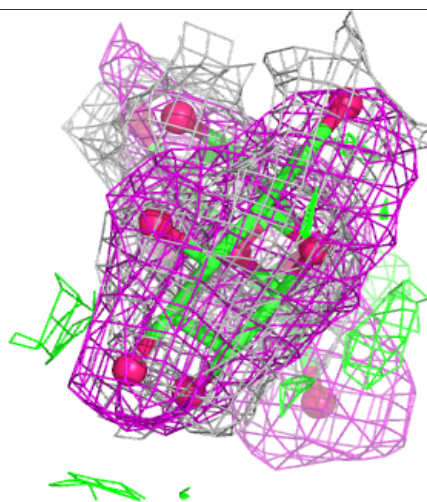
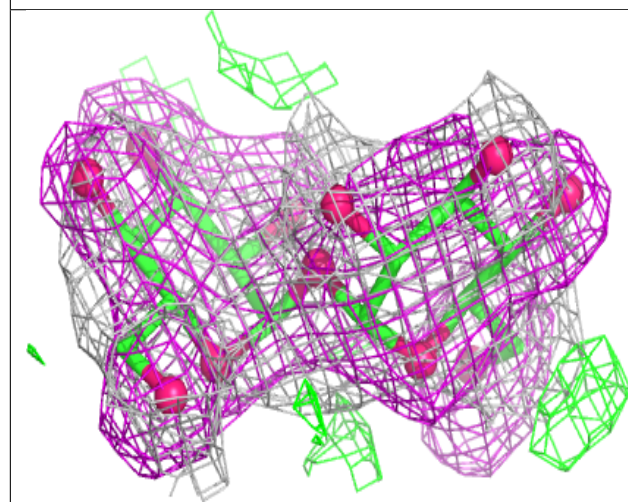
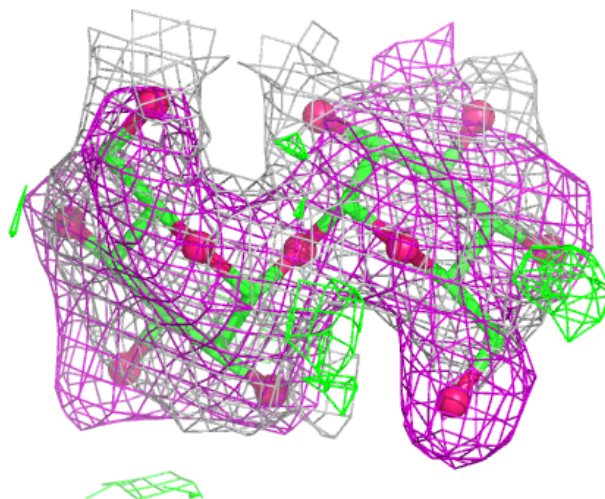
Electron density around Chain P:

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



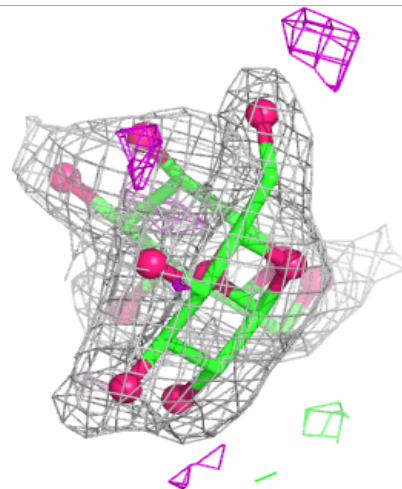
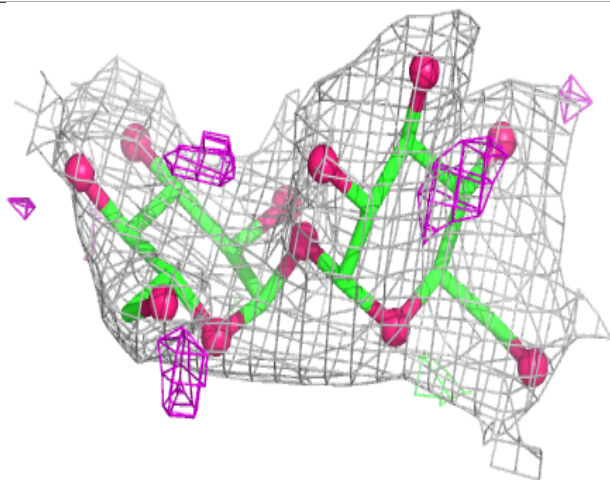
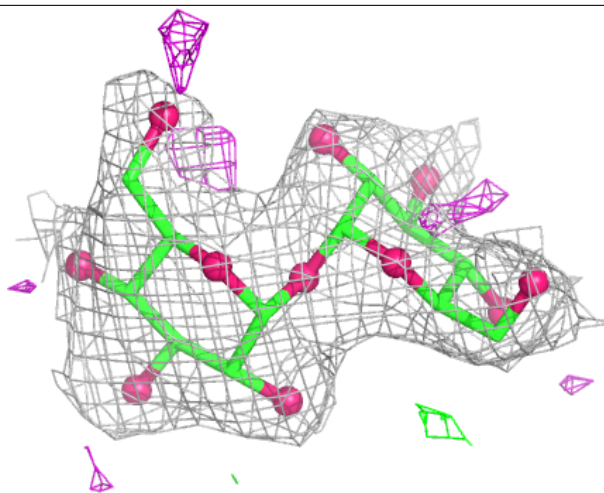
Electron density around Chain Q:

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



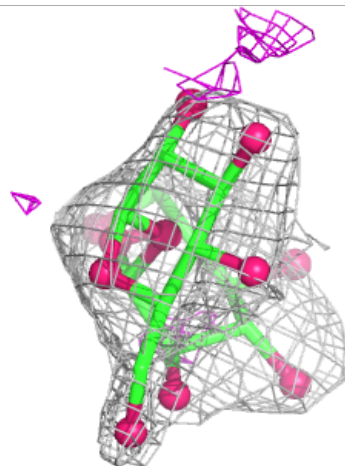
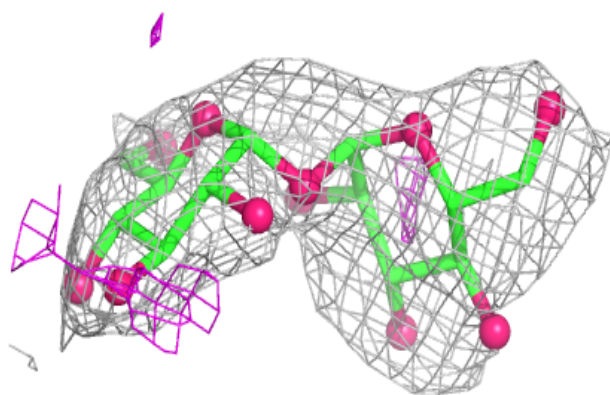
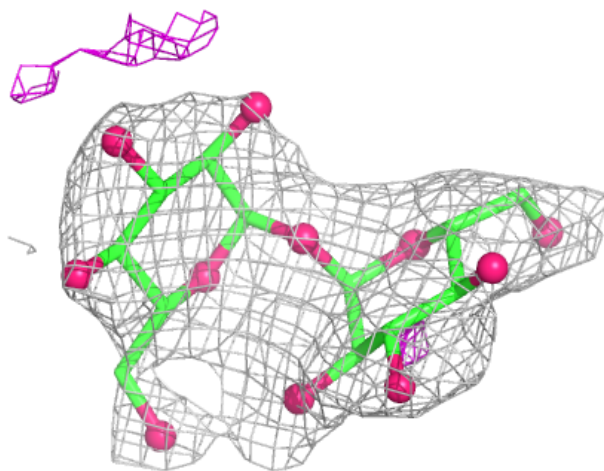
Electron density around Chain R:

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



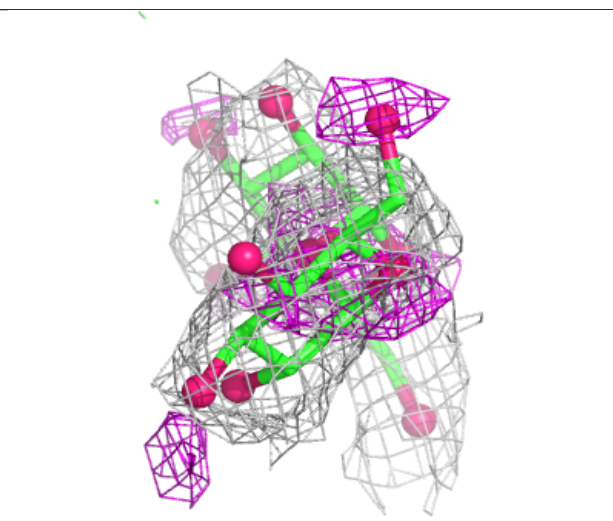
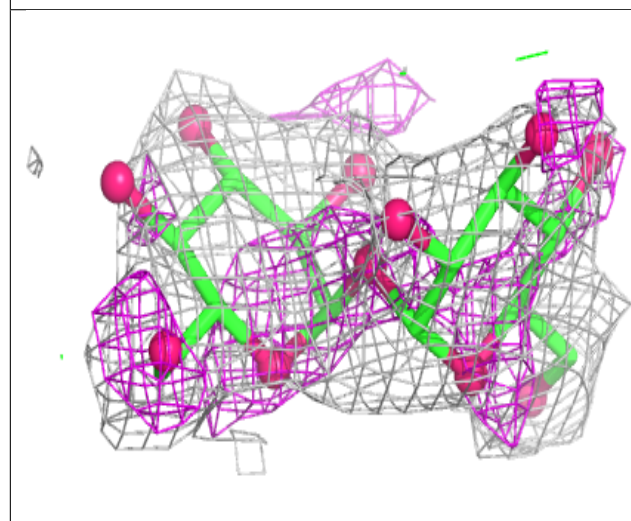
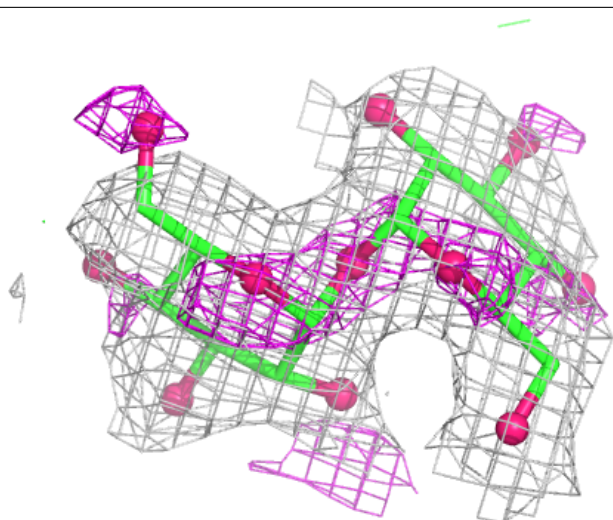
Electron density around Chain S:

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



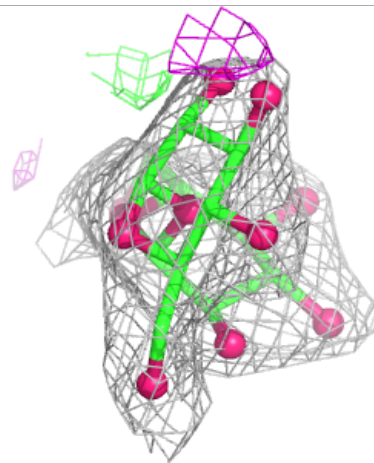
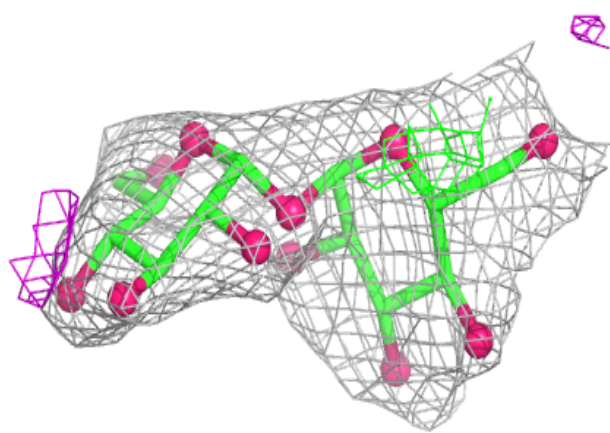
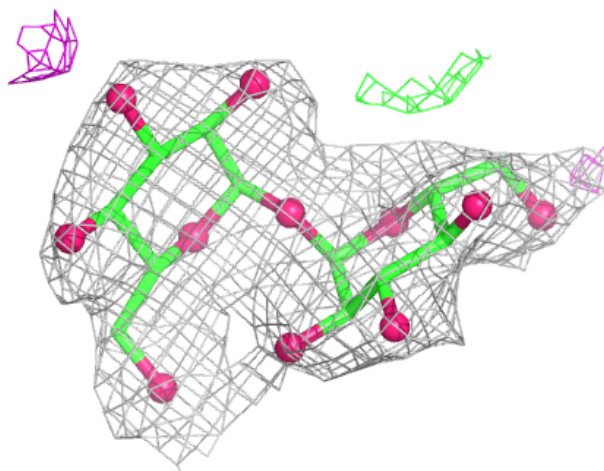
Electron density around Chain T:

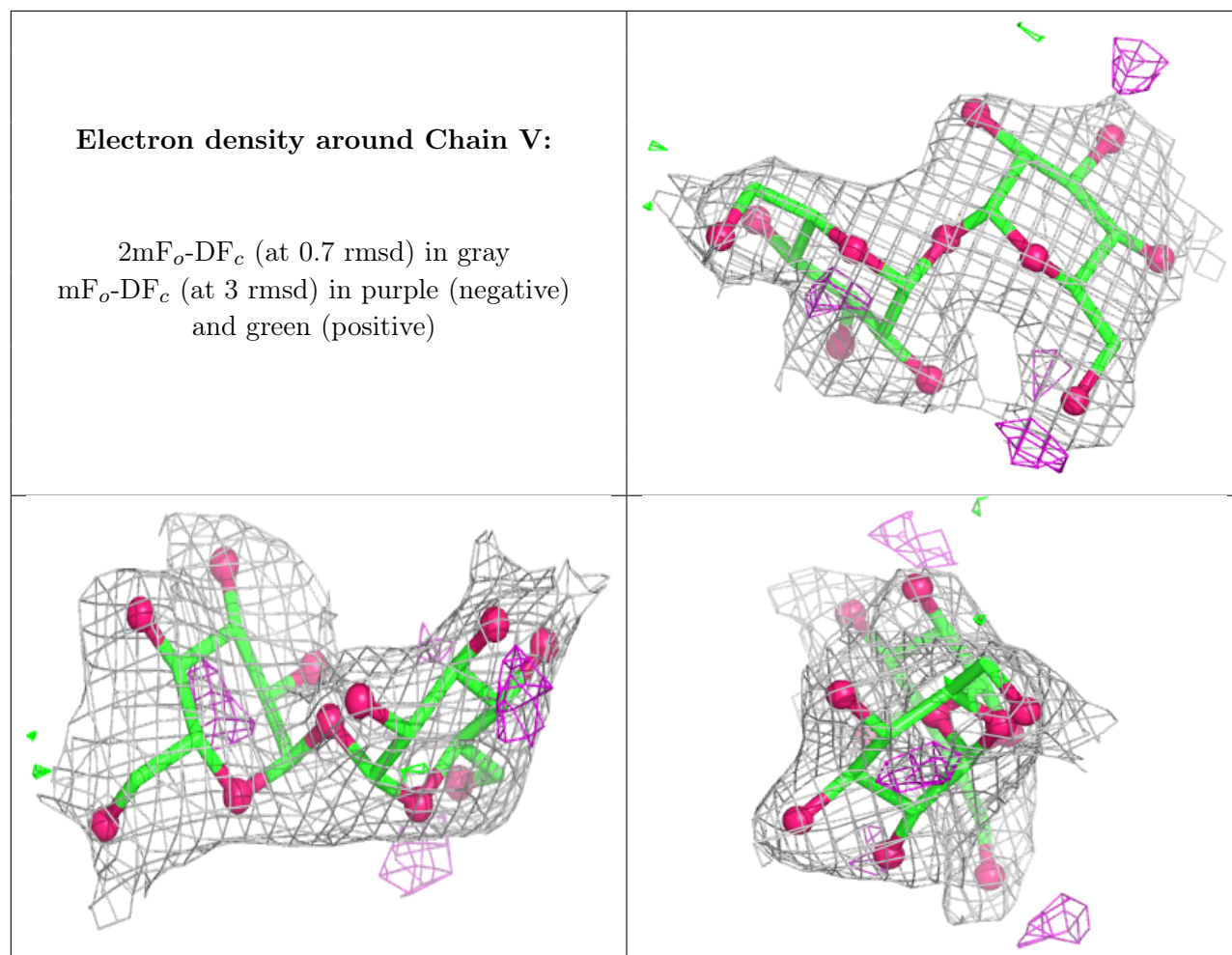
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain U:

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





6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.