



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:45 PM UTC

PDB ID : 7DRB / pdb_00007drb
Title : Crystal structure of plant receptor like protein RXEG1 with xyloglucanase XEG1
Authors : Sun, Y.; Wang, Y.; Zhang, X.X.; Chen, Z.D.; Xia, Y.Q.; Sun, Y.J.; Zhang, M.M.; Xiao, Y.; Han, Z.F.; Wang, Y.C.; Chai, J.J.
Deposited on : 2020-12-27
Resolution : 3.30 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

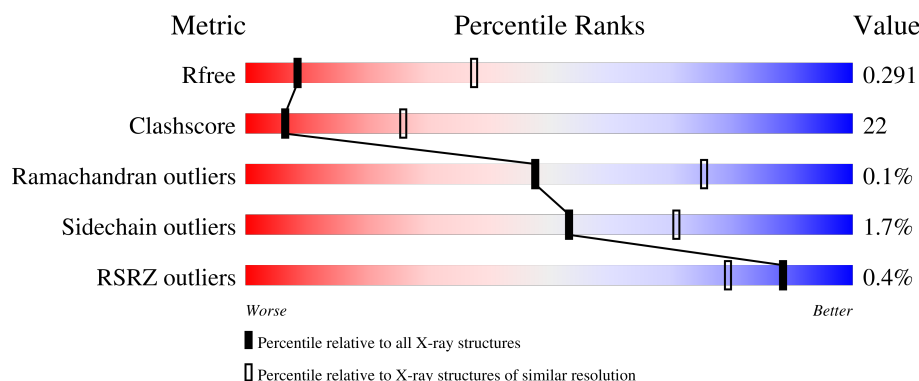
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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.



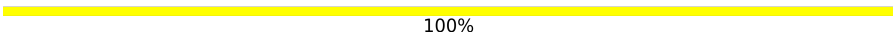
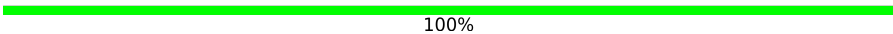
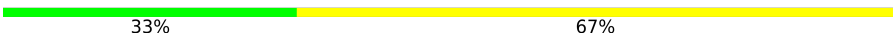
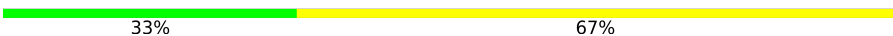
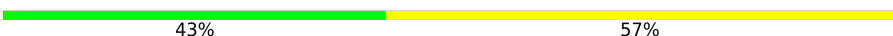
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)

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	241	54% 37% 8%
1	B	241	59% 33% 8%
2	C	934	48% 31% 19%
2	D	934	45% 33% 19%
3	E	10	10% 90%

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Mol	Chain	Length	Quality of chain
3	L	10	 40%50%10%
4	F	2	 100%
4	G	2	 50%50%
4	J	2	 50%50%
4	K	2	 100%
4	M	2	 100%
4	Q	2	 50%50%
5	H	3	 33%67%
5	N	3	 33%67%
5	O	3	 33%67%
5	R	3	 67%33%
6	I	7	 57%43%
6	P	7	 43%57%

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 16004 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.

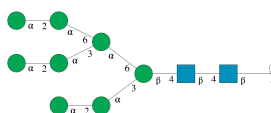
- Molecule 1 is a protein called Cell 12A endoglucanase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	222	Total	C	N	O	S	0	0	0
			1675	1068	269	333	5			
1	B	222	Total	C	N	O	S	0	0	0
			1675	1068	269	333	5			

- Molecule 2 is a protein called Membrane-localized LRR receptor-like protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	752	Total	C	N	O	S	0	0	0
			5924	3792	984	1122	26			
2	D	752	Total	C	N	O	S	0	0	0
			5924	3792	984	1122	26			

- Molecule 3 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	E	10	Total	C	N	O	0	0	0
			116	64	2	50			
3	L	10	Total	C	N	O	0	0	0
			116	64	2	50			

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



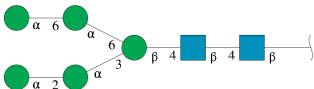
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	F	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	G	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	J	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	K	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	M	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	Q	2	Total	C	N	O	0	0	0
			28	16	2	10			

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



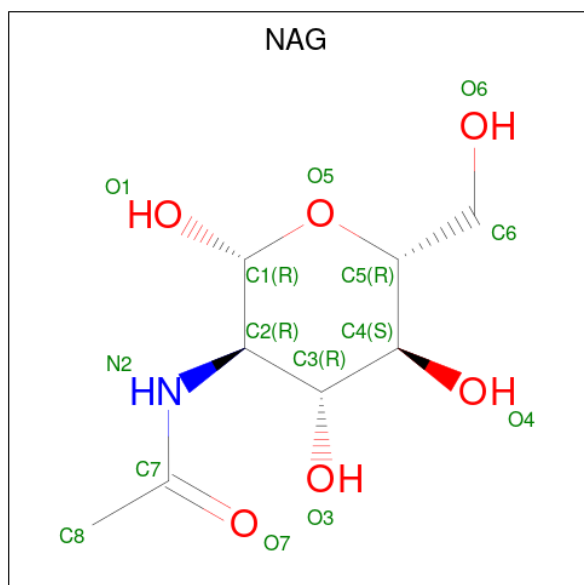
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	H	3	Total	C	N	O	0	0	0
			39	22	2	15			
5	N	3	Total	C	N	O	0	0	0
			39	22	2	15			
5	O	3	Total	C	N	O	0	0	0
			39	22	2	15			
5	R	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 6 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	I	7	Total	C	N	O	0	0	0
			83	46	2	35			
6	P	7	Total	C	N	O	0	0	0
			83	46	2	35			

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).

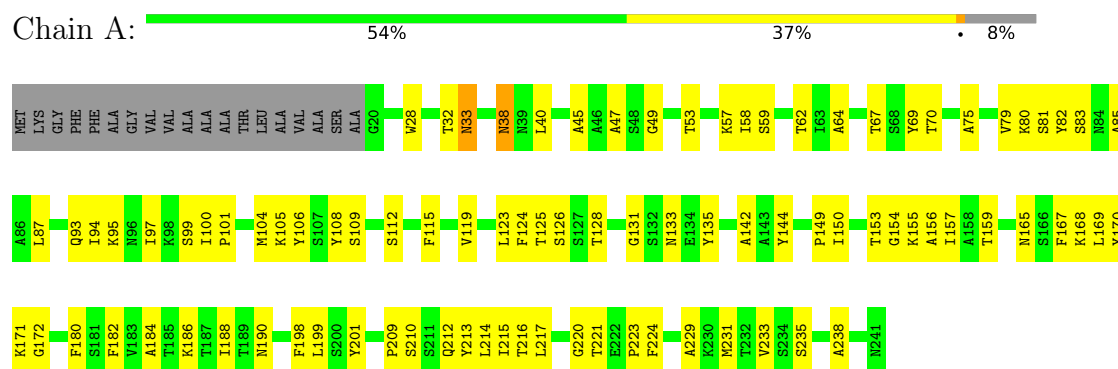


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	C	1	Total	C	N	O	0	0
			14	8	1	5		
7	C	1	Total	C	N	O	0	0
			14	8	1	5		
7	C	1	Total	C	N	O	0	0
			14	8	1	5		
7	D	1	Total	C	N	O	0	0
			14	8	1	5		
7	D	1	Total	C	N	O	0	0
			14	8	1	5		
7	D	1	Total	C	N	O	0	0
			14	8	1	5		

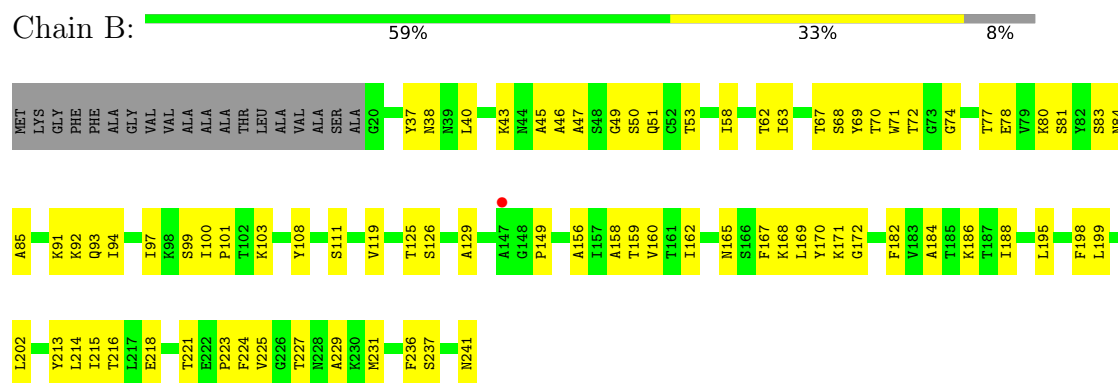
3 Residue-property plots [i](#)

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.

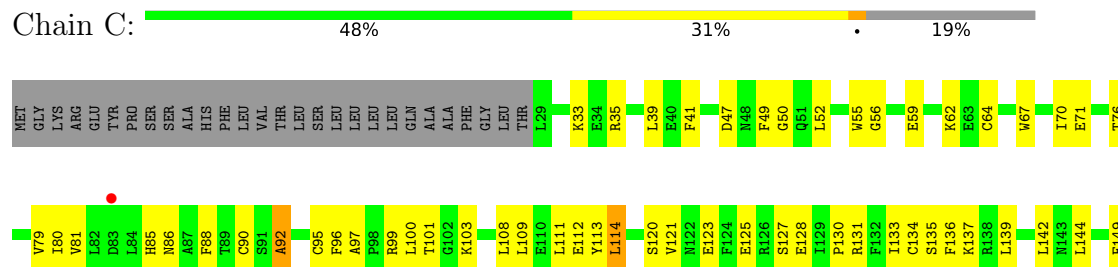
• Molecule 1: Cell 12A endoglucanase



• Molecule 1: Cell 12A endoglucanase



• Molecule 2: Membrane-localized LRR receptor-like protein





L366	L367	L368	L369	L370	L371	L372	L373	L374	L375	L376	L377	L378	L379	L380	L381	L382	L383	L384	L385	L386	L387	L388	L389	L390	L391	L392	L393	L394	L395	L396	L397	L398	L399	L400	L401	L402	L403	L404	L405	L406	L407	L408	L409	L410	L411	L412	L413	L414	L415	L416	L417	L418	L419	L420	L421	L422	L423	L424	L425	L426	L427	L428	L429	L430	L431	L432	L433	L434	L435	L436	L437	L438	L439	L440	L441	L442	L443	L444	L445	L446	L447	L448	L449	L450	L451	L452	L453	L454	L455	L456	L457	L458	L459	L460	L461	L462	L463	L464	L465	L466	L467	L468	L469	L470	L471	L472	L473	L474	L475	L476	L477	L478	L479	L480	L481	L482	L483	L484	L485	L486	L487	L488	L489	L490	L491	L492	L493	L494	L495	L496	L497	L498	L499	L500	L501	L502	L503	L504	L505	L506	L507	L508	L509	L510	L511	L512	L513	L514	L515	L516	L517	L518	L519	L520	L521	L522	L523	L524	L525	L526	L527	L528	L529	L530	L531	L532	L533	L534	L535	L536	L537	L538	L539	L540	L541	L542	L543	L544	L545	L546	L547	L548	L549	L550	L551	L552	L553	L554	L555	L556	L557	L558	L559	L560	L561	L562	L563	L564	L565	L566	L567	L568	L569	L570	L571	L572	L573	L574	L575	L576	L577	L578	L579	L580	L581	L582	L583	L584	L585	L586	L587	L588	L589	L590	L591	L592	L593	L594	L595	L596	L597	L598	L599	L600	L601	L602	L603	L604	L605	L606	L607	L608	L609	L610	L611	L612	L613	L614	L615	L616	L617	L618	L619	L620	L621	L622	L623	L624	L625	L626	L627	L628	L629	L630	L631	L632	L633	L634	L635	L636	L637	L638	L639	L640	L641	L642	L643	L644	L645	L646	L647	L648	L649	L650	L651	L652	L653	L654	L655	L656	L657	L658	L659	L660	L661	L662	L663	L664	L665	L666	L667	L668	L669	L670	L671	L672	L673	L674	L675	L676	L677	L678	L679	L680	L681	L682	L683	L684	L685	L686	L687	L688	L689	L690	L691	L692	L693	L694	L695	L696	L697	L698	L699	L700	L701	L702	L703	L704	L705	L706	L707	L708	L709	L710	L711	L712	L713	L714	L715	L716	L717	L718	L719	L720	L721	L722	L723	L724	L725	L726	L727	L728	L729	L730	L731	L732	L733	L734	L735	L736	L737	L738	L739	L740	L741	L742	L743	L744	L745	L746	L747	L748	L749	L750	L751	L752	L753	L754	L755	L756	L757	L758	L759	L760	L761	L762	L763	L764	L765	L766	L767	L768	L769	L770	L771	L772	L773	L774	L775	L776	L777	L778	L779	L780	L781	L782	L783	L784	L785	L786	L787	L788	L789	L790	L791	L792	L793	L794	L795	L796	L797	L798	L799	L800	L801	L802	L803	L804	L805	L806	L807	L808	L809	L810	L811	L812	L813	L814	L815	L816	L817	L818	L819	L820	L821	L822	L823	L824	L825	L826	L827	L828	L829	L830	L831	L832	L833	L834	L835	L836	L837	L838	L839	L840	L841	L842	L843	L844	L845	L846	L847	L848	L849	L850	L851	L852	L853	L854	L855	L856	L857	L858	L859	L860	L861	L862	L863	L864	L865	L866	L867	L868	L869	L870	L871	L872	L873	L874	L875	L876	L87
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- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:  50% 50%

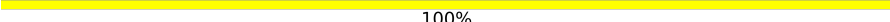
MAG1
MAG2

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

Chain J:  50% 50%

MAG1
MAG2

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

Chain K:  100%

MAG1
MAG2

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

Chain M:  100%

MAG1
MAG2

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

Chain Q:  50% 50%

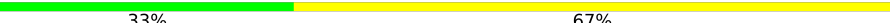
MAG1
MAG2

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

Chain H:  33% 67%

MAG1
MAG2
BMA3

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

Chain N:  33% 67%



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



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



- Molecule 6: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 6: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	103.89Å 92.84Å 154.53Å 90.00° 107.91° 90.00°	Depositor
Resolution (Å)	49.01 – 3.30 49.01 – 3.30	Depositor EDS
% Data completeness (in resolution range)	97.2 (49.01-3.30) 97.3 (49.01-3.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.80 (at 3.33Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.227 , 0.284 0.243 , 0.291	Depositor DCC
R_{free} test set	2066 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å ²)	93.4	Xtriage
Anisotropy	0.557	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 46.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.023 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	16004	wwPDB-VP
Average B, all atoms (Å ²)	99.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.32% 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: BMA, MAN, 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	0.62	0/1716	1.06	6/2333 (0.3%)
1	B	0.50	0/1716	0.84	0/2333
2	C	0.62	0/6051	1.05	14/8202 (0.2%)
2	D	0.58	0/6051	1.03	11/8202 (0.1%)
All	All	0.59	0/15534	1.02	31/21070 (0.1%)

There are no bond length outliers.

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	40	LEU	N-CA-C	-8.77	99.54	111.55
2	D	663	GLY	N-CA-C	8.66	121.89	111.93
2	D	625	THR	N-CA-C	7.15	119.08	111.28
2	D	169	GLY	N-CA-C	7.03	120.06	112.33
2	C	732	LYS	CA-C-N	-6.94	113.82	122.84
2	C	732	LYS	C-N-CA	-6.94	113.82	122.84
2	C	92	ALA	CB-CA-C	-6.68	108.88	116.63
2	D	692	LEU	N-CA-C	-6.48	104.69	112.59
2	D	570	GLY	CA-C-O	-6.25	117.81	122.37
2	D	115	ASN	N-CA-C	-6.03	104.57	113.61
2	D	666	PRO	N-CA-C	6.01	120.63	111.19
2	D	669	LEU	N-CA-C	-5.89	104.86	111.28
2	C	583	MET	N-CA-C	-5.85	107.95	114.62
2	C	541	ALA	CA-C-N	-5.84	114.73	122.85
2	C	541	ALA	C-N-CA	-5.84	114.73	122.85
2	C	170	TYR	CB-CA-C	5.83	119.55	111.63
1	A	38	ASN	CA-C-N	-5.78	114.85	122.99
1	A	38	ASN	C-N-CA	-5.78	114.85	122.99
2	D	637	PHE	CB-CA-C	-5.76	100.17	109.72
2	C	710	GLY	CA-C-O	-5.65	117.75	122.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	169	GLY	N-CA-C	5.59	119.36	112.14
2	C	168	LEU	N-CA-C	-5.59	104.10	112.54
1	A	154	GLY	N-CA-C	-5.55	107.70	114.92
2	D	575	LEU	N-CA-C	-5.46	105.33	111.28
1	A	112	SER	CB-CA-C	-5.46	110.30	116.63
2	C	659	ASN	CA-C-N	-5.43	115.20	122.42
2	C	659	ASN	C-N-CA	-5.43	115.20	122.42
2	C	163	LEU	N-CA-C	5.41	117.28	108.63
2	D	687	GLY	CA-C-O	-5.34	118.54	122.23
1	A	85	ALA	N-CA-C	-5.27	100.58	109.07
2	C	541	ALA	N-CA-C	-5.04	103.75	110.55

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	1675	0	1624	76	0
1	B	1675	0	1624	70	0
2	C	5924	0	5889	255	1
2	D	5924	0	5887	295	0
3	E	116	0	97	1	0
3	L	116	0	97	2	0
4	F	28	0	25	1	0
4	G	28	0	25	0	0
4	J	28	0	25	1	0
4	K	28	0	25	0	0
4	M	28	0	25	0	0
4	Q	28	0	25	0	0
5	H	39	0	34	3	0
5	N	39	0	34	0	0
5	O	39	0	34	0	0
5	R	39	0	34	6	0
6	I	83	0	70	0	0
6	P	83	0	70	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	C	42	0	39	1	0
7	D	42	0	39	1	0
All	All	16004	0	15722	692	1

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 22.

All (692) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:614:PHE:HA	2:D:637:PHE:HA	1.24	1.09
2:D:90:CYS:HA	2:D:95:CYS:HA	1.37	1.03
2:D:628:THR:HA	2:D:651:LEU:HA	1.49	0.94
2:C:479:LEU:HA	2:C:482:LEU:HD21	1.49	0.94
2:C:470:LEU:HB2	2:C:493:ASN:HD22	1.36	0.90
1:B:38:ASN:HB2	1:B:53:THR:HG21	1.53	0.90
2:C:498:LYS:HE2	2:C:520:GLY:HA2	1.55	0.87
2:C:313:THR:O	2:C:339:SER:HB3	1.76	0.86
1:B:84:ASN:ND2	1:B:218:GLU:OE1	2.09	0.86
2:D:349:ASN:HD22	2:D:372:GLN:NE2	1.75	0.84
1:B:119:VAL:HG22	1:B:221:THR:HG22	1.57	0.84
2:D:596:LEU:HD11	2:D:619:SER:HB2	1.60	0.84
1:A:159:THR:HG22	1:A:168:LYS:HD3	1.57	0.83
2:C:280:ILE:HD11	2:C:305:ILE:HA	1.60	0.83
1:B:159:THR:HG22	1:B:168:LYS:HD3	1.60	0.82
2:C:171:ASN:HB2	2:C:173:LEU:HD22	1.60	0.81
1:B:49:GLY:HA3	1:B:71:TRP:CE3	2.15	0.81
2:D:41:PHE:HB2	2:D:108:LEU:HD21	1.60	0.81
2:D:83:ASP:HB2	2:D:118:ASP:HB3	1.63	0.79
2:D:554:LEU:HD21	2:D:577:GLU:HB2	1.64	0.79
2:C:202:TRP:HD1	2:C:206:ILE:HD12	1.48	0.79
1:A:209:PRO:HG2	1:A:212:GLN:HG2	1.65	0.79
2:D:349:ASN:HD22	2:D:372:GLN:HE22	1.30	0.79
2:C:535:VAL:HG23	2:C:560:ILE:HB	1.65	0.79
2:C:617:ILE:HD11	2:C:641:LEU:HD22	1.65	0.79
2:D:165:ILE:HG23	2:D:189:LEU:HD22	1.65	0.79
1:B:149:PRO:HG2	1:B:170:TYR:CD2	2.18	0.78
2:D:468:ASN:HB2	2:D:470:LEU:HD23	1.64	0.78
1:A:108:TYR:HE2	1:A:115:PHE:HZ	1.30	0.78
2:D:280:ILE:HD11	2:D:305:ILE:HA	1.65	0.78
2:D:228:SER:HB3	2:D:231:GLU:HG3	1.65	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:149:PRO:HG2	1:A:170:TYR:HD2	1.49	0.77
2:D:476:GLU:OE1	2:D:500:SER:N	2.17	0.77
2:C:86:ASN:O	2:C:121:VAL:HB	1.85	0.77
2:D:630:LEU:HD23	2:D:651:LEU:HD11	1.66	0.76
2:D:655:ASN:HA	2:D:679:TYR:HB2	1.67	0.76
1:B:149:PRO:HG2	1:B:170:TYR:HD2	1.49	0.76
2:C:510:GLN:HA	2:C:533:TYR:HA	1.67	0.75
2:D:71:GLU:HB2	2:D:81:VAL:HB	1.68	0.75
2:C:165:ILE:HG23	2:C:189:LEU:HD22	1.69	0.75
2:D:45:LEU:HD23	2:D:100:LEU:HD23	1.67	0.75
2:C:90:CYS:HA	2:C:95:CYS:HA	1.68	0.75
2:D:458:SER:H	2:D:482:LEU:HD23	1.51	0.75
1:B:97:ILE:HD13	1:B:100:ILE:HD11	1.69	0.75
2:C:306:PRO:O	2:C:335:ARG:HD3	1.88	0.73
2:D:171:ASN:HB2	2:D:173:LEU:HD22	1.71	0.73
1:A:57:LYS:HB3	1:A:64:ALA:HB3	1.70	0.73
1:A:59:SER:OG	1:A:62:THR:HG23	1.89	0.73
1:A:108:TYR:CE2	1:A:115:PHE:HZ	2.06	0.73
2:C:134:CYS:SG	2:C:156:GLN:HB3	2.29	0.72
1:A:123:LEU:HD22	1:A:217:LEU:HG	1.70	0.72
2:C:202:TRP:CD1	2:C:206:ILE:HD12	2.25	0.72
2:D:299:LEU:O	2:D:324:ARG:NH1	2.22	0.72
2:C:470:LEU:HB2	2:C:493:ASN:ND2	2.03	0.72
2:D:491:SER:HA	2:D:515:PRO:HD2	1.73	0.71
2:D:86:ASN:HD22	2:D:122:ASN:HD21	1.37	0.71
1:A:97:ILE:HG21	1:A:100:ILE:HG13	1.72	0.71
1:B:93:GLN:HG2	1:B:213:TYR:CD1	2.26	0.71
2:D:237:LEU:HD11	7:D:1001:NAG:H81	1.73	0.70
2:D:379:PHE:HD1	2:D:402:GLY:HA3	1.57	0.70
2:C:519:LEU:HD12	2:C:538:ILE:HG23	1.74	0.70
1:B:53:THR:HA	1:B:67:THR:HA	1.74	0.70
3:L:9:MAN:H2	3:L:10:MAN:H5	1.74	0.69
2:C:248:ASN:O	2:C:274:ASN:ND2	2.20	0.69
2:C:738:SER:HB3	2:C:740:ILE:HG12	1.75	0.69
1:B:93:GLN:HG2	1:B:213:TYR:CE1	2.27	0.69
2:D:665:LEU:HB2	2:D:690:PRO:HD3	1.75	0.69
2:C:672:LEU:HD23	2:C:675:LEU:HD13	1.75	0.69
1:B:195:LEU:HA	1:B:198:PHE:HD2	1.57	0.69
2:C:515:PRO:HG3	2:C:537:ASP:OD1	1.93	0.69
2:D:86:ASN:HD22	2:D:122:ASN:ND2	1.91	0.68
2:D:512:ILE:HG23	2:D:536:LEU:HA	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:244:HIS:HA	2:C:270:ASP:HB3	1.75	0.68
1:B:169:LEU:HD13	1:B:182:PHE:CE1	2.29	0.68
2:D:500:SER:HB3	2:D:503:TRP:HB2	1.74	0.68
2:D:501:ILE:HD12	2:D:501:ILE:H	1.58	0.67
2:D:510:GLN:HA	2:D:533:TYR:HA	1.76	0.67
2:D:644:CYS:HB3	5:R:1:NAG:H82	1.77	0.67
2:C:638:SER:HA	2:C:660:ASN:O	1.95	0.67
1:A:124:PHE:HE2	2:C:792:TYR:HE1	1.43	0.67
1:A:171:LYS:HE2	1:A:180:PHE:CE1	2.28	0.67
2:D:351:ASN:O	2:D:374:ASN:HA	1.95	0.67
2:C:675:LEU:HD21	2:C:678:LEU:HD13	1.77	0.67
2:D:663:GLY:O	2:D:685:PHE:HD1	1.78	0.67
2:D:643:ASP:OD1	2:D:666:PRO:HB3	1.95	0.66
2:C:201:ASN:HB2	2:C:204:GLN:OE1	1.96	0.66
2:D:88:PHE:HB3	2:D:97:ALA:HB2	1.77	0.66
1:B:47:ALA:HB1	1:B:72:THR:O	1.96	0.65
2:D:288:MET:HG3	2:D:289:TYR:HD1	1.59	0.65
5:H:1:NAG:H61	5:H:2:NAG:H82	1.76	0.65
2:D:577:GLU:HG3	2:D:578:ASN:H	1.62	0.65
1:A:156:ALA:HB2	1:A:170:TYR:HE1	1.61	0.65
2:C:188:GLU:HA	2:C:211:LEU:O	1.96	0.65
1:A:75:ALA:O	1:A:80:LYS:NZ	2.23	0.64
2:D:191:SER:HA	2:D:216:ASP:HB3	1.79	0.64
2:C:460:LEU:HD21	2:C:463:PHE:HB2	1.79	0.64
2:C:605:ILE:HG22	2:C:629:SER:HB3	1.79	0.64
2:D:589:SER:H	2:D:610:LYS:HB2	1.63	0.64
2:C:681:ARG:HG2	2:C:704:GLY:H	1.63	0.64
1:B:182:PHE:CD2	1:B:198:PHE:HD1	2.16	0.64
2:D:246:CYS:SG	2:D:247:CYS:N	2.71	0.64
2:C:280:ILE:HD11	2:C:306:PRO:HD3	1.79	0.64
1:A:159:THR:HG23	2:C:219:LEU:HD21	1.80	0.64
2:C:709:THR:HA	2:C:732:LYS:O	1.97	0.63
2:C:79:VAL:HB	2:C:111:LEU:HD12	1.79	0.63
2:C:144:LEU:HB3	2:C:149:PHE:CE2	2.33	0.63
2:D:134:CYS:HG	2:D:157:PHE:HD1	1.46	0.63
2:D:86:ASN:ND2	2:D:122:ASN:HD21	1.97	0.63
2:C:458:SER:HA	2:C:482:LEU:HA	1.81	0.63
2:C:295:LEU:O	2:C:298:GLU:HG2	1.99	0.63
2:C:85:HIS:HB2	2:C:120:SER:OG	1.99	0.63
1:B:169:LEU:HD13	1:B:182:PHE:HE1	1.64	0.63
1:A:215:ILE:HG22	1:A:216:THR:HG23	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:83:ASP:CB	2:D:118:ASP:HB3	2.29	0.62
2:D:654:LEU:HD23	2:D:678:LEU:CD1	2.29	0.62
2:C:55:TRP:CZ2	2:C:70:ILE:HD11	2.34	0.62
2:C:503:TRP:CH2	2:C:505:PRO:HB3	2.35	0.62
1:B:165:ASN:OD1	1:B:186:LYS:HD2	1.98	0.62
2:D:515:PRO:HG3	2:D:537:ASP:OD1	1.99	0.62
1:B:67:THR:HG21	1:B:83:SER:OG	1.99	0.62
2:D:202:TRP:HE3	2:D:206:ILE:HD12	1.64	0.62
2:C:88:PHE:HB3	2:C:97:ALA:HB2	1.82	0.61
2:C:120:SER:HB2	3:E:1:NAG:H62	1.82	0.61
2:C:698:LEU:HD21	2:C:720:LEU:HD21	1.82	0.61
2:D:519:LEU:HD23	2:D:541:ALA:HB2	1.80	0.61
1:A:38:ASN:HB2	1:A:53:THR:HG21	1.82	0.61
2:C:467:TYR:CE1	2:C:492:PHE:HD2	2.19	0.61
2:C:197:PHE:HB3	2:C:220:CYS:O	2.00	0.61
2:C:178:LEU:HG	2:C:181:LEU:HD13	1.82	0.61
1:A:150:ILE:HD12	2:C:92:ALA:O	2.02	0.60
2:D:41:PHE:CB	2:D:108:LEU:HD21	2.31	0.60
2:C:680:MET:HB2	2:C:703:LEU:HD13	1.83	0.60
2:D:216:ASP:HA	2:D:244:HIS:HB2	1.83	0.60
5:H:2:NAG:H3	5:H:2:NAG:H83	1.82	0.60
1:B:50:SER:O	1:B:69:TYR:HA	2.01	0.60
2:C:351:ASN:O	2:C:374:ASN:HA	2.01	0.60
1:B:158:ALA:HA	2:D:219:LEU:HD21	1.83	0.60
2:D:376:LEU:HB2	2:D:398:ASN:HB3	1.84	0.60
1:A:169:LEU:HD13	1:A:182:PHE:CE1	2.36	0.60
1:B:126:SER:HB3	1:B:215:ILE:HD11	1.83	0.60
2:C:304:GLY:HA3	2:C:327:GLN:OE1	2.01	0.59
1:B:70:THR:HG23	1:B:227:THR:HA	1.83	0.59
2:D:164:ARG:HA	2:D:187:LEU:HA	1.85	0.59
2:C:665:LEU:HB2	2:C:690:PRO:HD3	1.84	0.59
2:C:722:ASN:O	2:C:723:LEU:HB2	2.01	0.59
2:C:327:GLN:HE21	2:C:331:GLU:HG3	1.68	0.59
2:D:508:GLN:NE2	2:D:529:SER:O	2.25	0.59
2:D:652:ALA:HA	2:D:675:LEU:HA	1.83	0.59
2:C:314:ARG:HA	2:C:342:THR:HG21	1.84	0.59
2:D:533:TYR:CE1	2:D:555:PRO:HG2	2.38	0.59
1:A:124:PHE:HE2	2:C:792:TYR:CE1	2.21	0.59
1:A:182:PHE:CD2	1:A:198:PHE:HD2	2.20	0.59
2:C:88:PHE:HB2	2:C:96:PHE:O	2.02	0.59
2:C:581:ASP:OD1	2:C:602:ASN:ND2	2.34	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:128:THR:HG23	1:A:131:GLY:CA	2.32	0.59
2:D:139:LEU:HD13	2:D:142:LEU:HD12	1.85	0.59
2:C:577:GLU:HG2	2:C:580:TYR:CZ	2.37	0.59
1:A:108:TYR:HE2	1:A:115:PHE:CZ	2.18	0.59
1:A:149:PRO:HG2	1:A:170:TYR:CD2	2.35	0.59
1:A:182:PHE:CE2	1:A:198:PHE:HD2	2.21	0.59
2:C:668:SER:O	2:C:671:SER:HB3	2.03	0.59
2:C:655:ASN:HA	2:C:679:TYR:HB2	1.84	0.58
2:D:666:PRO:HD2	2:D:669:LEU:HD12	1.85	0.58
2:C:498:LYS:NZ	2:C:521:PRO:HD3	2.18	0.58
2:D:99:ARG:HA	2:D:122:ASN:HD22	1.67	0.58
2:C:33:LYS:HB3	2:D:328:TRP:CD2	2.38	0.58
2:C:479:LEU:HD12	2:C:503:TRP:CH2	2.39	0.58
2:C:596:LEU:HD23	2:C:617:ILE:HG22	1.85	0.58
1:B:69:TYR:CZ	1:B:223:PRO:HB3	2.38	0.58
2:D:622:LYS:HD3	5:R:1:NAG:H2	1.85	0.58
2:D:86:ASN:O	2:D:121:VAL:HB	2.04	0.58
1:B:186:LYS:O	1:B:188:ILE:HG13	2.03	0.58
2:D:665:LEU:HD11	2:D:708:LEU:HD11	1.84	0.58
2:C:349:ASN:HD22	2:C:372:GLN:HE22	1.51	0.57
2:D:487:ASP:HA	2:D:511:VAL:HG13	1.86	0.57
1:A:156:ALA:HA	1:A:170:TYR:CD1	2.39	0.57
2:C:112:GLU:HG2	2:C:113:TYR:CE1	2.39	0.57
2:C:59:GLU:O	2:C:62:LYS:HB3	2.05	0.57
2:D:645:TRP:HE1	2:D:666:PRO:HG2	1.70	0.57
2:D:664:LYS:HA	2:D:686:SER:O	2.04	0.57
2:D:41:PHE:CG	2:D:108:LEU:HD21	2.40	0.57
2:C:512:ILE:HG23	2:C:536:LEU:HA	1.86	0.57
2:C:103:LYS:HD2	2:C:125:GLU:HB2	1.87	0.57
2:D:658:TYR:HD1	2:D:682:GLN:HB2	1.70	0.57
1:A:128:THR:HG23	1:A:131:GLY:HA3	1.87	0.56
2:C:101:THR:N	2:C:123:GLU:O	2.37	0.56
2:C:131:ARG:HD2	2:C:156:GLN:NE2	2.20	0.56
2:C:479:LEU:HD12	2:C:503:TRP:HH2	1.70	0.56
2:C:652:ALA:HA	2:C:675:LEU:HA	1.86	0.56
2:D:348:LEU:HB2	2:D:371:LEU:HD23	1.86	0.56
2:D:509:LEU:HD23	2:D:530:GLN:HG2	1.85	0.56
1:B:108:TYR:CE1	1:B:231:MET:HB2	2.39	0.56
2:C:329:LEU:HD21	2:C:333:PHE:CE2	2.40	0.56
2:C:41:PHE:CD2	2:C:108:LEU:HD21	2.41	0.56
2:D:243:LEU:HB3	2:D:245:LEU:HD23	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:161:THR:O	2:D:186:SER:OG	2.17	0.56
2:D:600:PRO:HB2	2:D:603:VAL:HB	1.88	0.56
2:C:130:PRO:HD2	2:C:133:ILE:HD11	1.88	0.56
2:D:200:LYS:HA	2:D:225:LEU:HD22	1.88	0.56
2:D:644:CYS:HA	2:D:646:MET:SD	2.46	0.56
1:A:57:LYS:HE2	1:A:64:ALA:HB2	1.87	0.55
2:C:664:LYS:HD3	2:C:687:GLY:HA3	1.87	0.55
2:C:163:LEU:HD13	2:C:166:LEU:HG	1.87	0.55
2:D:295:LEU:O	2:D:298:GLU:HG2	2.06	0.55
2:D:521:PRO:HA	2:D:542:ASN:O	2.05	0.55
2:C:164:ARG:HG2	2:C:165:ILE:HG13	1.88	0.55
2:C:336:LEU:HD23	2:C:343:LEU:HD11	1.89	0.55
2:D:277:ASP:HB2	2:D:299:LEU:HD23	1.87	0.55
2:D:313:THR:O	2:D:339:SER:OG	2.15	0.55
1:A:47:ALA:HB2	1:A:80:LYS:HE2	1.89	0.55
2:C:508:GLN:HA	2:C:530:GLN:OE1	2.07	0.55
2:D:418:LEU:HB2	2:D:442:VAL:HG12	1.89	0.55
2:C:166:LEU:HD22	2:C:168:LEU:HD11	1.89	0.55
2:C:681:ARG:NE	2:C:702:ASP:OD2	2.31	0.55
2:D:475:THR:O	2:D:478:HIS:HB3	2.05	0.55
2:C:702:ASP:C	2:C:703:LEU:HD22	2.32	0.55
2:D:689:LEU:HD21	2:D:713:PRO:HD3	1.89	0.55
1:B:77:THR:HG23	1:B:78:GLU:HG3	1.88	0.55
2:D:558:ILE:HD11	2:D:582:TYR:OH	2.07	0.55
2:C:491:SER:HA	2:C:515:PRO:HD2	1.88	0.55
2:D:100:LEU:HD13	2:D:122:ASN:OD1	2.07	0.55
2:C:109:LEU:HD21	2:C:135:SER:HB2	1.90	0.54
2:C:192:LEU:O	2:C:220:CYS:SG	2.65	0.54
2:D:184:LEU:HB3	2:D:187:LEU:HG	1.88	0.54
2:D:301:LEU:HB2	2:D:325:THR:HG22	1.90	0.54
2:D:654:LEU:HD23	2:D:678:LEU:HD11	1.89	0.54
1:B:38:ASN:HB2	1:B:53:THR:CG2	2.31	0.54
2:D:410:PHE:O	2:D:434:LEU:HD21	2.06	0.54
2:C:246:CYS:HG	2:C:247:CYS:HG	1.53	0.54
1:A:105:LYS:HE3	1:A:190:ASN:ND2	2.22	0.54
2:C:47:ASP:O	2:C:49:PHE:N	2.38	0.54
2:C:103:LYS:HD3	2:C:125:GLU:OE2	2.08	0.54
1:A:109:SER:O	1:A:229:ALA:HA	2.08	0.54
2:D:101:THR:N	2:D:123:GLU:O	2.40	0.54
2:D:507:PHE:CE1	2:D:509:LEU:HD22	2.43	0.54
2:D:100:LEU:HD13	2:D:122:ASN:CG	2.33	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:794:ARG:HD3	2:D:796:TYR:CZ	2.43	0.54
1:A:79:VAL:HG22	1:A:224:PHE:CE1	2.42	0.53
1:A:95:LYS:HG2	1:A:210:SER:HB3	1.89	0.53
2:C:479:LEU:N	2:C:479:LEU:HD23	2.23	0.53
2:D:457:LEU:HB2	2:D:482:LEU:HD21	1.89	0.53
2:D:170:TYR:HE1	2:D:219:LEU:HD12	1.74	0.53
2:D:511:VAL:HG23	2:D:535:VAL:CG1	2.38	0.53
1:B:195:LEU:HA	1:B:198:PHE:CD2	2.40	0.53
2:D:445:ASN:O	2:D:468:ASN:HA	2.08	0.53
2:D:622:LYS:HD3	5:R:1:NAG:C2	2.37	0.53
2:C:266:LEU:HD13	2:C:269:ILE:HD11	1.90	0.53
2:D:168:LEU:O	2:D:171:ASN:ND2	2.41	0.53
2:D:429:GLN:OE1	2:D:451:PRO:HB2	2.09	0.53
2:D:266:LEU:HD13	2:D:269:ILE:HD11	1.90	0.53
2:D:547:LEU:HD22	2:D:575:LEU:HD13	1.90	0.53
2:D:664:LYS:HE3	2:D:687:GLY:HA3	1.88	0.53
2:D:535:VAL:HG23	2:D:560:ILE:HB	1.90	0.53
1:A:126:SER:HB3	1:A:215:ILE:HD11	1.89	0.53
2:D:343:LEU:HD21	2:D:346:LEU:HB2	1.90	0.53
2:D:450:LEU:HB3	2:D:478:HIS:HE1	1.74	0.53
2:C:571:ARG:NH1	2:C:595:PRO:HD3	2.24	0.53
2:D:46:SER:OG	2:D:101:THR:HG23	2.09	0.53
2:D:642:PRO:HB2	2:D:644:CYS:SG	2.49	0.53
1:B:91:LYS:NZ	1:B:129:ALA:O	2.26	0.53
1:B:182:PHE:CE2	1:B:198:PHE:HD1	2.26	0.53
2:C:658:TYR:N	2:C:658:TYR:HD1	2.07	0.52
2:C:47:ASP:HB2	2:C:50:GLY:O	2.09	0.52
2:D:140:GLU:HA	2:D:163:LEU:HA	1.89	0.52
2:C:246:CYS:SG	2:C:247:CYS:SG	3.02	0.52
2:C:685:PHE:O	2:C:706:ASN:O	2.28	0.52
1:A:28:TRP:HE1	2:C:674:ASN:ND2	2.07	0.52
2:C:298:GLU:HB2	2:C:323:THR:HG22	1.90	0.52
2:C:596:LEU:HD22	2:C:620:ILE:HD11	1.90	0.52
2:C:33:LYS:HB3	2:D:328:TRP:CE3	2.44	0.52
2:C:800:GLY:O	2:C:802:LEU:HD12	2.10	0.52
1:A:69:TYR:CZ	1:A:223:PRO:HB3	2.44	0.52
2:C:681:ARG:HG2	2:C:704:GLY:N	2.24	0.52
2:C:710:GLY:HA2	2:C:734:TYR:CZ	2.45	0.52
1:B:72:THR:HA	1:B:225:VAL:HG13	1.90	0.52
2:D:508:GLN:OE1	2:D:530:GLN:HA	2.11	0.52
2:C:658:TYR:N	2:C:658:TYR:CD1	2.78	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:703:LEU:HD23	2:C:728:LEU:CD2	2.39	0.51
2:D:289:TYR:HB3	2:D:314:ARG:HH11	1.74	0.51
2:D:471:LYS:HD2	2:D:471:LYS:C	2.35	0.51
1:A:231:MET:HE3	1:A:233:VAL:CG2	2.39	0.51
2:D:35:ARG:NH1	2:D:62:LYS:HB2	2.25	0.51
2:D:99:ARG:HA	2:D:122:ASN:ND2	2.25	0.51
2:D:458:SER:HA	2:D:482:LEU:HA	1.93	0.51
2:C:559:LYS:NZ	2:C:788:PHE:O	2.44	0.51
2:D:503:TRP:CH2	2:D:505:PRO:HA	2.45	0.51
2:D:354:PHE:HA	2:D:375:VAL:O	2.11	0.51
1:A:28:TRP:CH2	2:C:650:ASN:HB3	2.45	0.51
2:D:240:LEU:HD23	2:D:262:PHE:CZ	2.46	0.51
2:D:291:GLU:HA	2:D:315:LEU:HA	1.91	0.51
1:A:87:LEU:HD11	1:A:238:ALA:HB3	1.91	0.51
2:C:305:ILE:HD11	2:C:332:LEU:HG	1.92	0.51
1:B:92:LYS:NZ	1:B:241:ASN:O	2.33	0.51
2:D:613:PHE:O	2:D:636:GLN:HB2	2.11	0.51
2:C:501:ILE:HG13	2:C:502:ASP:N	2.25	0.51
1:A:94:ILE:HG12	1:A:199:LEU:HD23	1.92	0.51
1:B:40:LEU:CD2	1:B:51:GLN:HB3	2.41	0.51
1:B:182:PHE:HD2	1:B:198:PHE:CD1	2.27	0.51
2:D:658:TYR:HE1	2:D:682:GLN:HG3	1.76	0.51
1:A:128:THR:HG23	1:A:131:GLY:N	2.27	0.50
2:D:139:LEU:HB3	2:D:163:LEU:HD21	1.93	0.50
2:C:142:LEU:HD22	2:C:166:LEU:HD21	1.94	0.50
2:D:289:TYR:HB2	2:D:314:ARG:HD2	1.93	0.50
2:D:356:SER:OG	2:D:378:GLY:HA3	2.11	0.50
2:D:164:ARG:HG3	2:D:165:ILE:HG13	1.92	0.50
2:D:659:ASN:O	2:D:683:ASN:HA	2.11	0.50
1:A:53:THR:HA	1:A:67:THR:HA	1.94	0.50
1:A:97:ILE:HG21	1:A:100:ILE:CG1	2.39	0.50
2:C:434:LEU:HD12	2:C:437:LEU:HD22	1.94	0.50
2:D:618:SER:HA	2:D:642:PRO:HG3	1.93	0.50
1:B:111:SER:HB2	1:B:227:THR:O	2.11	0.50
2:D:328:TRP:O	2:D:331:GLU:HG2	2.11	0.50
1:A:125:THR:OG1	1:A:135:TYR:HB2	2.11	0.50
2:C:680:MET:O	2:C:706:ASN:ND2	2.44	0.50
2:C:114:LEU:O	2:C:114:LEU:HD12	2.12	0.50
2:D:572:VAL:HG21	2:D:587:LEU:HD13	1.93	0.50
1:A:53:THR:OG1	1:A:67:THR:HG22	2.12	0.50
1:A:167:PHE:HE1	1:A:184:ALA:HB2	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:45:ALA:CB	1:B:80:LYS:HE3	2.42	0.50
2:D:476:GLU:HB3	2:D:499:THR:HA	1.94	0.50
2:D:794:ARG:HD3	2:D:796:TYR:CE2	2.47	0.50
1:A:231:MET:HE3	1:A:233:VAL:HG23	1.93	0.49
2:C:160:LEU:HD13	2:C:163:LEU:HD11	1.94	0.49
2:C:306:PRO:C	2:C:335:ARG:HD3	2.37	0.49
1:B:125:THR:HG22	1:B:214:LEU:HA	1.94	0.49
2:D:320:MET:HE2	2:D:348:LEU:HD22	1.95	0.49
2:D:646:MET:SD	5:R:1:NAG:H81	2.53	0.49
2:D:676:GLU:OE1	2:D:781:MET:HE3	2.13	0.49
2:D:133:ILE:O	2:D:160:LEU:HD11	2.12	0.49
1:A:157:ILE:HD11	1:A:169:LEU:HG	1.94	0.49
2:C:59:GLU:O	2:C:62:LYS:HD2	2.13	0.49
2:D:641:LEU:HB3	2:D:645:TRP:HZ2	1.77	0.49
2:D:641:LEU:HG	2:D:685:PHE:HE1	1.77	0.49
2:D:747:LEU:HD21	2:D:750:LEU:HD13	1.93	0.49
2:C:445:ASN:O	2:C:468:ASN:HA	2.13	0.49
1:A:59:SER:HG	1:A:62:THR:HG23	1.76	0.49
2:D:173:LEU:HD23	2:D:173:LEU:H	1.78	0.49
2:D:645:TRP:HB2	2:D:668:SER:C	2.38	0.49
2:C:99:ARG:HB3	2:C:123:GLU:H	1.77	0.49
2:C:379:PHE:HD1	2:C:402:GLY:HA3	1.78	0.49
2:C:689:LEU:H	2:C:689:LEU:HD23	1.78	0.49
2:D:505:PRO:HG3	2:D:529:SER:OG	2.12	0.49
1:B:45:ALA:O	1:B:46:ALA:HB3	2.13	0.49
1:B:108:TYR:CD1	1:B:231:MET:HB2	2.48	0.49
2:C:525:LYS:HE2	2:C:528:GLN:NE2	2.28	0.49
2:C:664:LYS:CD	2:C:687:GLY:HA3	2.43	0.49
2:D:462:SER:HA	2:D:487:ASP:HB3	1.95	0.49
2:D:599:VAL:HG11	2:D:625:THR:HB	1.95	0.49
2:C:306:PRO:HD2	2:C:309:PHE:CD1	2.47	0.48
2:D:219:LEU:HG	2:D:247:CYS:CB	2.43	0.48
2:C:651:LEU:O	2:C:674:ASN:O	2.32	0.48
2:C:698:LEU:CD1	2:C:723:LEU:HD13	2.43	0.48
1:B:94:ILE:HG12	1:B:199:LEU:HD23	1.93	0.48
2:D:144:LEU:HB3	2:D:149:PHE:HE2	1.78	0.48
2:D:559:LYS:HG2	2:D:560:ILE:HG13	1.94	0.48
2:C:35:ARG:HG2	2:C:64:CYS:HB3	1.94	0.48
1:A:119:VAL:HG22	1:A:221:THR:HG22	1.96	0.48
1:B:97:ILE:HG21	1:B:100:ILE:HG13	1.95	0.48
1:B:182:PHE:CD2	1:B:198:PHE:CD1	2.98	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:90:CYS:HB3	2:D:94:ALA:O	2.14	0.48
2:D:562:ASN:HA	2:D:586:ASP:OD1	2.13	0.48
2:D:630:LEU:HD11	2:D:654:LEU:HD12	1.95	0.48
2:C:202:TRP:O	2:C:203:PHE:C	2.57	0.48
2:D:156:GLN:O	2:D:159:ASN:HB2	2.13	0.48
2:D:612:GLN:HA	2:D:636:GLN:HG3	1.96	0.48
2:D:645:TRP:HD1	2:D:668:SER:HB2	1.78	0.48
2:C:323:THR:OG1	2:C:325:THR:HG23	2.12	0.48
2:D:104:LEU:HD11	2:D:130:PRO:HG2	1.96	0.48
2:D:487:ASP:HA	2:D:511:VAL:CG1	2.44	0.48
2:D:617:ILE:HD11	2:D:641:LEU:HD22	1.94	0.48
1:A:83:SER:O	1:A:220:GLY:HA3	2.13	0.48
1:A:169:LEU:HD13	1:A:182:PHE:CD1	2.48	0.48
2:D:306:PRO:HD2	2:D:309:PHE:CE1	2.48	0.48
2:D:313:THR:HA	2:D:338:GLY:O	2.14	0.48
1:B:160:VAL:HG12	1:B:162:ILE:HG13	1.96	0.48
2:C:470:LEU:HD13	2:C:493:ASN:HD21	1.77	0.48
2:C:572:VAL:HG23	2:C:597:PRO:HG3	1.94	0.48
2:C:228:SER:HB3	2:C:231:GLU:HG3	1.94	0.48
2:D:585:ILE:HD11	2:D:600:PRO:HG2	1.95	0.48
2:C:39:LEU:HD11	2:C:56:GLY:HA2	1.95	0.47
2:D:450:LEU:HB3	2:D:478:HIS:CE1	2.49	0.47
2:C:558:ILE:HD11	2:C:582:TYR:CE1	2.50	0.47
2:D:215:LEU:HB2	2:D:240:LEU:HD11	1.96	0.47
2:D:592:PHE:O	2:D:612:GLN:HB2	2.14	0.47
2:D:693:SER:HB3	2:D:719:ASP:OD2	2.15	0.47
2:C:202:TRP:CH2	2:C:227:PRO:HD3	2.48	0.47
2:C:451:PRO:O	2:C:454:MET:HG2	2.14	0.47
2:D:470:LEU:HB3	2:D:495:LEU:HD13	1.97	0.47
2:D:558:ILE:HG13	2:D:582:TYR:CE1	2.49	0.47
1:A:104:MET:HE2	1:A:106:TYR:CD1	2.48	0.47
1:A:156:ALA:HA	1:A:170:TYR:HD1	1.79	0.47
2:C:210:PRO:HB2	2:C:211:LEU:HD22	1.96	0.47
2:C:237:LEU:HD21	7:C:1001:NAG:H81	1.95	0.47
1:A:97:ILE:HD13	1:A:100:ILE:HD11	1.95	0.47
2:C:180:TRP:H	2:C:180:TRP:CD1	2.31	0.47
1:B:169:LEU:HD12	1:B:170:TYR:N	2.30	0.47
2:D:106:PRO:HB3	2:D:132:PHE:CD2	2.50	0.47
2:D:143:ASN:OD1	2:D:167:ASP:HB3	2.15	0.47
2:D:218:SER:HB2	2:D:246:CYS:HB3	1.96	0.47
2:D:511:VAL:HG23	2:D:535:VAL:HG11	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:244:HIS:C	2:C:245:LEU:HD22	2.39	0.47
2:C:181:LEU:O	2:C:182:SER:C	2.56	0.47
2:D:80:ILE:HG13	2:D:81:VAL:HG23	1.96	0.47
2:D:144:LEU:HB3	2:D:149:PHE:CE2	2.50	0.47
2:D:415:GLU:CD	2:D:439:ILE:HD12	2.40	0.47
2:C:698:LEU:HD21	2:C:720:LEU:CD2	2.45	0.47
1:A:108:TYR:CE1	1:A:231:MET:HB2	2.50	0.47
1:A:142:ALA:HB1	1:A:144:TYR:CE1	2.50	0.47
1:A:214:LEU:HD21	1:A:217:LEU:HD11	1.97	0.47
2:C:301:LEU:HB2	2:C:325:THR:HG22	1.97	0.47
1:B:99:SER:OG	1:B:101:PRO:HD3	2.15	0.47
2:D:492:PHE:HA	2:D:516:SER:HB3	1.96	0.47
2:C:572:VAL:HA	2:C:575:LEU:HB2	1.97	0.47
2:C:698:LEU:HD11	2:C:720:LEU:HG	1.96	0.47
2:C:782:GLU:HB2	2:C:796:TYR:O	2.14	0.47
1:B:62:THR:HG22	1:B:237:SER:HB2	1.97	0.47
2:D:305:ILE:HD11	2:D:332:LEU:HG	1.97	0.47
2:C:289:TYR:O	2:C:290:LEU:C	2.58	0.46
2:C:373:LYS:HE3	2:C:373:LYS:HB3	1.82	0.46
1:B:85:ALA:HB3	1:B:236:PHE:CE2	2.51	0.46
2:D:313:THR:HG22	2:D:314:ARG:H	1.80	0.46
2:C:336:LEU:HD23	2:C:343:LEU:CD1	2.45	0.46
2:C:469:VAL:HG12	2:C:469:VAL:O	2.16	0.46
2:D:133:ILE:CG2	2:D:142:LEU:HD11	2.46	0.46
2:D:219:LEU:HG	2:D:247:CYS:HB2	1.97	0.46
2:D:280:ILE:HD11	2:D:306:PRO:HD3	1.98	0.46
1:A:93:GLN:HG2	1:A:213:TYR:CE1	2.51	0.46
2:D:366:LEU:HD23	2:D:390:LEU:HD11	1.97	0.46
1:A:171:LYS:HE2	1:A:180:PHE:CZ	2.50	0.46
2:C:88:PHE:HB2	2:C:96:PHE:C	2.41	0.46
1:B:37:TYR:HB2	1:B:84:ASN:OD1	2.16	0.46
2:D:572:VAL:HG13	2:D:576:ILE:HG23	1.97	0.46
2:C:251:SER:HA	2:C:276:LEU:HA	1.96	0.46
1:B:216:THR:HG22	1:B:218:GLU:HG3	1.98	0.46
2:C:281:ASP:CG	2:C:283:ARG:HE	2.24	0.46
2:C:299:LEU:O	2:C:324:ARG:NH1	2.49	0.46
2:C:514:LEU:N	2:C:515:PRO:HD3	2.30	0.46
1:B:167:PHE:HE1	1:B:184:ALA:HB2	1.79	0.46
2:D:586:ASP:HB2	2:D:607:TYR:HB2	1.97	0.46
1:A:45:ALA:HB3	1:A:80:LYS:HE3	1.98	0.46
1:A:62:THR:OG1	1:A:235:SER:OG	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:212:LEU:O	2:C:240:LEU:HD12	2.15	0.46
2:D:42:LYS:HE3	2:D:52:LEU:O	2.15	0.46
2:D:102:GLY:O	2:D:124:PHE:HB3	2.16	0.46
2:D:599:VAL:CG1	2:D:625:THR:HB	2.46	0.46
2:C:35:ARG:HH22	2:C:62:LYS:HA	1.81	0.46
2:C:479:LEU:CA	2:C:482:LEU:HD21	2.33	0.46
2:C:509:LEU:HD21	2:C:512:ILE:HD12	1.97	0.46
2:D:153:ILE:HD11	2:D:168:LEU:HD22	1.97	0.46
2:D:400:MET:N	2:D:421:ASN:OD1	2.33	0.46
2:C:131:ARG:HG2	2:C:154:PRO:HB3	1.98	0.46
2:D:313:THR:HG22	2:D:314:ARG:N	2.31	0.46
2:C:139:LEU:HD13	2:C:142:LEU:HD12	1.98	0.45
2:D:35:ARG:HE	2:D:35:ARG:HB3	1.38	0.45
2:D:187:LEU:O	2:D:211:LEU:HB2	2.16	0.45
2:D:799:LEU:HD12	2:D:799:LEU:HA	1.80	0.45
1:A:99:SER:OG	1:A:101:PRO:HD3	2.16	0.45
2:D:122:ASN:HD22	2:D:122:ASN:HA	1.46	0.45
2:D:285:GLY:HA2	2:D:312:LEU:HD21	1.97	0.45
2:C:50:GLY:O	2:C:52:LEU:N	2.42	0.45
2:C:361:THR:HG21	2:C:386:GLN:C	2.41	0.45
2:C:509:LEU:O	2:C:533:TYR:HB3	2.16	0.45
2:C:693:SER:HB3	2:C:719:ASP:OD2	2.17	0.45
2:D:486:VAL:HG13	2:D:510:GLN:HB2	1.98	0.45
2:D:528:GLN:HG2	2:D:550:TRP:CD2	2.52	0.45
2:D:669:LEU:O	2:D:672:LEU:HB2	2.17	0.45
3:L:9:MAN:H2	3:L:10:MAN:C5	2.43	0.45
1:A:57:LYS:O	1:A:58:ILE:HD13	2.16	0.45
2:C:349:ASN:HD22	2:C:372:GLN:NE2	2.12	0.45
2:C:384:PHE:HD2	2:C:386:GLN:HB2	1.81	0.45
2:D:288:MET:HG3	2:D:289:TYR:CD1	2.47	0.45
2:D:322:ASN:HA	2:D:350:ASP:O	2.16	0.45
2:D:586:ASP:CB	2:D:607:TYR:HB2	2.47	0.45
2:C:541:ALA:O	2:C:566:ASN:OD1	2.34	0.45
2:C:617:ILE:HD11	2:C:641:LEU:CD2	2.42	0.45
2:C:688:MET:HA	2:C:709:THR:O	2.17	0.45
2:D:118:ASP:O	2:D:119:LEU:HD23	2.17	0.45
2:D:583:MET:HG3	2:D:584:VAL:HG23	1.98	0.45
2:C:503:TRP:CZ3	2:C:505:PRO:HB3	2.52	0.45
1:B:40:LEU:HD22	1:B:51:GLN:HB3	1.98	0.45
1:B:156:ALA:HB2	1:B:170:TYR:HE1	1.81	0.45
2:D:88:PHE:HB3	2:D:97:ALA:CB	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:695:CYS:O	2:D:698:LEU:HD23	2.17	0.45
2:C:180:TRP:CZ3	2:C:181:LEU:HD12	2.52	0.45
2:C:558:ILE:HG13	2:C:558:ILE:O	2.16	0.45
1:B:49:GLY:HA2	1:B:70:THR:O	2.17	0.45
2:D:505:PRO:HG3	2:D:530:GLN:OE1	2.16	0.45
2:D:622:LYS:HD3	5:R:1:NAG:N2	2.32	0.45
1:A:49:GLY:HA3	1:A:70:THR:O	2.16	0.45
2:C:166:LEU:HD13	2:C:168:LEU:HD11	1.98	0.45
2:D:41:PHE:HB2	2:D:108:LEU:CD2	2.39	0.45
2:D:645:TRP:CD1	2:D:668:SER:HB2	2.52	0.45
1:A:82:TYR:O	1:A:83:SER:C	2.58	0.45
2:C:381:MET:HE2	2:C:381:MET:HB3	1.89	0.45
1:B:171:LYS:HG2	1:B:172:GLY:N	2.32	0.45
2:D:78:HIS:CG	2:D:113:TYR:HD2	2.34	0.45
2:D:470:LEU:HB2	2:D:493:ASN:ND2	2.31	0.45
1:A:153:THR:HG22	1:A:155:LYS:HG3	1.99	0.44
2:C:180:TRP:O	2:C:181:LEU:C	2.60	0.44
2:C:313:THR:HA	2:C:338:GLY:O	2.17	0.44
2:D:309:PHE:CD2	2:D:312:LEU:HD11	2.53	0.44
2:D:427:ILE:HD12	2:D:450:LEU:HD22	1.98	0.44
2:C:80:ILE:HA	2:C:114:LEU:HA	1.99	0.44
2:D:509:LEU:CD2	2:D:530:GLN:HG2	2.47	0.44
2:D:622:LYS:NZ	2:D:644:CYS:HB3	2.32	0.44
2:D:514:LEU:N	2:D:515:PRO:HD3	2.33	0.44
2:D:658:TYR:CE1	2:D:682:GLN:HG3	2.53	0.44
1:A:79:VAL:HG22	1:A:224:PHE:HE1	1.82	0.44
2:C:114:LEU:HD11	2:C:136:PHE:CE1	2.52	0.44
2:C:317:TYR:HD2	2:C:345:VAL:HB	1.82	0.44
2:D:105:SER:O	2:D:108:LEU:HD23	2.17	0.44
2:D:683:ASN:HD22	2:D:685:PHE:HE2	1.65	0.44
2:D:702:ASP:CB	2:D:727:SER:HB3	2.48	0.44
2:C:498:LYS:HE2	2:C:521:PRO:HD3	1.99	0.44
2:C:513:ASN:C	2:C:515:PRO:HD3	2.42	0.44
2:D:654:LEU:HD23	2:D:678:LEU:HD12	1.98	0.44
2:C:291:GLU:HA	2:C:315:LEU:HA	1.99	0.44
2:C:324:ARG:CZ	2:C:324:ARG:HB2	2.45	0.44
2:D:287:LEU:HB2	2:D:290:LEU:HD22	1.98	0.44
2:D:357:LEU:HG	2:D:360:VAL:HG22	1.98	0.44
2:D:641:LEU:HB2	2:D:666:PRO:CG	2.48	0.44
1:A:186:LYS:O	1:A:188:ILE:HG13	2.16	0.44
2:C:64:CYS:HA	2:C:67:TRP:CE2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:243:LEU:HB3	2:C:245:LEU:CD2	2.47	0.44
2:D:738:SER:HB3	2:D:740:ILE:HG12	2.00	0.44
2:C:680:MET:HB2	2:C:703:LEU:CD1	2.47	0.44
2:C:614:PHE:HA	2:C:637:PHE:HA	1.99	0.43
2:C:677:ALA:HB1	2:C:679:TYR:CE1	2.53	0.43
1:B:53:THR:OG1	1:B:67:THR:HG22	2.17	0.43
2:D:73:ASN:HB3	2:D:76:THR:O	2.18	0.43
1:A:28:TRP:HE1	2:C:674:ASN:HD21	1.63	0.43
2:C:128:GLU:OE1	2:C:151:GLY:HA3	2.17	0.43
2:C:659:ASN:O	2:C:683:ASN:OD1	2.35	0.43
2:D:533:TYR:CZ	2:D:555:PRO:HG2	2.54	0.43
2:D:645:TRP:CD1	2:D:669:LEU:HG	2.53	0.43
2:C:724:ARG:HH12	2:C:780:PRO:HG2	1.84	0.43
2:D:379:PHE:HA	2:D:401:ARG:O	2.18	0.43
2:D:467:TYR:CE1	2:D:492:PHE:HD2	2.36	0.43
2:D:468:ASN:CB	2:D:470:LEU:HD23	2.42	0.43
2:D:715:TRP:CZ3	2:D:716:ILE:HG12	2.54	0.43
2:C:41:PHE:CG	2:C:108:LEU:HD21	2.53	0.43
2:C:199:VAL:O	2:C:225:LEU:HD13	2.19	0.43
2:D:170:TYR:CE1	2:D:219:LEU:HD12	2.50	0.43
2:C:508:GLN:NE2	2:C:529:SER:O	2.52	0.43
2:D:202:TRP:CE3	2:D:206:ILE:HD12	2.47	0.43
2:D:215:LEU:HB3	2:D:243:LEU:HD23	2.00	0.43
2:C:710:GLY:HA2	2:C:734:TYR:CE2	2.54	0.43
2:D:596:LEU:HD21	2:D:619:SER:HB2	2.00	0.43
2:C:39:LEU:HD21	2:C:67:TRP:HH2	1.83	0.43
2:C:86:ASN:O	2:C:121:VAL:CB	2.62	0.43
2:C:394:ASP:HA	2:C:417:HIS:HB2	2.01	0.43
2:D:380:PHE:O	2:D:405:PRO:HD3	2.19	0.43
2:C:339:SER:HB2	2:C:342:THR:OG1	2.19	0.43
2:C:523:PHE:O	2:C:524:PRO:C	2.61	0.43
2:D:190:LEU:HD21	2:D:192:LEU:CD1	2.49	0.43
2:D:353:MET:HE2	2:D:353:MET:HB3	1.82	0.43
2:D:689:LEU:H	2:D:689:LEU:HG	1.43	0.43
1:A:201:TYR:CD1	1:A:201:TYR:C	2.97	0.43
2:C:724:ARG:HA	2:C:747:LEU:HA	2.01	0.43
2:D:111:LEU:O	2:D:112:GLU:HB2	2.18	0.43
2:D:399:GLN:N	2:D:421:ASN:OD1	2.52	0.43
2:D:613:PHE:HB3	2:D:637:PHE:CE2	2.54	0.43
2:C:698:LEU:HD11	2:C:720:LEU:HD23	2.00	0.42
1:B:69:TYR:C	1:B:70:THR:HG1	2.26	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:617:ILE:HD11	2:D:641:LEU:CD2	2.49	0.42
1:B:69:TYR:HB2	1:B:71:TRP:NE1	2.33	0.42
2:D:646:MET:HG2	2:D:647:ASN:N	2.33	0.42
2:C:361:THR:HB	2:C:382:GLU:OE2	2.19	0.42
1:B:40:LEU:HD21	1:B:51:GLN:HG2	2.01	0.42
2:D:111:LEU:H	2:D:111:LEU:HG	1.61	0.42
2:D:665:LEU:HA	2:D:666:PRO:HD3	1.72	0.42
2:C:130:PRO:HD2	2:C:133:ILE:CD1	2.50	0.42
2:D:99:ARG:HB3	2:D:123:GLU:H	1.84	0.42
2:C:71:GLU:HB2	2:C:81:VAL:HB	2.00	0.42
2:C:498:LYS:CE	2:C:521:PRO:HD3	2.50	0.42
2:D:414:ARG:HA	2:D:437:LEU:HA	2.01	0.42
2:D:434:LEU:HA	2:D:434:LEU:HD23	1.79	0.42
2:D:517:CYS:O	2:D:519:LEU:HD22	2.19	0.42
2:D:621:CYS:HB2	2:D:644:CYS:HB2	1.64	0.42
2:D:622:LYS:HD3	5:R:1:NAG:HN2	1.85	0.42
2:C:303:GLY:O	2:C:325:THR:HB	2.20	0.42
1:B:103:LYS:HE2	1:B:103:LYS:HB3	1.76	0.42
2:D:100:LEU:HD13	2:D:122:ASN:ND2	2.34	0.42
2:C:652:ALA:C	2:C:675:LEU:HD12	2.45	0.42
1:B:169:LEU:HD13	1:B:182:PHE:CD1	2.54	0.42
2:C:114:LEU:HD21	2:C:136:PHE:CE1	2.55	0.42
2:D:622:LYS:HE2	2:D:622:LYS:HB2	1.85	0.42
5:H:2:NAG:H3	5:H:2:NAG:C8	2.50	0.42
2:C:187:LEU:HD23	2:C:187:LEU:HA	1.75	0.42
2:C:312:LEU:HD23	2:C:312:LEU:HA	1.92	0.42
1:B:69:TYR:HB2	1:B:71:TRP:CD1	2.55	0.42
2:D:448:GLU:O	2:D:471:LYS:HG3	2.20	0.42
2:D:498:LYS:HE2	2:D:520:GLY:HA2	2.02	0.42
2:D:606:PHE:O	2:D:630:LEU:HA	2.19	0.42
2:D:663:GLY:O	2:D:685:PHE:CD1	2.65	0.42
2:C:134:CYS:HA	2:C:160:LEU:HG	2.01	0.42
2:C:312:LEU:O	2:C:313:THR:C	2.61	0.42
1:B:156:ALA:HA	1:B:170:TYR:CD1	2.55	0.42
2:D:289:TYR:CB	2:D:314:ARG:HD2	2.48	0.42
2:D:379:PHE:CD1	2:D:402:GLY:HA3	2.47	0.42
2:D:802:LEU:HD12	2:D:802:LEU:HA	1.82	0.42
2:C:210:PRO:C	2:C:211:LEU:HD13	2.45	0.41
2:C:547:LEU:N	2:C:569:SER:O	2.45	0.41
1:B:58:ILE:HD13	1:B:63:ILE:HG13	2.02	0.41
2:D:543:ILE:HG22	2:D:568:ILE:HG12	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:572:VAL:O	2:D:573:SER:C	2.62	0.41
2:C:125:GLU:O	2:C:127:SER:N	2.54	0.41
2:C:560:ILE:HG12	2:C:584:VAL:HB	2.02	0.41
2:D:88:PHE:HB2	2:D:96:PHE:O	2.20	0.41
2:D:104:LEU:HD23	2:D:104:LEU:H	1.85	0.41
2:D:212:LEU:HD12	2:D:212:LEU:HA	1.90	0.41
2:D:519:LEU:CD2	2:D:538:ILE:HG23	2.51	0.41
2:D:728:LEU:HB2	2:D:752:LEU:HD23	2.01	0.41
2:C:222:LEU:HA	2:C:222:LEU:HD12	1.80	0.41
2:C:224:LYS:HD2	2:C:224:LYS:HA	1.83	0.41
2:C:250:PHE:O	2:C:251:SER:HB2	2.20	0.41
2:C:280:ILE:CG1	2:C:306:PRO:HD3	2.50	0.41
2:C:353:MET:HE2	2:C:353:MET:HB3	1.80	0.41
2:D:52:LEU:HD13	2:D:52:LEU:HA	1.88	0.41
2:D:240:LEU:HD23	2:D:262:PHE:CE2	2.54	0.41
2:D:560:ILE:HG12	2:D:584:VAL:HB	2.02	0.41
2:D:702:ASP:HB3	2:D:727:SER:HB3	2.01	0.41
2:C:282:ASP:OD2	2:C:282:ASP:N	2.53	0.41
2:C:467:TYR:CE1	2:C:492:PHE:CD2	3.05	0.41
2:C:715:TRP:HA	2:C:718:THR:HB	2.01	0.41
2:D:35:ARG:CG	2:D:64:CYS:HB3	2.50	0.41
2:D:407:LEU:HD12	2:D:431:ILE:HD12	2.02	0.41
2:D:413:LEU:HD13	2:D:416:LEU:HD13	2.01	0.41
2:D:424:ASN:HA	2:D:446:ARG:O	2.21	0.41
2:D:609:HIS:HB2	2:D:633:SER:OG	2.21	0.41
2:C:76:THR:HG23	4:J:1:NAG:O6	2.20	0.41
2:C:375:VAL:O	2:C:375:VAL:HG23	2.20	0.41
2:C:617:ILE:O	2:C:642:PRO:HG3	2.21	0.41
1:B:81:SER:O	1:B:223:PRO:HD2	2.19	0.41
2:D:143:ASN:CG	2:D:167:ASP:HB3	2.45	0.41
2:D:713:PRO:HG2	2:D:716:ILE:HG13	2.02	0.41
4:F:1:NAG:H61	4:F:2:NAG:H82	2.02	0.41
1:A:123:LEU:HA	1:A:216:THR:O	2.21	0.41
2:C:137:LYS:HB3	2:C:137:LYS:HE2	1.92	0.41
1:B:202:LEU:HD23	1:B:202:LEU:HA	1.93	0.41
2:D:621:CYS:SG	2:D:622:LYS:N	2.94	0.41
2:D:681:ARG:HG2	2:D:704:GLY:H	1.85	0.41
1:A:81:SER:O	1:A:223:PRO:HD2	2.20	0.41
2:C:288:MET:HG3	2:C:314:ARG:HH12	1.86	0.41
2:C:645:TRP:HD1	2:C:668:SER:HB2	1.85	0.41
1:A:133:ASN:H	1:A:133:ASN:ND2	2.18	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:100:LEU:O	2:C:101:THR:C	2.64	0.41
2:C:689:LEU:HD11	2:C:713:PRO:CD	2.51	0.41
2:C:698:LEU:HD11	2:C:720:LEU:CD2	2.51	0.41
1:B:45:ALA:O	1:B:74:GLY:HA3	2.20	0.41
1:B:68:SER:HA	1:B:229:ALA:O	2.21	0.41
1:B:80:LYS:NZ	1:B:224:PHE:O	2.50	0.41
2:D:394:ASP:OD1	2:D:417:HIS:HB2	2.20	0.41
2:C:142:LEU:CD2	2:C:144:LEU:HG	2.51	0.41
2:C:166:LEU:HD22	2:C:168:LEU:CD1	2.50	0.41
2:C:201:ASN:HB2	2:C:204:GLN:CD	2.46	0.41
2:C:280:ILE:HG22	2:C:301:LEU:HD22	2.03	0.41
1:B:43:LYS:HE3	1:B:43:LYS:HB2	1.76	0.41
1:B:100:ILE:HG22	1:B:100:ILE:O	2.21	0.41
2:D:120:SER:O	2:D:121:VAL:C	2.64	0.41
2:D:382:GLU:OE1	2:D:382:GLU:HA	2.21	0.41
2:D:609:HIS:HD2	2:D:610:LYS:HG2	1.85	0.41
2:D:645:TRP:O	2:D:672:LEU:HD11	2.21	0.41
1:A:165:ASN:OD1	1:A:186:LYS:HD2	2.21	0.41
2:C:343:LEU:HD23	2:C:343:LEU:C	2.45	0.41
2:C:368:ARG:HG2	2:C:392:TYR:HB2	2.02	0.41
2:C:698:LEU:HD11	2:C:720:LEU:CG	2.51	0.41
2:D:50:GLY:O	2:D:52:LEU:N	2.49	0.41
2:D:190:LEU:HD21	2:D:192:LEU:HD12	2.02	0.41
2:D:507:PHE:CD1	2:D:509:LEU:HD22	2.55	0.41
2:C:191:SER:HA	2:C:216:ASP:HB3	2.03	0.40
2:C:217:LEU:HD13	2:C:222:LEU:HD11	2.02	0.40
2:C:501:ILE:HG13	2:C:502:ASP:H	1.86	0.40
1:A:32:THR:OG1	1:A:33:ASN:N	2.54	0.40
2:C:535:VAL:O	2:C:535:VAL:HG13	2.22	0.40
2:D:596:LEU:HD21	2:D:619:SER:CB	2.51	0.40
2:D:643:ASP:CG	2:D:668:SER:H	2.29	0.40
2:C:478:HIS:HB2	2:C:479:LEU:HD23	2.04	0.40
2:C:526:TRP:H	2:C:526:TRP:CD1	2.37	0.40
2:C:631:ASP:HA	2:C:655:ASN:HB3	2.03	0.40
2:D:137:LYS:H	2:D:160:LEU:HD23	1.87	0.40
2:D:219:LEU:HD23	2:D:219:LEU:HA	1.91	0.40
2:D:596:LEU:HD21	2:D:619:SER:H	1.85	0.40
2:C:357:LEU:HA	2:C:357:LEU:HD12	1.88	0.40
2:C:434:LEU:CD1	2:C:437:LEU:HD22	2.51	0.40
2:C:571:ARG:O	2:C:571:ARG:HG3	2.21	0.40
2:C:582:TYR:CG	2:C:585:ILE:HD11	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:218:SER:HA	2:D:246:CYS:O	2.21	0.40
1:A:171:LYS:HG2	1:A:172:GLY:N	2.36	0.40
2:D:368:ARG:HD3	2:D:370:TYR:HE2	1.86	0.40
2:D:578:ASN:OD1	2:D:598:LEU:HB2	2.21	0.40
2:D:630:LEU:HD11	2:D:654:LEU:CD1	2.52	0.40

All (1) 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)
2:C:234:ASN:OD1	2:C:711:ARG:NH1[1_455]	2.14	0.06

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	220/241 (91%)	202 (92%)	18 (8%)	0	100	100
1	B	220/241 (91%)	204 (93%)	16 (7%)	0	100	100
2	C	748/934 (80%)	681 (91%)	67 (9%)	0	100	100
2	D	748/934 (80%)	676 (90%)	71 (10%)	1 (0%)	48	75
All	All	1936/2350 (82%)	1763 (91%)	172 (9%)	1 (0%)	48	75

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	306	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	181/191 (95%)	180 (99%)	1 (1%)	78	81
1	B	181/191 (95%)	181 (100%)	0	100	100
2	C	680/839 (81%)	665 (98%)	15 (2%)	45	66
2	D	680/839 (81%)	667 (98%)	13 (2%)	50	68
All	All	1722/2060 (84%)	1693 (98%)	29 (2%)	53	71

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	ASN
2	C	114	LEU
2	C	166	LEU
2	C	167	ASP
2	C	179	THR
2	C	181	LEU
2	C	211	LEU
2	C	219	LEU
2	C	222	LEU
2	C	245	LEU
2	C	282	ASP
2	C	479	LEU
2	C	482	LEU
2	C	660	ASN
2	C	698	LEU
2	C	707	LYS
2	D	122	ASN
2	D	157	PHE
2	D	240	LEU
2	D	377	ASN
2	D	572	VAL
2	D	622	LYS
2	D	624	THR
2	D	628	THR

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Mol	Chain	Res	Type
2	D	643	ASP
2	D	644	CYS
2	D	689	LEU
2	D	698	LEU
2	D	799	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	133	ASN
2	C	244	HIS
2	C	273	ASN
2	C	275	GLN
2	C	372	GLN
2	C	493	ASN
2	C	531	ASN
2	C	565	ASN
2	C	591	ASN
2	C	722	ASN
2	D	85	HIS
2	D	122	ASN
2	D	275	GLN
2	D	349	ASN
2	D	478	HIS
2	D	655	ASN

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 ⓘ

58 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	$\# Z > 2$
3	NAG	E	1	2,3	14,14,15	0.47	0	17,19,21	0.73	0
3	MAN	E	10	3	11,11,12	1.91	4 (36%)	15,15,17	2.24	4 (26%)
3	NAG	E	2	3	14,14,15	0.22	0	17,19,21	0.63	0
3	BMA	E	3	3	11,11,12	1.77	2 (18%)	15,15,17	1.44	3 (20%)
3	MAN	E	4	3	11,11,12	1.56	2 (18%)	15,15,17	2.16	2 (13%)
3	MAN	E	5	3	11,11,12	1.47	2 (18%)	15,15,17	1.68	2 (13%)
3	MAN	E	6	3	11,11,12	1.26	1 (9%)	15,15,17	1.32	2 (13%)
3	MAN	E	7	3	11,11,12	1.23	1 (9%)	15,15,17	2.55	3 (20%)
3	MAN	E	8	3	11,11,12	2.34	5 (45%)	15,15,17	1.94	4 (26%)
3	MAN	E	9	3	11,11,12	1.66	3 (27%)	15,15,17	1.58	4 (26%)
4	NAG	F	1	4,2	14,14,15	0.32	0	17,19,21	0.90	1 (5%)
4	NAG	F	2	4	14,14,15	0.67	1 (7%)	17,19,21	0.58	0
4	NAG	G	1	4,2	14,14,15	0.81	2 (14%)	17,19,21	0.85	1 (5%)
4	NAG	G	2	4	14,14,15	0.58	0	17,19,21	0.71	0
5	NAG	H	1	5,2	14,14,15	0.72	1 (7%)	17,19,21	1.10	1 (5%)
5	NAG	H	2	5	14,14,15	0.51	0	17,19,21	1.71	2 (11%)
5	BMA	H	3	5	11,11,12	0.84	0	15,15,17	0.87	0
6	NAG	I	1	6,2	14,14,15	0.68	0	17,19,21	1.06	1 (5%)
6	NAG	I	2	6	14,14,15	0.56	0	17,19,21	1.27	2 (11%)
6	BMA	I	3	6	11,11,12	0.46	0	15,15,17	0.82	0
6	MAN	I	4	6	11,11,12	0.47	0	15,15,17	0.71	0
6	MAN	I	5	6	11,11,12	0.38	0	15,15,17	0.74	0
6	MAN	I	6	6	11,11,12	0.29	0	15,15,17	0.85	0
6	MAN	I	7	6	11,11,12	0.40	0	15,15,17	0.90	1 (6%)
4	NAG	J	1	4,2	14,14,15	0.41	0	17,19,21	0.70	1 (5%)
4	NAG	J	2	4	14,14,15	0.41	0	17,19,21	0.80	1 (5%)
4	NAG	K	1	4,2	14,14,15	0.70	1 (7%)	17,19,21	0.63	0
4	NAG	K	2	4	14,14,15	0.63	1 (7%)	17,19,21	0.84	1 (5%)
3	NAG	L	1	2,3	14,14,15	0.48	0	17,19,21	0.56	0
3	MAN	L	10	3	11,11,12	0.24	0	15,15,17	0.68	0
3	NAG	L	2	3	14,14,15	0.31	0	17,19,21	0.85	0
3	BMA	L	3	3	11,11,12	1.66	2 (18%)	15,15,17	1.31	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	MAN	L	4	3	11,11,12	0.75	0	15,15,17	1.35	3 (20%)
3	MAN	L	5	3	11,11,12	0.62	0	15,15,17	1.53	2 (13%)
3	MAN	L	6	3	11,11,12	0.49	0	15,15,17	0.79	0
3	MAN	L	7	3	11,11,12	0.54	0	15,15,17	1.03	1 (6%)
3	MAN	L	8	3	11,11,12	0.31	0	15,15,17	0.78	0
3	MAN	L	9	3	11,11,12	1.66	3 (27%)	15,15,17	1.22	2 (13%)
4	NAG	M	1	4,2	14,14,15	0.31	0	17,19,21	0.76	0
4	NAG	M	2	4	14,14,15	0.40	0	17,19,21	0.80	0
5	NAG	N	1	5,2	14,14,15	0.42	0	17,19,21	0.93	1 (5%)
5	NAG	N	2	5	14,14,15	0.45	0	17,19,21	0.98	2 (11%)
5	BMA	N	3	5	11,11,12	0.37	0	15,15,17	0.57	0
5	NAG	O	1	5,2	14,14,15	0.78	1 (7%)	17,19,21	1.35	2 (11%)
5	NAG	O	2	5	14,14,15	0.40	0	17,19,21	0.69	0
5	BMA	O	3	5	11,11,12	1.47	2 (18%)	15,15,17	1.01	0
6	NAG	P	1	6,2	14,14,15	0.52	0	17,19,21	0.95	1 (5%)
6	NAG	P	2	6	14,14,15	0.63	0	17,19,21	1.01	1 (5%)
6	BMA	P	3	6	11,11,12	0.49	0	15,15,17	1.19	1 (6%)
6	MAN	P	4	6	11,11,12	0.48	0	15,15,17	0.77	0
6	MAN	P	5	6	11,11,12	0.34	0	15,15,17	0.84	0
6	MAN	P	6	6	11,11,12	0.34	0	15,15,17	0.75	0
6	MAN	P	7	6	11,11,12	0.22	0	15,15,17	1.09	1 (6%)
4	NAG	Q	1	4,2	14,14,15	0.58	0	17,19,21	0.79	0
4	NAG	Q	2	4	14,14,15	0.36	0	17,19,21	1.01	1 (5%)
5	NAG	R	1	5,2	14,14,15	0.52	0	17,19,21	0.82	1 (5%)
5	NAG	R	2	5	14,14,15	0.40	0	17,19,21	0.67	0
5	BMA	R	3	5	11,11,12	0.29	0	15,15,17	0.79	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
3	NAG	E	1	2,3	-	4/6/23/26	0/1/1/1
3	MAN	E	10	3	-	0/2/19/22	0/1/1/1
3	NAG	E	2	3	-	0/6/23/26	0/1/1/1
3	BMA	E	3	3	-	1/2/19/22	0/1/1/1
3	MAN	E	4	3	-	2/2/19/22	0/1/1/1
3	MAN	E	5	3	-	2/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	MAN	E	6	3	-	0/2/19/22	0/1/1/1
3	MAN	E	7	3	-	0/2/19/22	0/1/1/1
3	MAN	E	8	3	-	2/2/19/22	0/1/1/1
3	MAN	E	9	3	-	0/2/19/22	0/1/1/1
4	NAG	F	1	4,2	-	0/6/23/26	0/1/1/1
4	NAG	F	2	4	-	3/6/23/26	0/1/1/1
4	NAG	G	1	4,2	-	0/6/23/26	0/1/1/1
4	NAG	G	2	4	-	2/6/23/26	0/1/1/1
5	NAG	H	1	5,2	-	0/6/23/26	0/1/1/1
5	NAG	H	2	5	-	5/6/23/26	0/1/1/1
5	BMA	H	3	5	-	0/2/19/22	0/1/1/1
6	NAG	I	1	6,2	-	2/6/23/26	0/1/1/1
6	NAG	I	2	6	-	0/6/23/26	0/1/1/1
6	BMA	I	3	6	-	0/2/19/22	0/1/1/1
6	MAN	I	4	6	-	1/2/19/22	0/1/1/1
6	MAN	I	5	6	-	0/2/19/22	0/1/1/1
6	MAN	I	6	6	-	2/2/19/22	0/1/1/1
6	MAN	I	7	6	-	0/2/19/22	0/1/1/1
4	NAG	J	1	4,2	-	2/6/23/26	0/1/1/1
4	NAG	J	2	4	-	2/6/23/26	0/1/1/1
4	NAG	K	1	4,2	-	0/6/23/26	0/1/1/1
4	NAG	K	2	4	-	2/6/23/26	0/1/1/1
3	NAG	L	1	2,3	-	2/6/23/26	0/1/1/1
3	MAN	L	10	3	-	0/2/19/22	0/1/1/1
3	NAG	L	2	3	-	2/6/23/26	0/1/1/1
3	BMA	L	3	3	-	1/2/19/22	0/1/1/1
3	MAN	L	4	3	-	0/2/19/22	0/1/1/1
3	MAN	L	5	3	-	0/2/19/22	0/1/1/1
3	MAN	L	6	3	-	0/2/19/22	0/1/1/1
3	MAN	L	7	3	-	0/2/19/22	0/1/1/1
3	MAN	L	8	3	-	0/2/19/22	0/1/1/1
3	MAN	L	9	3	-	0/2/19/22	0/1/1/1
4	NAG	M	1	4,2	-	0/6/23/26	0/1/1/1
4	NAG	M	2	4	-	1/6/23/26	0/1/1/1
5	NAG	N	1	5,2	-	3/6/23/26	0/1/1/1
5	NAG	N	2	5	-	2/6/23/26	0/1/1/1
5	BMA	N	3	5	-	0/2/19/22	0/1/1/1
5	NAG	O	1	5,2	-	0/6/23/26	0/1/1/1
5	NAG	O	2	5	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	BMA	O	3	5	-	0/2/19/22	0/1/1/1
6	NAG	P	1	6,2	-	0/6/23/26	0/1/1/1
6	NAG	P	2	6	-	0/6/23/26	0/1/1/1
6	BMA	P	3	6	-	0/2/19/22	0/1/1/1
6	MAN	P	4	6	-	1/2/19/22	0/1/1/1
6	MAN	P	5	6	-	0/2/19/22	0/1/1/1
6	MAN	P	6	6	-	0/2/19/22	0/1/1/1
6	MAN	P	7	6	-	1/2/19/22	0/1/1/1
4	NAG	Q	1	4,2	-	4/6/23/26	0/1/1/1
4	NAG	Q	2	4	-	0/6/23/26	0/1/1/1
5	NAG	R	1	5,2	-	3/6/23/26	0/1/1/1
5	NAG	R	2	5	-	5/6/23/26	0/1/1/1
5	BMA	R	3	5	-	0/2/19/22	0/1/1/1

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	8	MAN	C1-C2	5.17	1.64	1.52
3	E	3	BMA	C4-C5	4.19	1.61	1.53
3	L	3	BMA	O5-C1	-3.89	1.37	1.43
3	L	9	MAN	O5-C5	3.69	1.50	1.43
3	E	4	MAN	C4-C3	3.60	1.61	1.52
3	E	9	MAN	O5-C5	3.40	1.50	1.43
3	E	10	MAN	O5-C1	3.40	1.49	1.43
3	E	8	MAN	O5-C1	3.23	1.49	1.43
3	E	10	MAN	O5-C5	3.22	1.49	1.43
3	E	8	MAN	C4-C5	3.13	1.59	1.53
3	L	3	BMA	C4-C5	3.07	1.59	1.53
5	O	3	BMA	C1-C2	2.92	1.59	1.52
3	E	9	MAN	C4-C3	2.74	1.59	1.52
3	E	3	BMA	C2-C3	-2.67	1.48	1.52
3	E	9	MAN	O2-C2	2.60	1.48	1.43
3	E	10	MAN	C1-C2	2.56	1.58	1.52
3	E	10	MAN	C4-C3	2.43	1.58	1.52
3	L	9	MAN	C4-C5	2.42	1.58	1.53
3	E	8	MAN	O5-C5	2.38	1.48	1.43
3	E	5	MAN	O5-C1	-2.22	1.40	1.43
3	E	6	MAN	C1-C2	2.20	1.57	1.52
3	E	5	MAN	C2-C3	2.14	1.55	1.52
5	O	1	NAG	O5-C1	2.14	1.47	1.43
4	K	1	NAG	C1-C2	2.12	1.55	1.52
4	K	2	NAG	C1-C2	2.09	1.55	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	H	1	NAG	C1-C2	2.08	1.55	1.52
3	E	4	MAN	C4-C5	2.08	1.57	1.53
3	E	8	MAN	C2-C3	2.08	1.55	1.52
4	G	1	NAG	C1-C2	2.07	1.55	1.52
3	E	7	MAN	C6-C5	2.07	1.58	1.51
3	L	9	MAN	O5-C1	-2.05	1.40	1.43
5	O	3	BMA	O5-C1	2.03	1.47	1.43
4	F	2	NAG	O5-C1	2.03	1.47	1.43
4	G	1	NAG	O5-C1	2.01	1.47	1.43

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	7	MAN	C1-O5-C5	8.40	123.45	112.19
3	E	10	MAN	C1-O5-C5	6.81	121.31	112.19
3	E	4	MAN	C1-O5-C5	6.20	120.50	112.19
5	H	2	NAG	C2-N2-C7	5.52	130.29	122.90
3	E	8	MAN	C1-O5-C5	4.92	118.78	112.19
3	E	5	MAN	O2-C2-C3	-4.67	100.48	110.15
3	E	4	MAN	C3-C4-C5	4.30	118.03	110.23
6	I	2	NAG	C2-N2-C7	-3.99	117.55	122.90
5	O	1	NAG	O4-C4-C5	3.88	118.89	109.32
3	E	6	MAN	O2-C2-C3	-3.49	102.93	110.15
3	E	9	MAN	C1-C2-C3	-3.43	104.65	109.64
5	O	1	NAG	C1-O5-C5	3.36	116.69	112.19
3	L	5	MAN	C2-C3-C4	-3.28	105.10	110.86
3	E	3	BMA	O2-C2-C3	-3.20	103.52	110.15
3	L	5	MAN	O2-C2-C3	-3.15	103.62	110.15
6	P	3	BMA	O3-C3-C2	-3.15	103.63	110.05
6	P	7	MAN	C1-O5-C5	3.10	116.34	112.19
3	E	7	MAN	O5-C5-C4	2.97	118.05	110.83
3	L	3	BMA	O5-C5-C6	-2.91	102.00	107.66
3	E	8	MAN	C1-C2-C3	2.86	113.81	109.64
3	E	9	MAN	C1-O5-C5	2.72	115.83	112.19
3	L	4	MAN	O3-C3-C2	-2.70	104.55	110.05
4	J	2	NAG	C1-O5-C5	2.67	115.76	112.19
3	E	5	MAN	O3-C3-C2	2.65	115.46	110.05
3	L	9	MAN	O2-C2-C3	-2.62	104.73	110.15
3	E	3	BMA	C6-C5-C4	2.59	119.38	113.02
5	H	2	NAG	C1-C2-N2	2.58	114.49	110.43
3	E	3	BMA	O5-C5-C6	-2.57	102.65	107.66
6	I	1	NAG	C1-C2-N2	-2.57	106.38	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	K	2	NAG	C1-O5-C5	2.57	115.63	112.19
4	F	1	NAG	C1-O5-C5	2.47	115.49	112.19
3	L	3	BMA	C6-C5-C4	2.38	118.85	113.02
3	L	4	MAN	C1-O5-C5	2.37	115.36	112.19
5	N	2	NAG	O4-C4-C3	-2.37	104.80	110.38
3	E	8	MAN	O2-C2-C1	2.36	114.62	109.22
3	E	6	MAN	O2-C2-C1	2.33	114.56	109.22
3	E	10	MAN	O3-C3-C4	2.23	115.64	110.38
6	P	1	NAG	C4-C3-C2	-2.23	107.76	111.02
3	E	10	MAN	O4-C4-C3	2.20	115.56	110.38
3	L	9	MAN	C1-C2-C3	-2.17	106.48	109.64
3	E	9	MAN	O2-C2-C3	-2.17	105.66	110.15
3	L	7	MAN	O2-C2-C3	-2.16	105.68	110.15
3	E	8	MAN	O3-C3-C2	2.12	114.38	110.05
5	H	1	NAG	C1-O5-C5	2.10	115.00	112.19
3	L	4	MAN	O3-C3-C4	-2.10	105.43	110.38
4	J	1	NAG	C1-O5-C5	2.10	115.00	112.19
6	I	7	MAN	C2-C3-C4	-2.08	107.20	110.86
3	E	9	MAN	O3-C3-C2	2.07	114.28	110.05
4	Q	2	NAG	C2-N2-C7	-2.05	120.16	122.90
5	N	2	NAG	C2-N2-C7	-2.04	120.16	122.90
3	E	7	MAN	O5-C1-C2	2.04	115.65	110.79
5	N	1	NAG	O4-C4-C3	-2.04	105.57	110.38
4	G	1	NAG	C1-O5-C5	2.03	114.91	112.19
5	R	1	NAG	C4-C3-C2	-2.02	108.05	111.02
3	E	10	MAN	C3-C4-C5	-2.02	106.56	110.23
6	P	2	NAG	O4-C4-C3	-2.00	105.66	110.38
6	I	2	NAG	C4-C3-C2	-2.00	108.08	111.02

There are no chirality outliers.

All (57) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	N	2	NAG	C8-C7-N2-C2
5	N	2	NAG	O7-C7-N2-C2
5	R	1	NAG	C1-C2-N2-C7
5	R	1	NAG	C8-C7-N2-C2
5	R	1	NAG	O7-C7-N2-C2
5	R	2	NAG	C8-C7-N2-C2
5	R	2	NAG	O7-C7-N2-C2
3	E	8	MAN	C4-C5-C6-O6
4	Q	1	NAG	C8-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
4	Q	1	NAG	O7-C7-N2-C2
4	J	1	NAG	O5-C5-C6-O6
5	H	2	NAG	O5-C5-C6-O6
4	F	2	NAG	O5-C5-C6-O6
4	G	2	NAG	O5-C5-C6-O6
6	I	6	MAN	O5-C5-C6-O6
4	J	1	NAG	C4-C5-C6-O6
3	E	8	MAN	O5-C5-C6-O6
4	F	2	NAG	C4-C5-C6-O6
4	J	2	NAG	O5-C5-C6-O6
3	L	2	NAG	C4-C5-C6-O6
4	K	2	NAG	O5-C5-C6-O6
4	J	2	NAG	C4-C5-C6-O6
3	E	1	NAG	C8-C7-N2-C2
3	E	1	NAG	O7-C7-N2-C2
3	L	1	NAG	C8-C7-N2-C2
3	L	1	NAG	O7-C7-N2-C2
5	H	2	NAG	C8-C7-N2-C2
5	H	2	NAG	O7-C7-N2-C2
3	L	2	NAG	O5-C5-C6-O6
5	H	2	NAG	C4-C5-C6-O6
4	Q	1	NAG	O5-C5-C6-O6
5	N	1	NAG	C4-C5-C6-O6
3	E	5	MAN	O5-C5-C6-O6
4	Q	1	NAG	C4-C5-C6-O6
6	I	6	MAN	C4-C5-C6-O6
4	G	2	NAG	C4-C5-C6-O6
4	K	2	NAG	C4-C5-C6-O6
3	E	1	NAG	C4-C5-C6-O6
3	E	4	MAN	C4-C5-C6-O6
4	M	2	NAG	O5-C5-C6-O6
5	N	1	NAG	O5-C5-C6-O6
6	P	4	MAN	O5-C5-C6-O6
3	E	1	NAG	O5-C5-C6-O6
3	L	3	BMA	O5-C5-C6-O6
3	E	3	BMA	O5-C5-C6-O6
6	P	7	MAN	O5-C5-C6-O6
5	R	2	NAG	O5-C5-C6-O6
6	I	4	MAN	O5-C5-C6-O6
6	I	1	NAG	C4-C5-C6-O6
6	I	1	NAG	O5-C5-C6-O6
5	R	2	NAG	C1-C2-N2-C7

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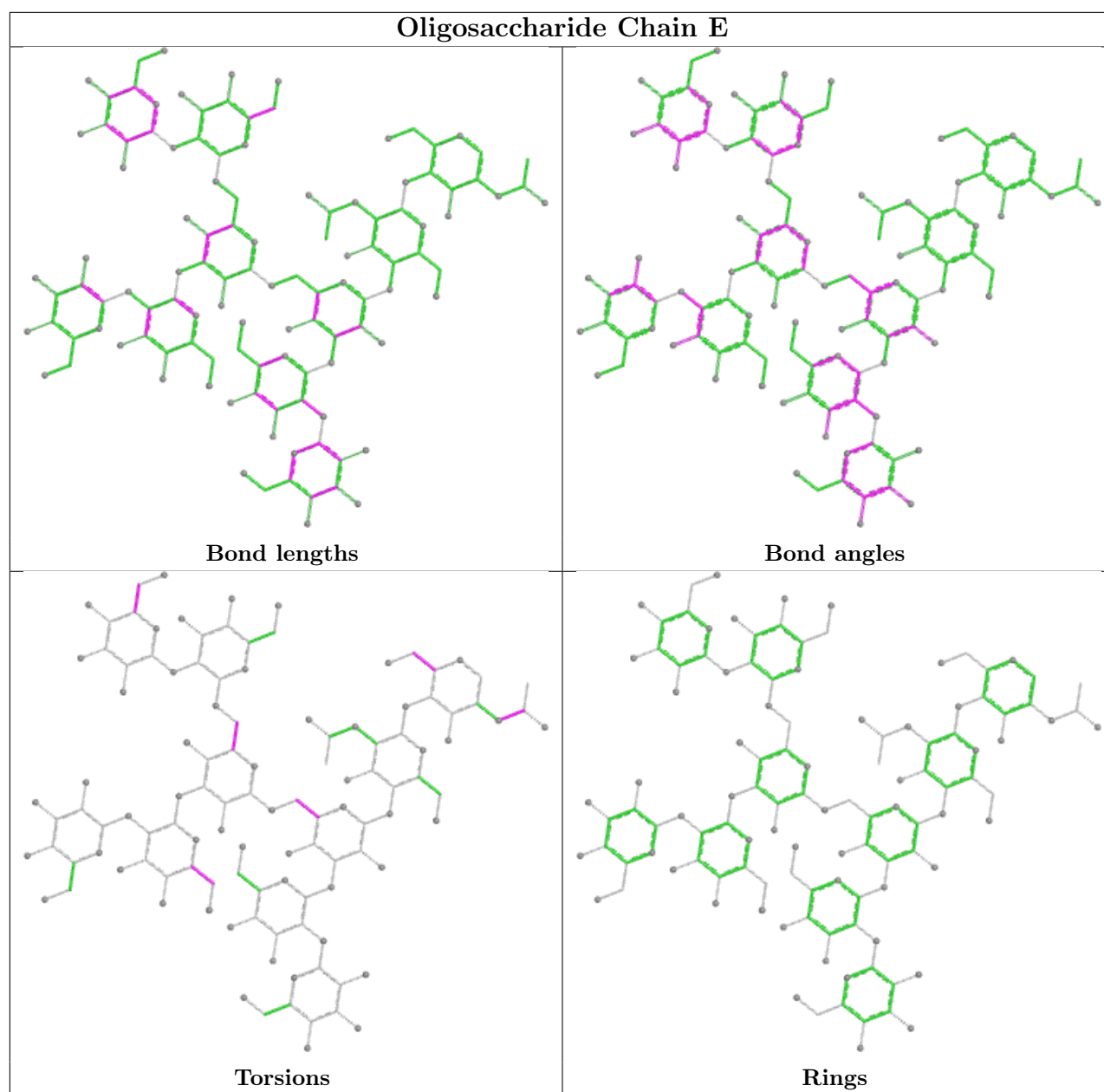
Mol	Chain	Res	Type	Atoms
5	H	2	NAG	C3-C2-N2-C7
5	R	2	NAG	C3-C2-N2-C7
4	F	2	NAG	C1-C2-N2-C7
5	N	1	NAG	C3-C2-N2-C7
3	E	5	MAN	C4-C5-C6-O6
3	E	4	MAN	O5-C5-C6-O6

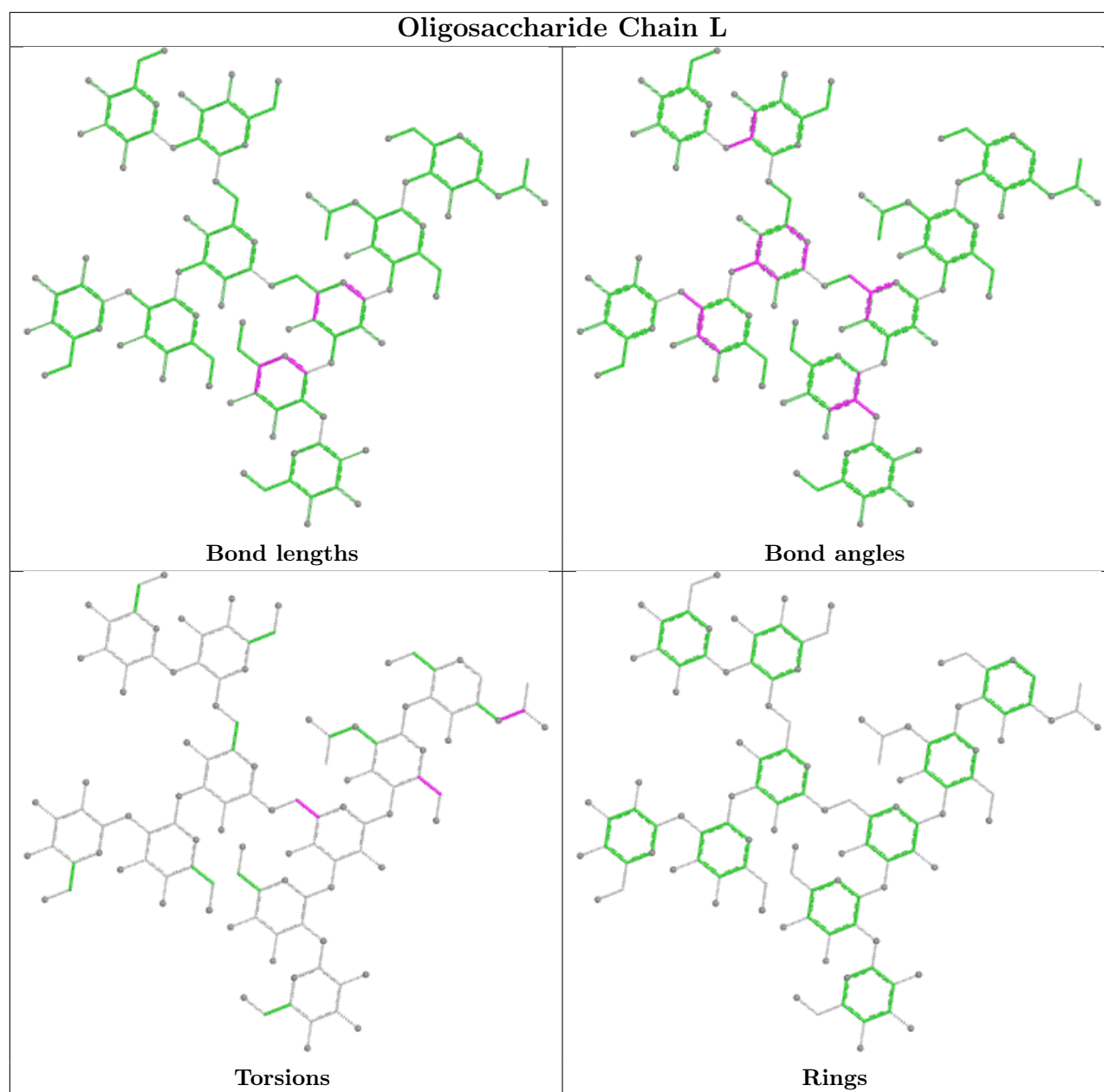
There are no ring outliers.

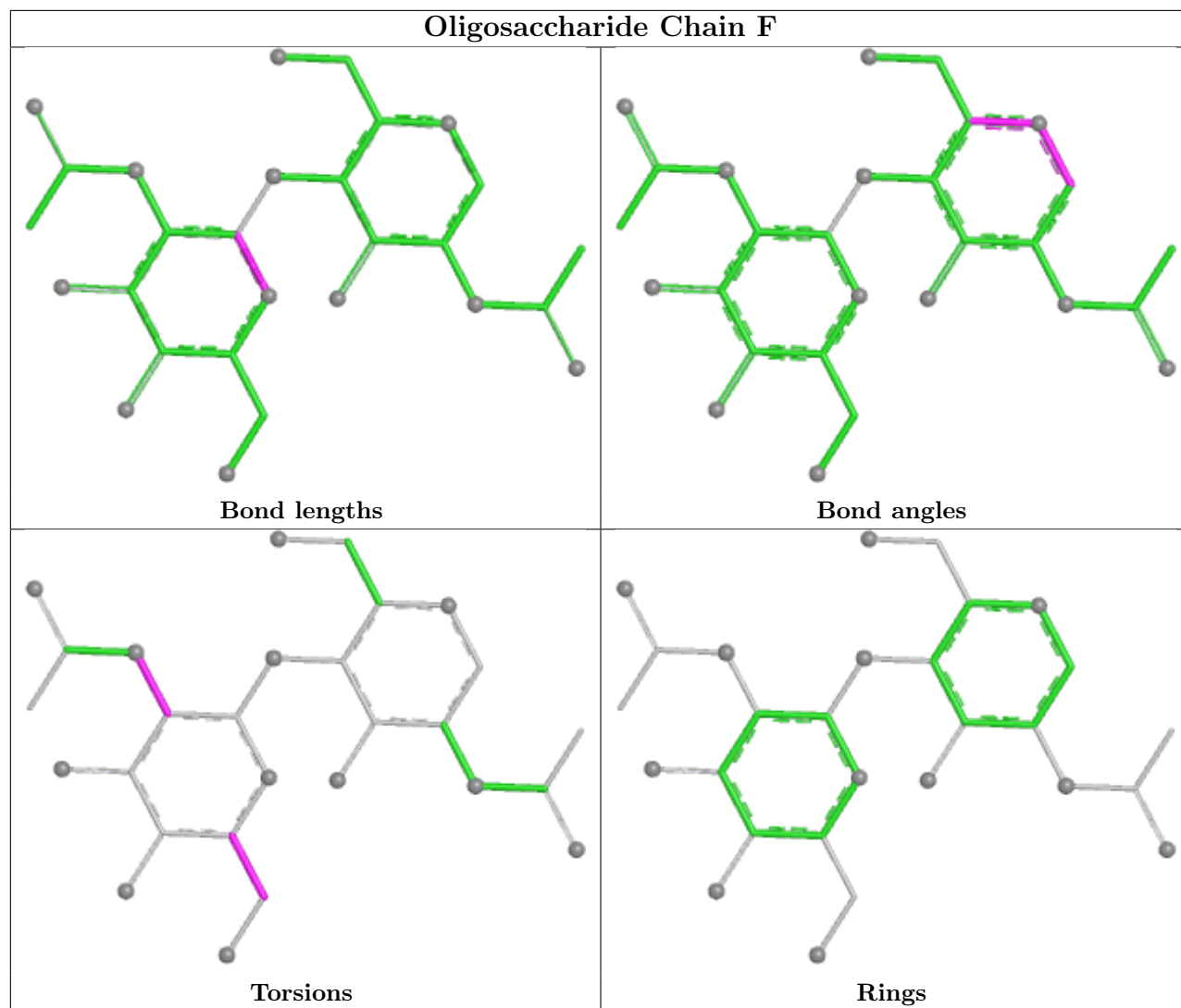
9 monomers are involved in 14 short contacts:

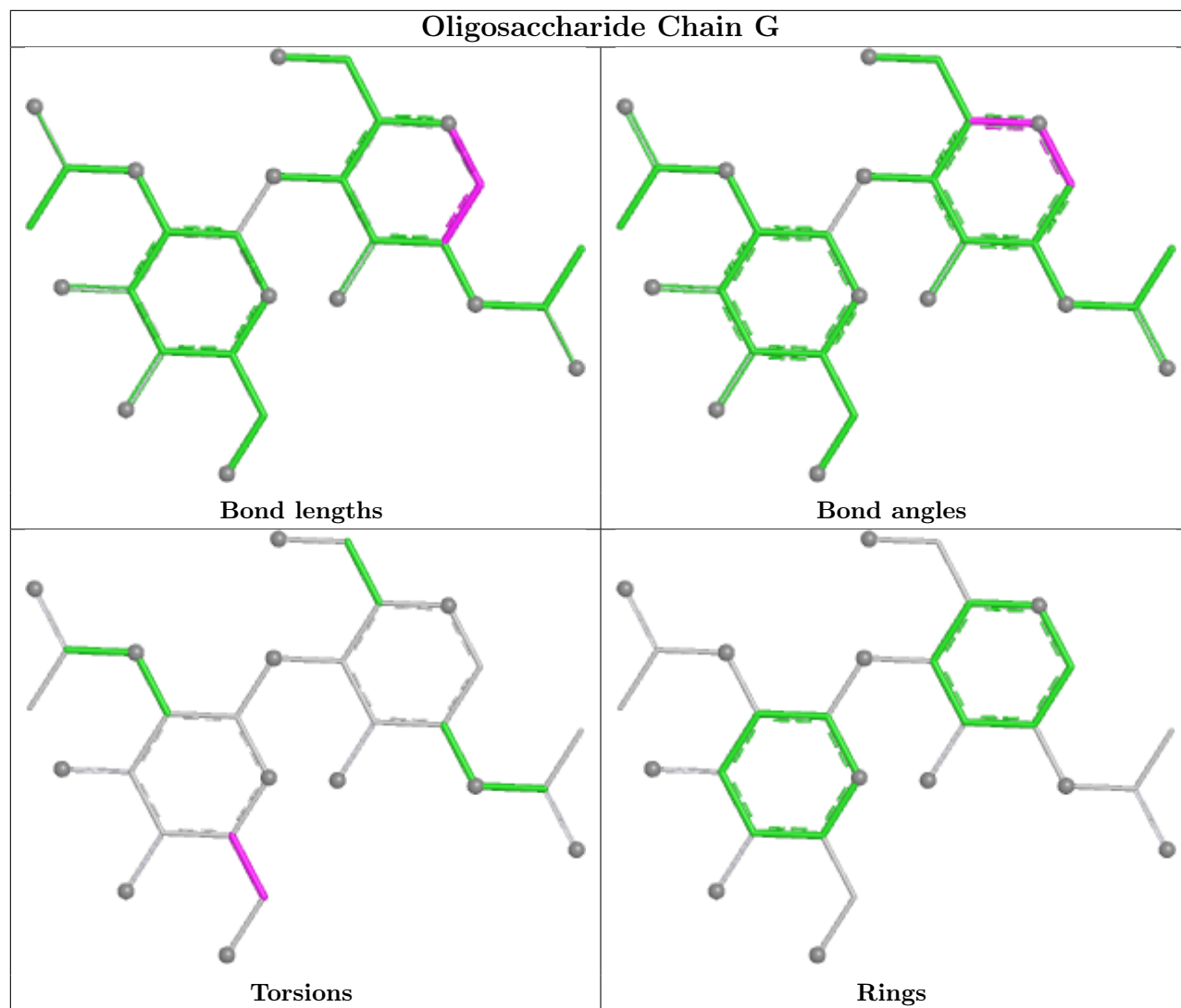
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	L	9	MAN	2	0
4	F	1	NAG	1	0
5	R	1	NAG	6	0
4	F	2	NAG	1	0
4	J	1	NAG	1	0
5	H	1	NAG	1	0
3	E	1	NAG	1	0
3	L	10	MAN	2	0
5	H	2	NAG	3	0

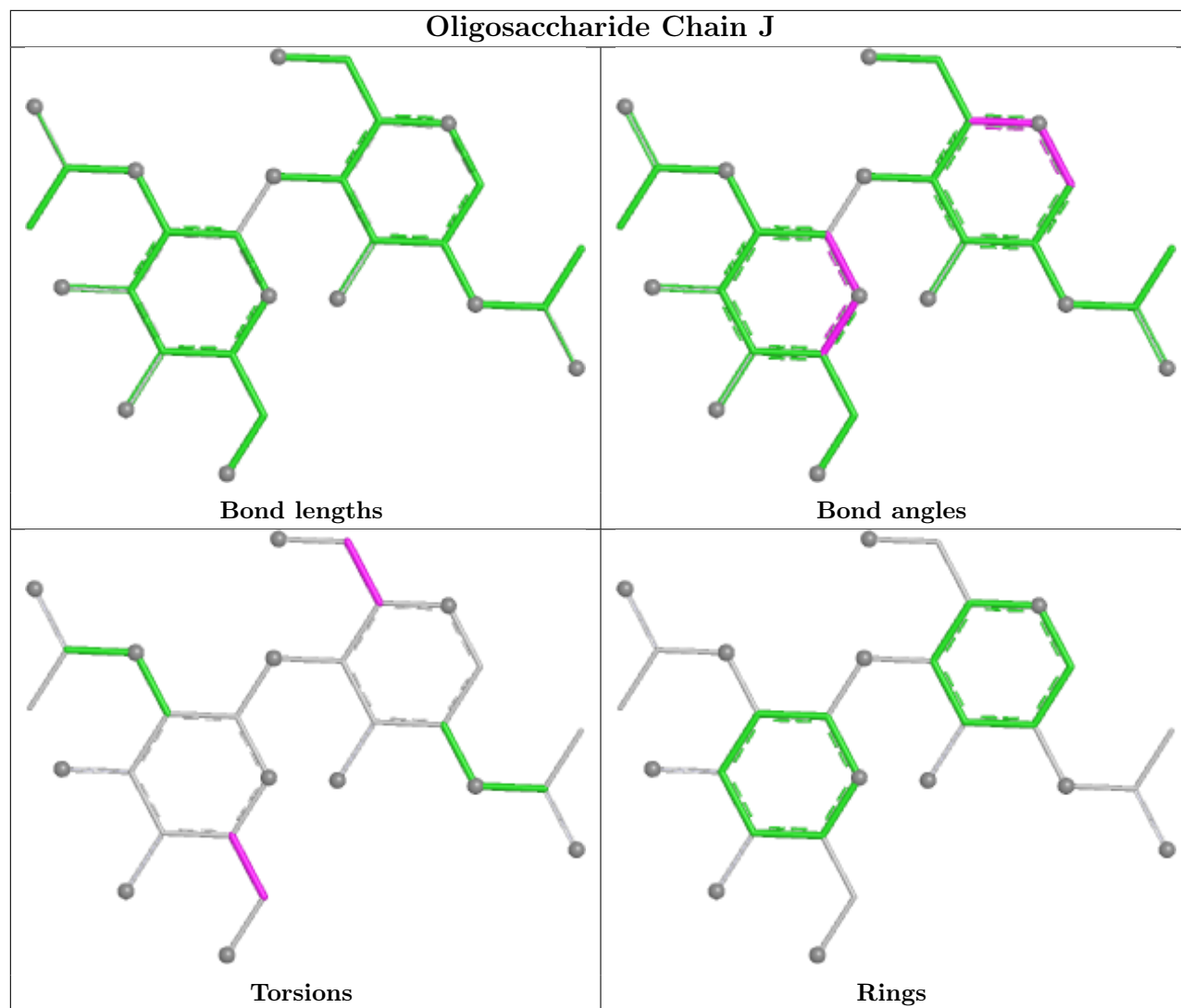
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

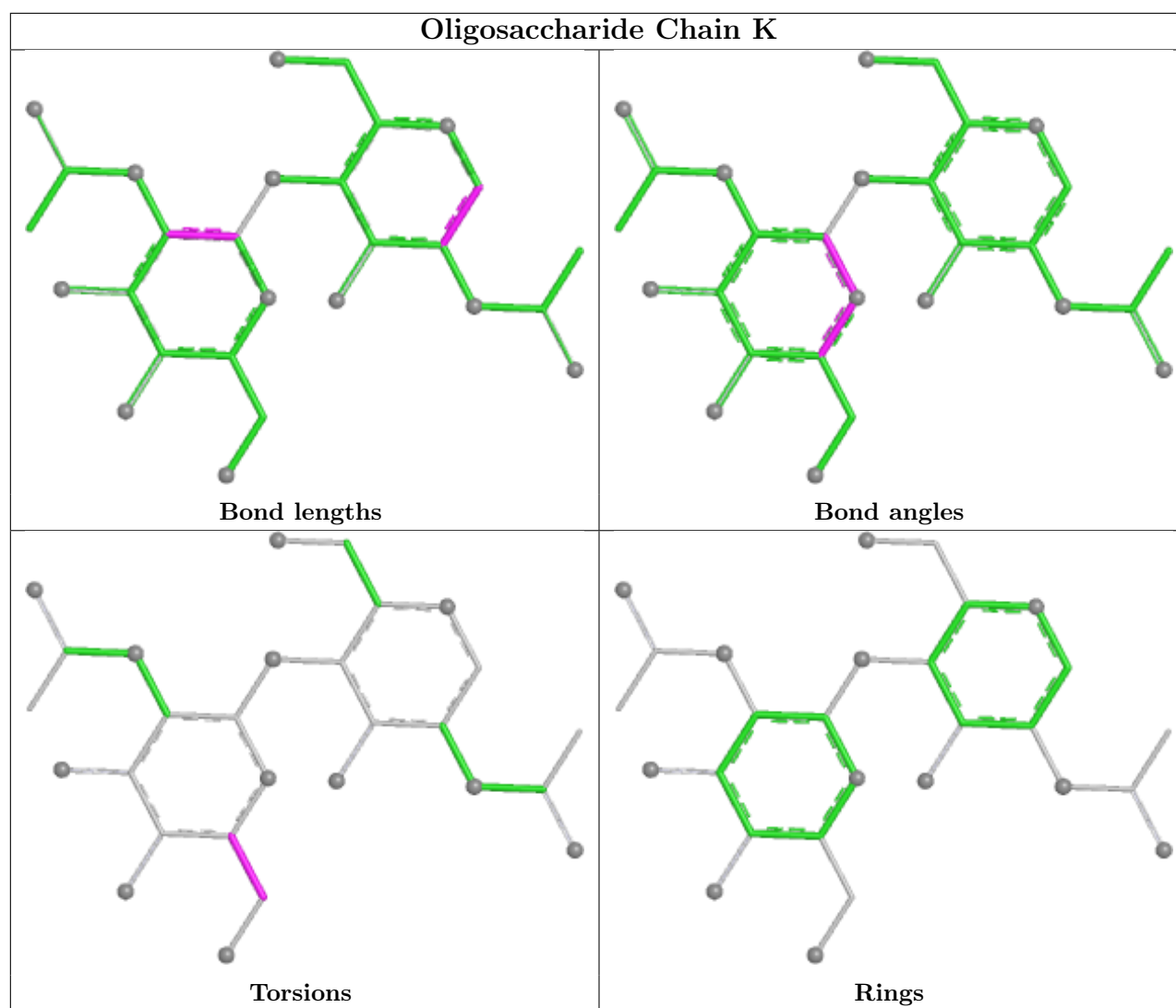


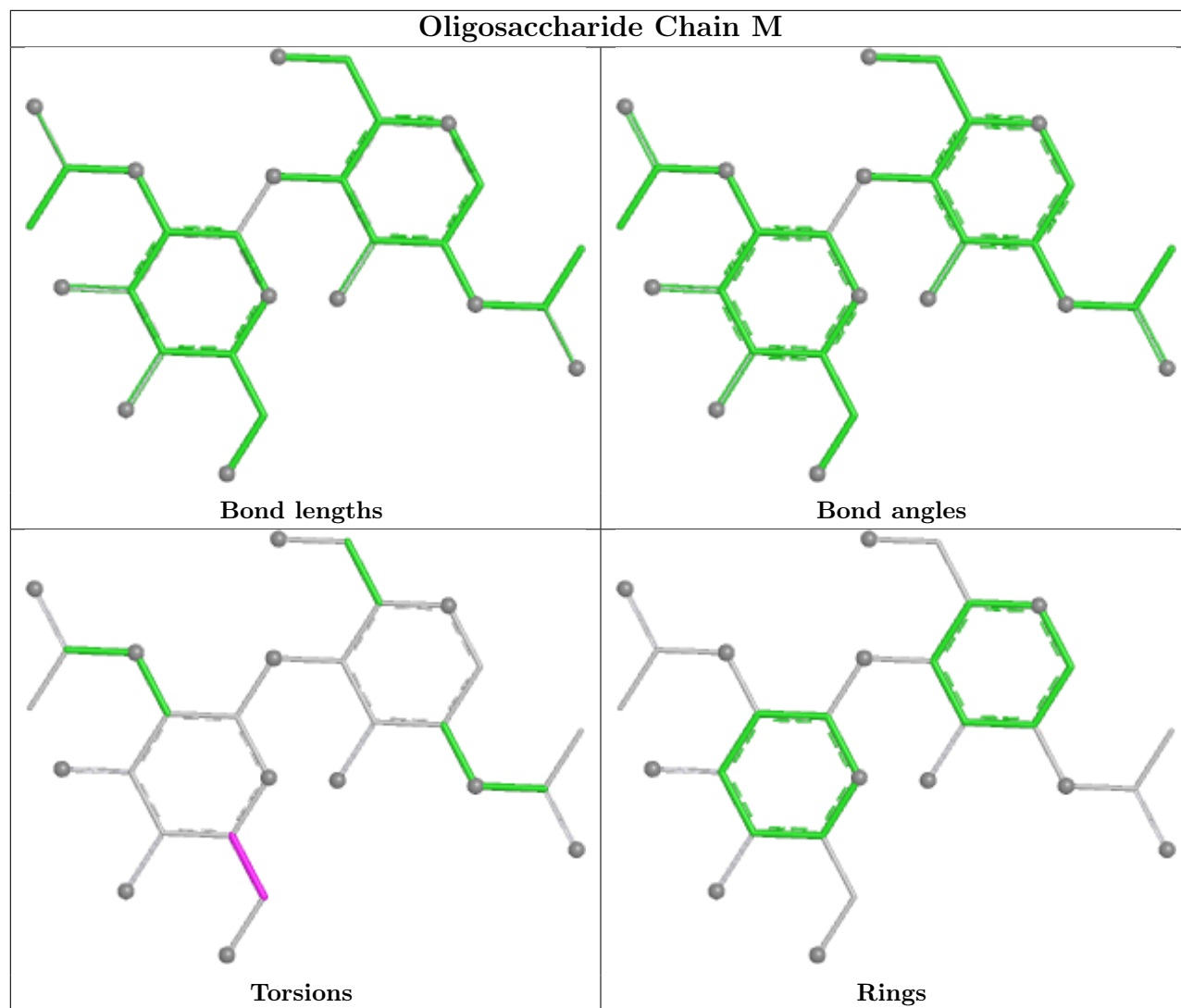


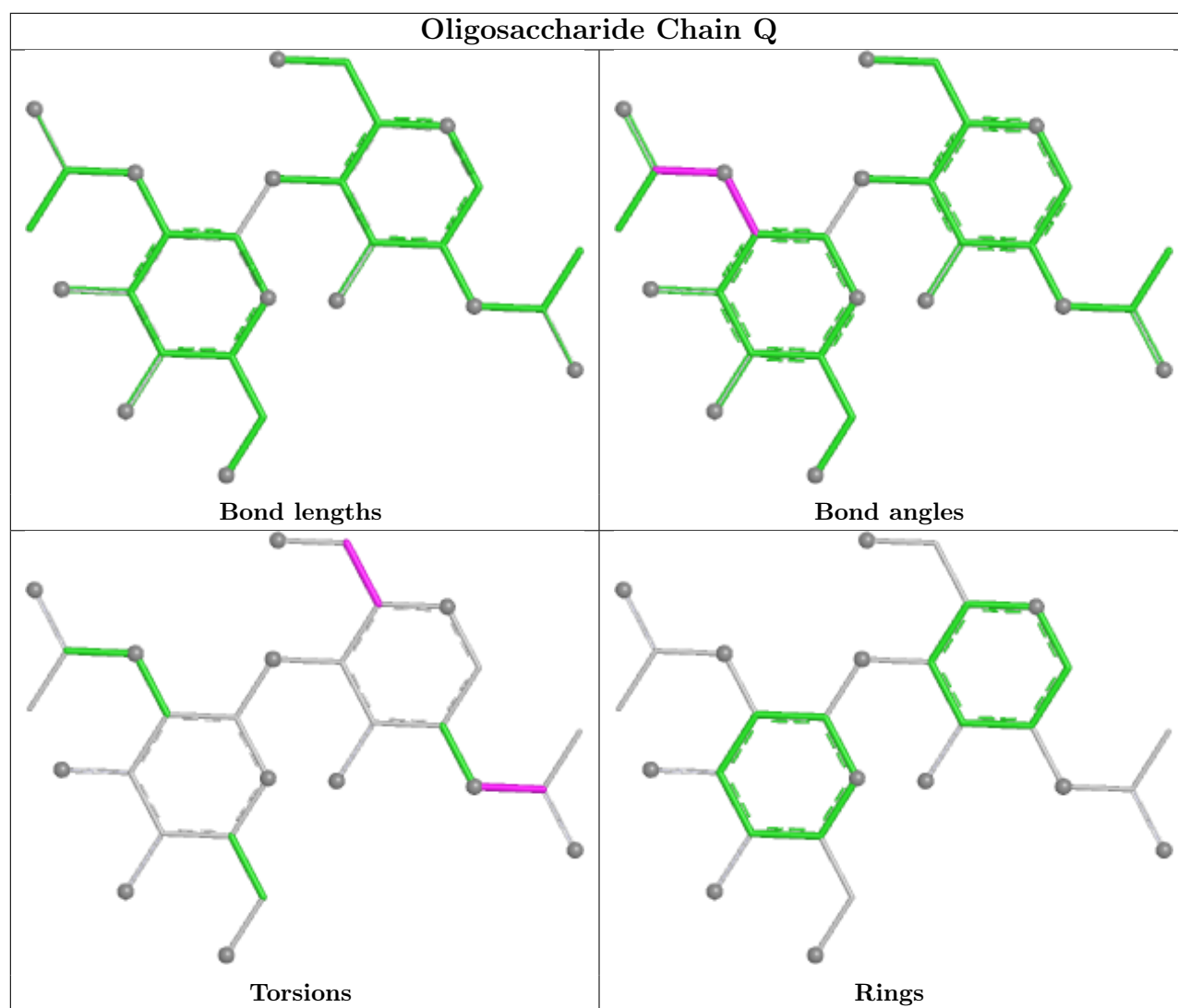


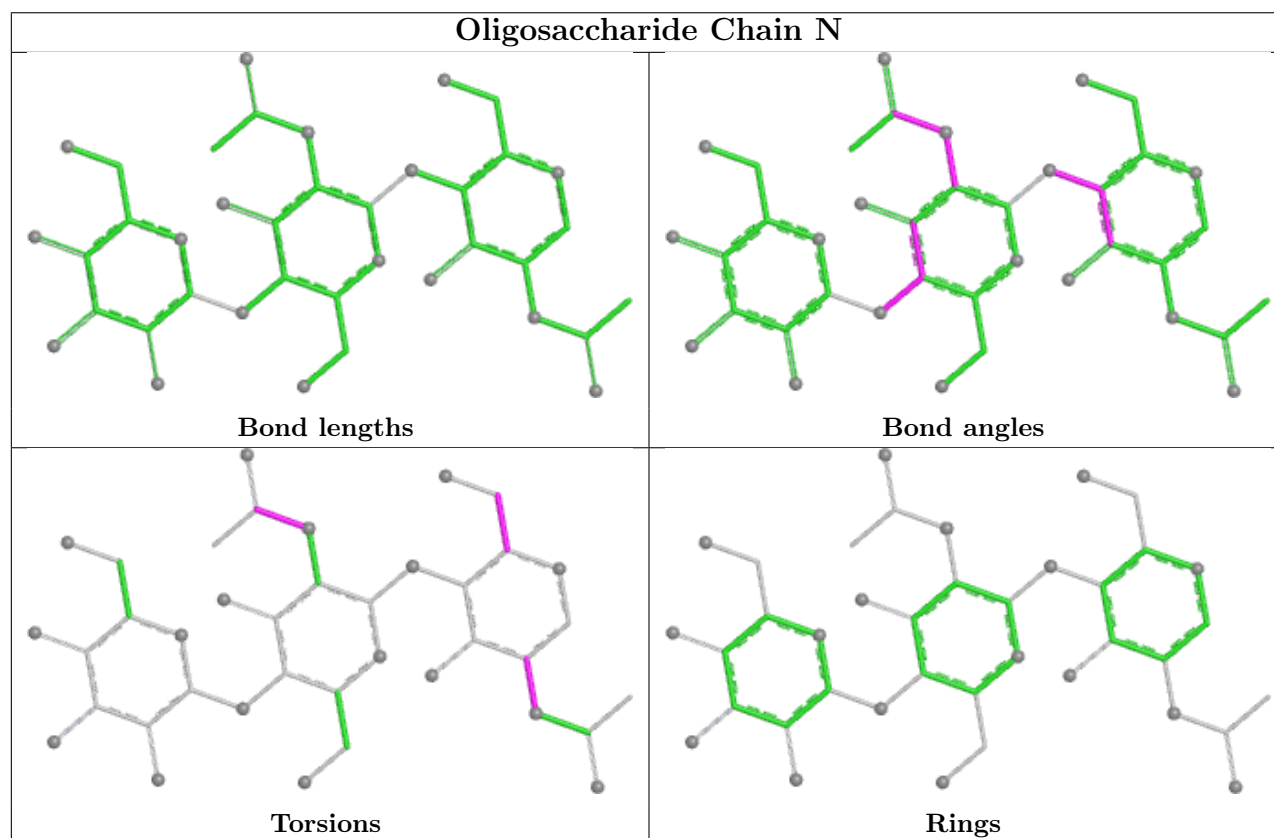
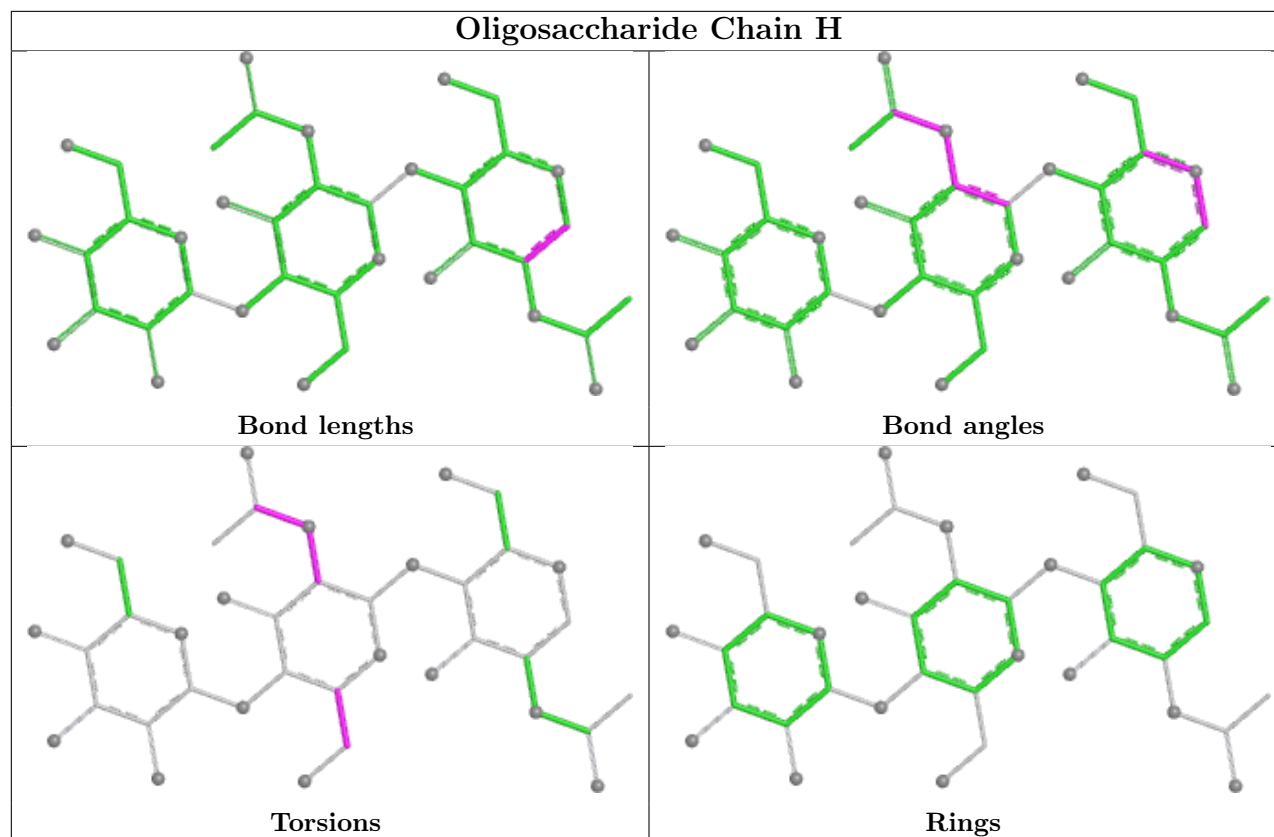


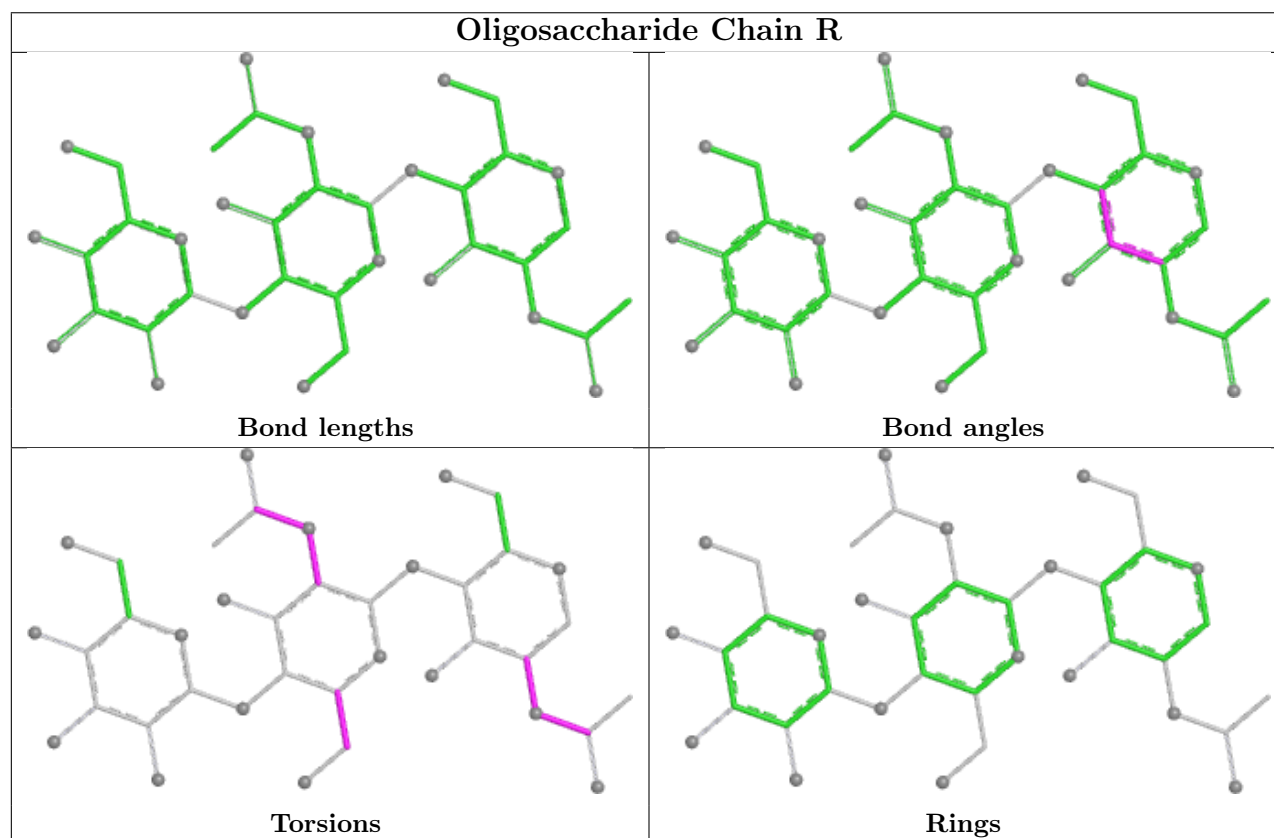
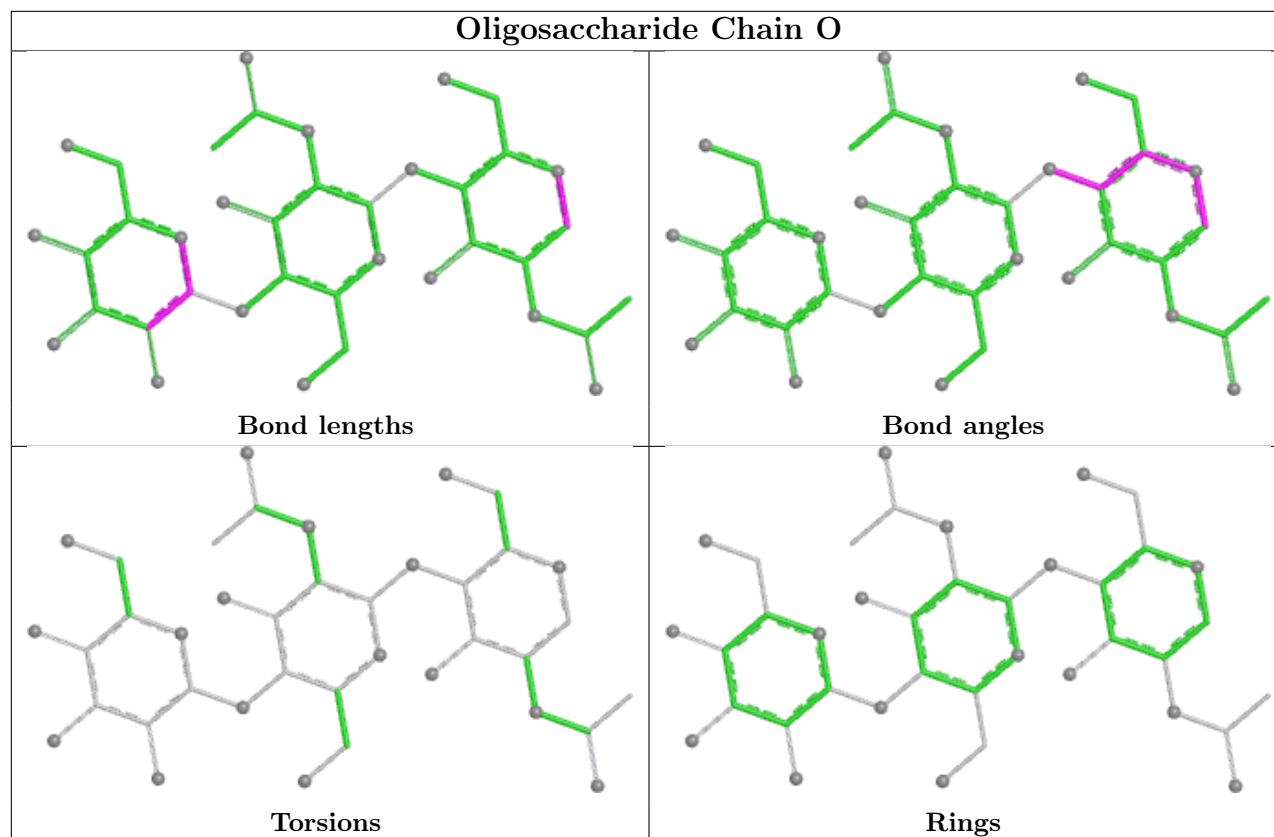


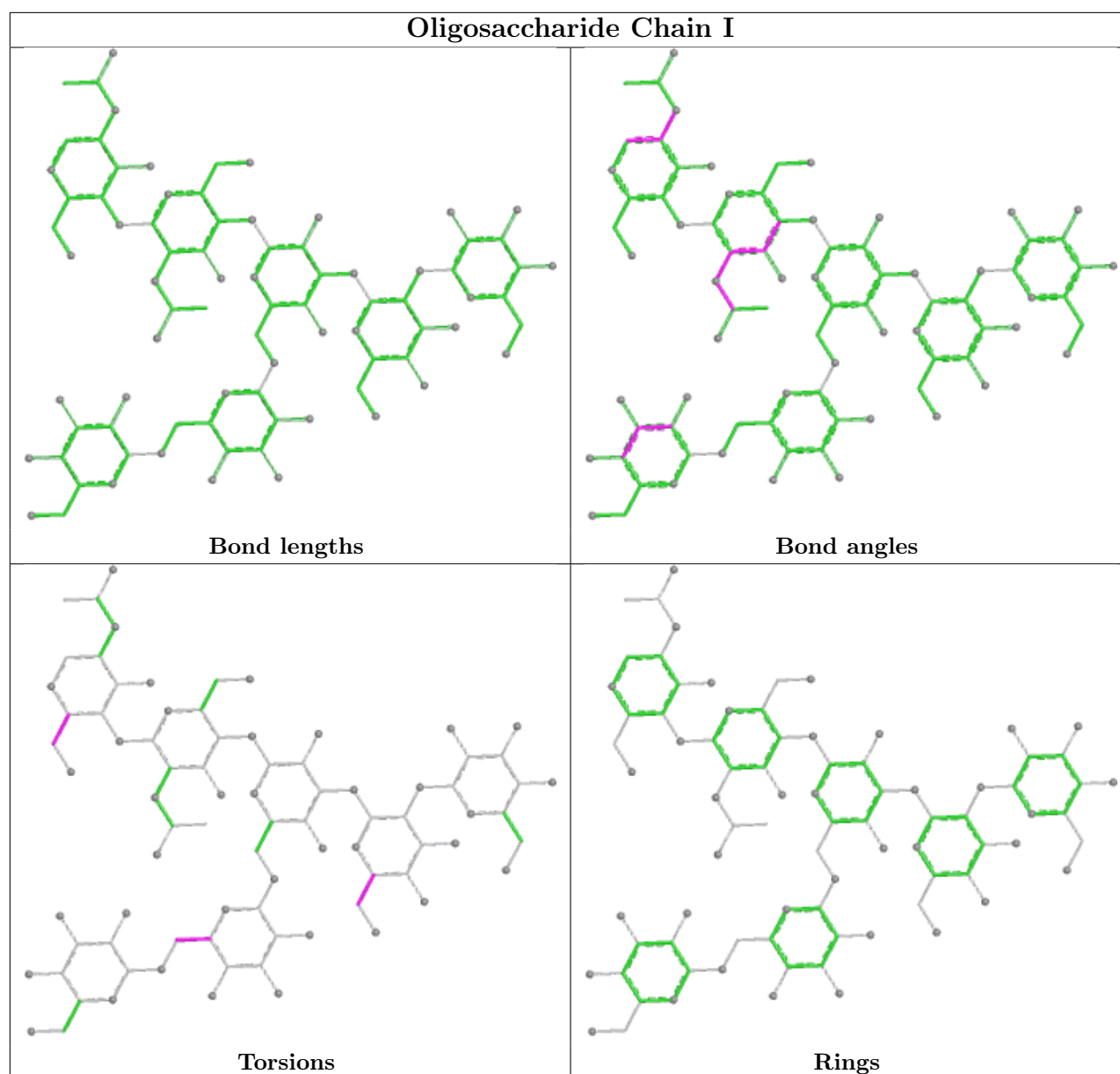


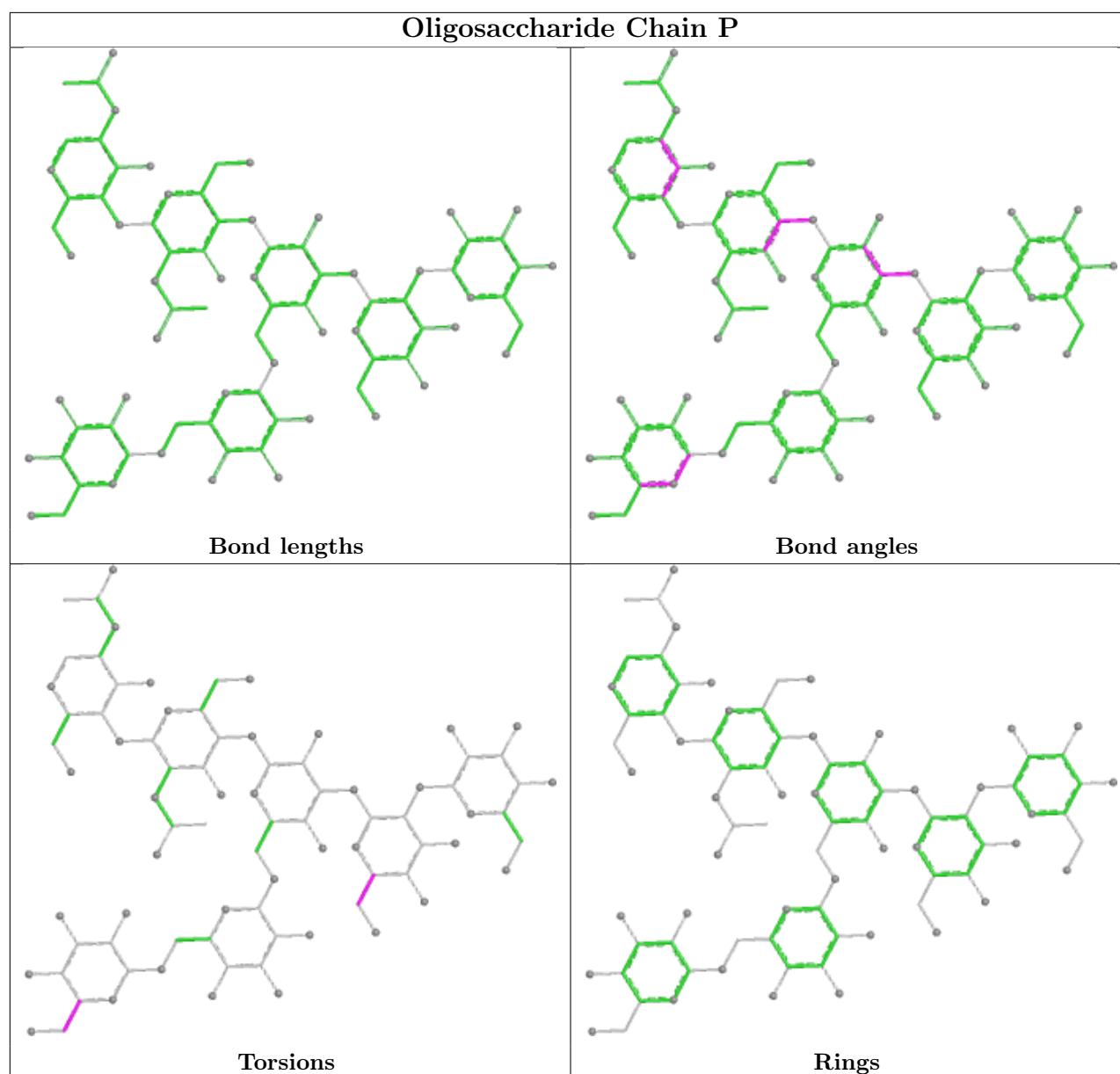












5.6 Ligand geometry [i](#)

6 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	NAG	D	1003	2	14,14,15	0.39	0	17,19,21	0.58	0
7	NAG	C	1002	2	14,14,15	0.65	1 (7%)	17,19,21	0.85	1 (5%)
7	NAG	D	1002	2	14,14,15	0.37	0	17,19,21	0.99	2 (11%)
7	NAG	C	1001	2	14,14,15	0.49	0	17,19,21	0.97	1 (5%)
7	NAG	C	1003	2	14,14,15	0.81	1 (7%)	17,19,21	0.80	0
7	NAG	D	1001	2	14,14,15	0.44	0	17,19,21	0.75	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
7	NAG	D	1003	2	-	2/6/23/26	0/1/1/1
7	NAG	C	1002	2	-	0/6/23/26	0/1/1/1
7	NAG	D	1002	2	-	1/6/23/26	0/1/1/1
7	NAG	C	1001	2	-	2/6/23/26	0/1/1/1
7	NAG	C	1003	2	-	2/6/23/26	0/1/1/1
7	NAG	D	1001	2	-	2/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	C	1003	NAG	C1-C2	2.56	1.55	1.52
7	C	1002	NAG	O5-C1	2.01	1.47	1.43

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	C	1002	NAG	C1-O5-C5	2.26	115.21	112.19
7	C	1001	NAG	C1-O5-C5	2.24	115.19	112.19
7	D	1002	NAG	C2-N2-C7	-2.21	119.94	122.90
7	D	1002	NAG	C1-O5-C5	2.00	114.87	112.19

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	D	1003	NAG	C8-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
7	D	1003	NAG	O7-C7-N2-C2
7	C	1001	NAG	O5-C5-C6-O6
7	C	1001	NAG	C4-C5-C6-O6
7	C	1003	NAG	C8-C7-N2-C2
7	C	1003	NAG	O7-C7-N2-C2
7	D	1001	NAG	C8-C7-N2-C2
7	D	1001	NAG	O7-C7-N2-C2
7	D	1002	NAG	C1-C2-N2-C7

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	C	1001	NAG	1	0
7	D	1001	NAG	1	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	222/241 (92%)	-0.35	0 100 100	56, 89, 116, 128	0
1	B	222/241 (92%)	-0.37	1 (0%) 87 76	68, 105, 132, 147	0
2	C	752/934 (80%)	-0.40	3 (0%) 88 79	59, 84, 119, 157	0
2	D	752/934 (80%)	-0.21	4 (0%) 87 76	76, 109, 144, 160	0
All	All	1948/2350 (82%)	-0.32	8 (0%) 88 79	56, 97, 138, 160	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	752	LEU	3.0
2	D	121	VAL	2.9
2	C	83	ASP	2.8
2	C	178	LEU	2.4
2	D	574	ASP	2.3
2	D	606	PHE	2.3
2	C	346	LEU	2.2
1	B	147	ALA	2.2

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.

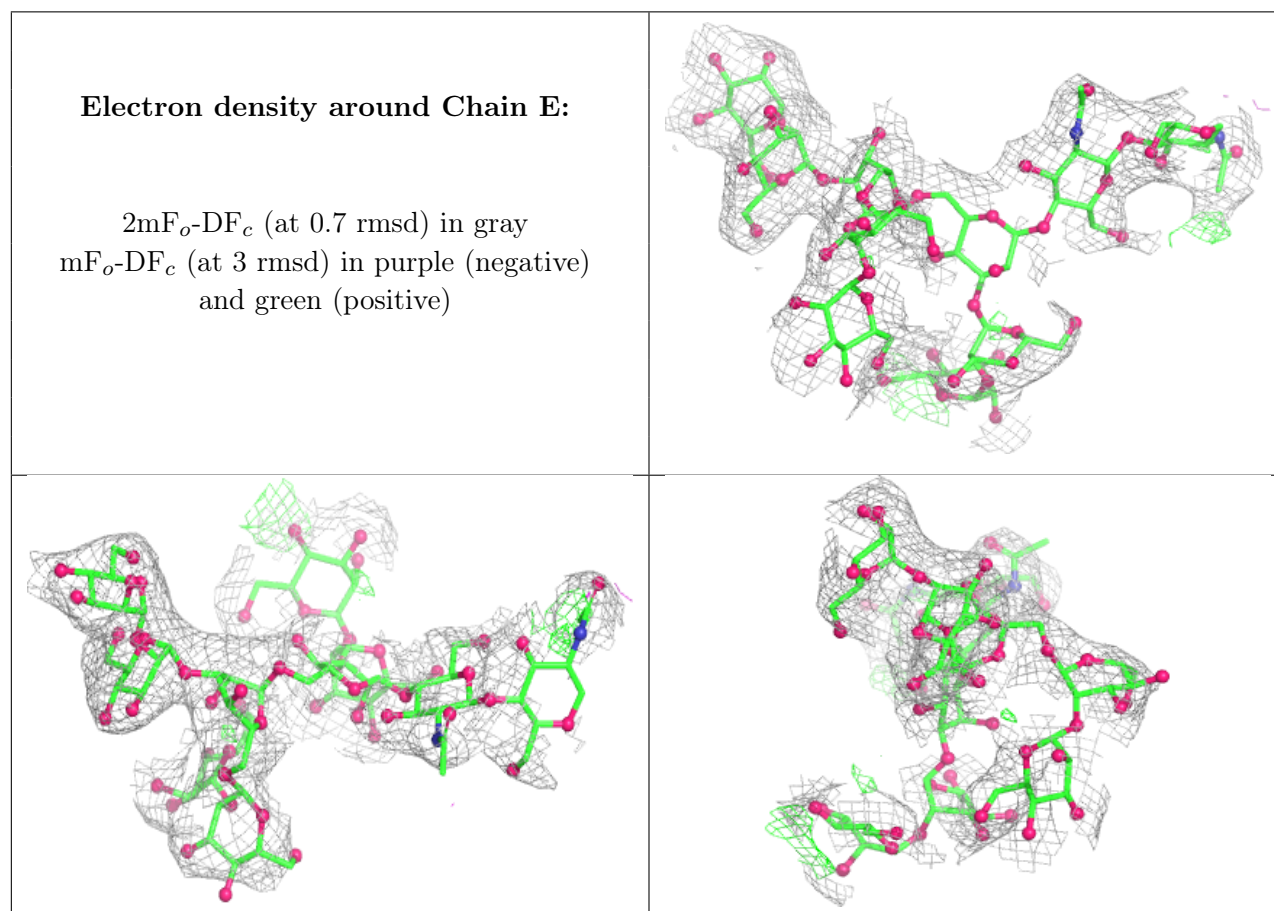
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	NAG	M	1	14/15	0.09	0.17	135,148,163,165	0
3	MAN	L	10	11/12	0.21	0.11	116,131,143,145	0
5	NAG	O	2	14/15	0.37	0.08	148,166,173,175	0
5	NAG	R	1	14/15	0.37	0.10	128,149,157,159	0
3	MAN	L	8	11/12	0.41	0.10	124,131,139,141	0
5	NAG	R	2	14/15	0.46	0.09	148,161,165,165	0
5	BMA	O	3	11/12	0.47	0.08	163,174,176,178	0
4	NAG	M	2	14/15	0.48	0.09	159,170,174,177	0
5	BMA	N	3	11/12	0.50	0.09	128,143,150,152	0
5	NAG	N	2	14/15	0.51	0.10	119,138,147,148	0
5	BMA	R	3	11/12	0.52	0.07	150,155,161,164	0
5	NAG	O	1	14/15	0.55	0.10	126,144,155,156	0
3	MAN	E	8	11/12	0.57	0.09	113,117,127,133	0
6	MAN	P	5	11/12	0.57	0.09	127,134,143,145	0
3	MAN	E	10	11/12	0.58	0.10	91,110,115,120	0
4	NAG	F	2	14/15	0.60	0.10	130,142,151,151	0
4	NAG	Q	2	14/15	0.62	0.07	129,146,150,151	0
6	MAN	I	5	11/12	0.64	0.09	107,114,118,120	0
5	BMA	H	3	11/12	0.64	0.07	137,150,153,157	0
5	NAG	H	2	14/15	0.67	0.08	116,136,143,151	0
4	NAG	K	2	14/15	0.67	0.07	129,141,143,147	0
4	NAG	G	2	14/15	0.67	0.10	92,111,122,127	0
6	BMA	P	3	11/12	0.68	0.10	118,123,125,125	0
5	NAG	N	1	14/15	0.72	0.10	113,131,140,142	0
6	MAN	I	6	11/12	0.72	0.15	30,30,30,30	0
3	MAN	E	9	11/12	0.74	0.10	105,108,116,118	0
3	MAN	L	9	11/12	0.74	0.09	111,123,126,126	0
4	NAG	F	1	14/15	0.75	0.09	118,133,142,144	0
6	BMA	I	3	11/12	0.75	0.09	99,101,104,110	0
4	NAG	K	1	14/15	0.75	0.08	117,126,129,131	0
3	MAN	L	4	11/12	0.76	0.10	95,101,112,116	0
6	MAN	P	7	11/12	0.76	0.17	30,30,30,30	0
4	NAG	J	2	14/15	0.78	0.08	135,140,145,146	0
6	MAN	P	4	11/12	0.79	0.07	115,124,134,137	0
3	BMA	L	3	11/12	0.81	0.08	104,108,113,123	0
3	MAN	E	7	11/12	0.81	0.12	114,119,126,127	0
4	NAG	G	1	14/15	0.82	0.09	79,86,100,102	0
6	MAN	I	4	11/12	0.82	0.08	83,97,106,108	0
3	MAN	L	7	11/12	0.83	0.08	118,126,130,132	0
6	MAN	P	6	11/12	0.84	0.15	30,30,30,30	0
6	MAN	I	7	11/12	0.84	0.16	30,30,30,30	0
5	NAG	H	1	14/15	0.86	0.06	79,102,112,122	0
4	NAG	Q	1	14/15	0.86	0.07	101,124,132,142	0

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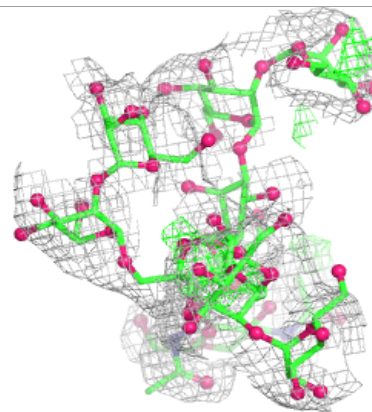
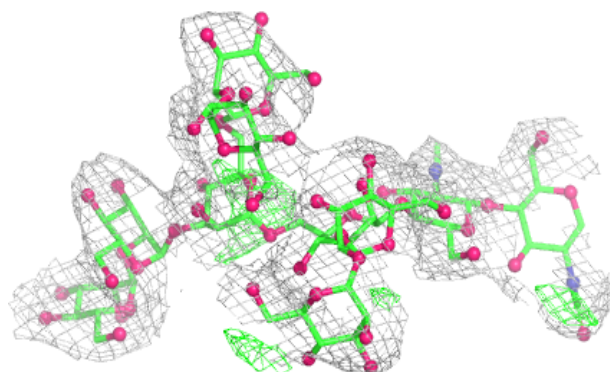
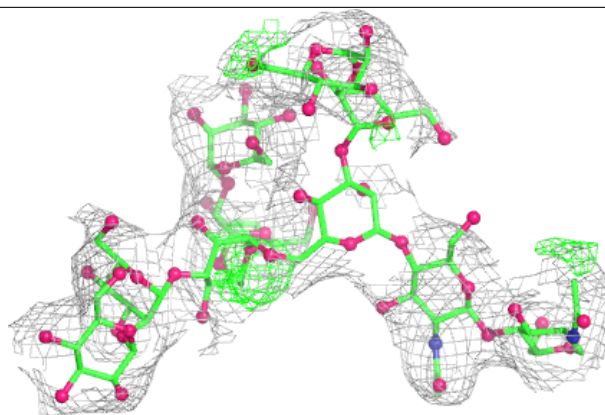
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	MAN	L	6	11/12	0.87	0.09	72,84,92,96	0
3	MAN	E	4	11/12	0.88	0.07	77,85,95,100	0
3	NAG	L	1	14/15	0.88	0.08	80,89,92,98	0
3	MAN	L	5	11/12	0.89	0.08	79,87,90,91	0
6	NAG	I	2	14/15	0.89	0.07	72,88,100,100	0
6	NAG	P	2	14/15	0.90	0.07	111,116,126,129	0
3	BMA	E	3	11/12	0.91	0.06	89,98,100,106	0
6	NAG	P	1	14/15	0.91	0.07	98,113,120,121	0
3	NAG	E	1	14/15	0.92	0.08	60,70,76,85	0
3	NAG	L	2	14/15	0.92	0.08	77,92,102,109	0
3	MAN	E	5	11/12	0.93	0.08	63,67,69,72	0
4	NAG	J	1	14/15	0.93	0.05	116,125,136,137	0
3	MAN	E	6	11/12	0.95	0.06	59,67,75,75	0
3	NAG	E	2	14/15	0.95	0.07	76,80,92,95	0
6	NAG	I	1	14/15	0.96	0.06	54,61,74,74	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.



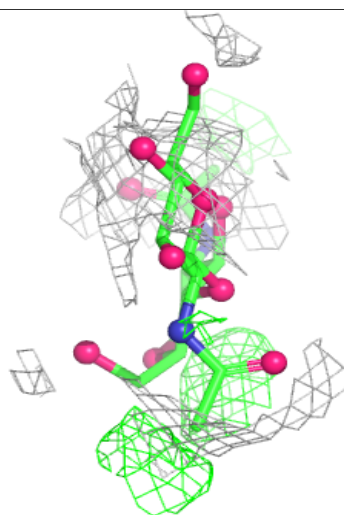
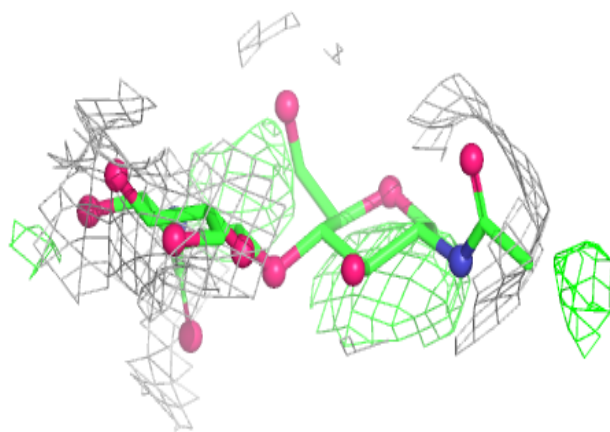
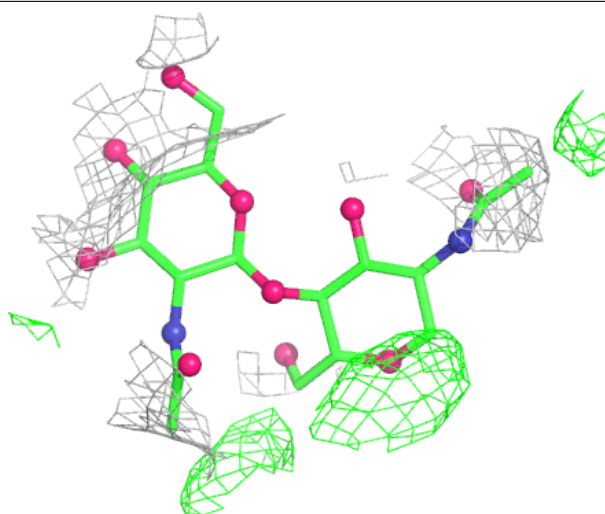
Electron density around Chain L:

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



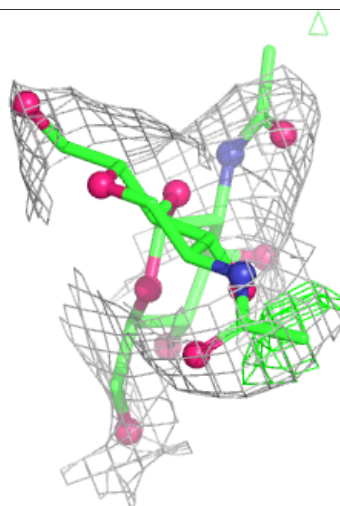
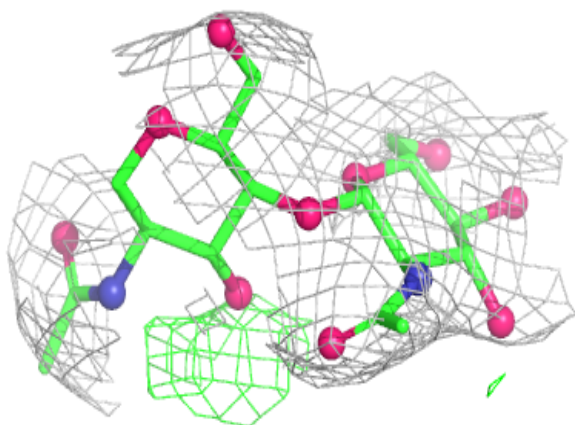
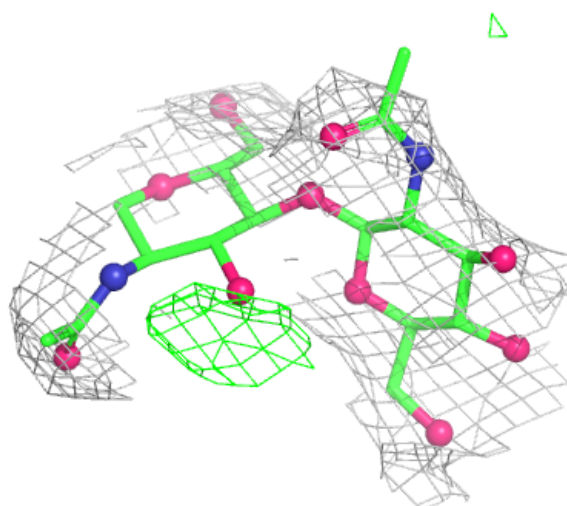
Electron density around Chain F:

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



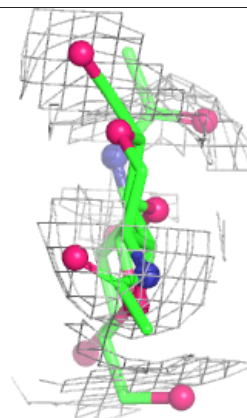
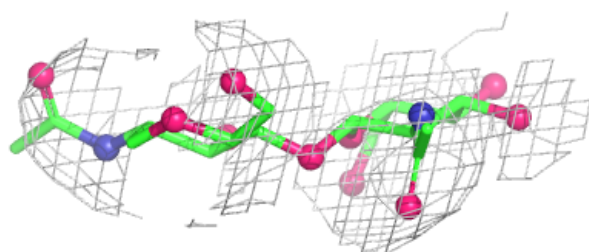
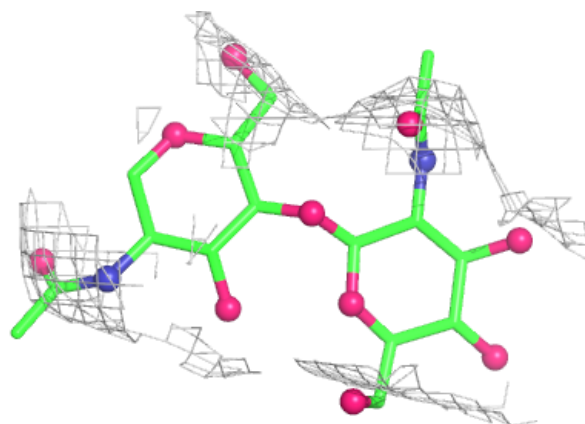
Electron density around Chain G:

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



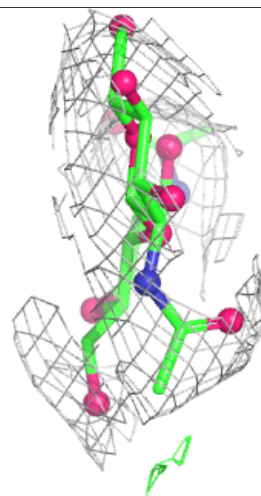
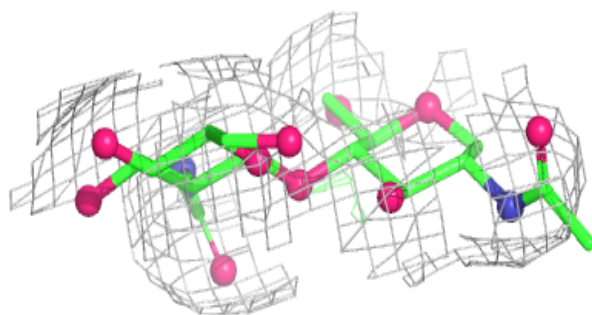
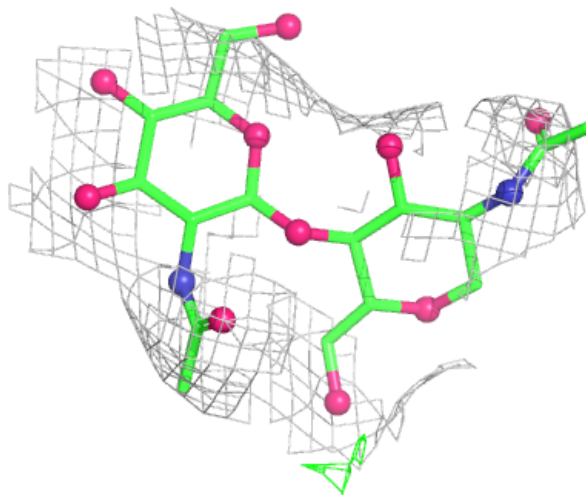
Electron density around Chain J:

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



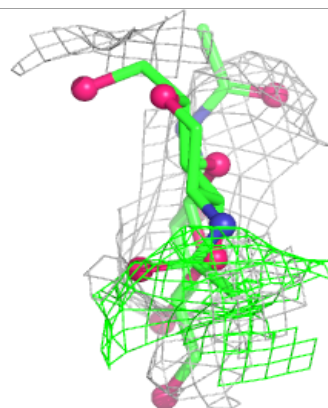
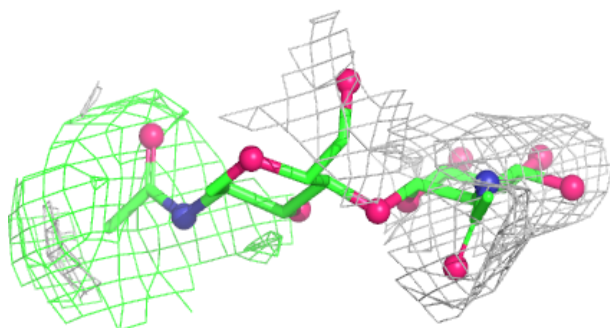
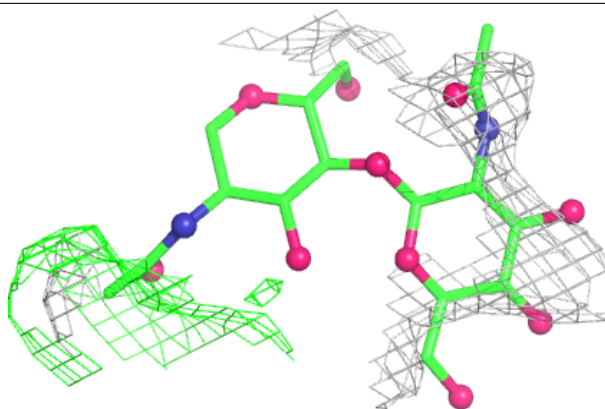
Electron density around Chain K:

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

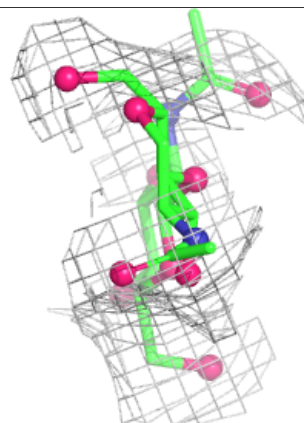
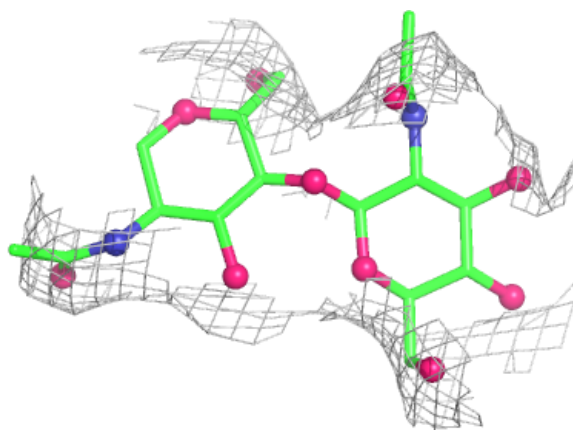


Electron density around Chain M:

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

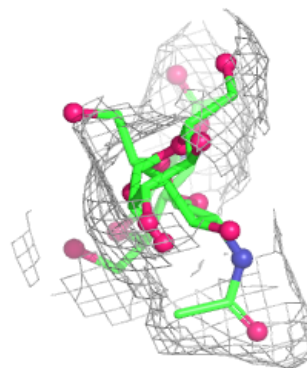
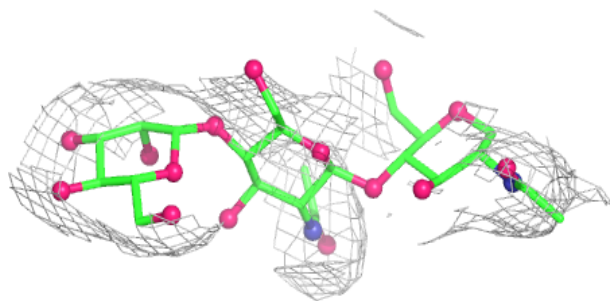
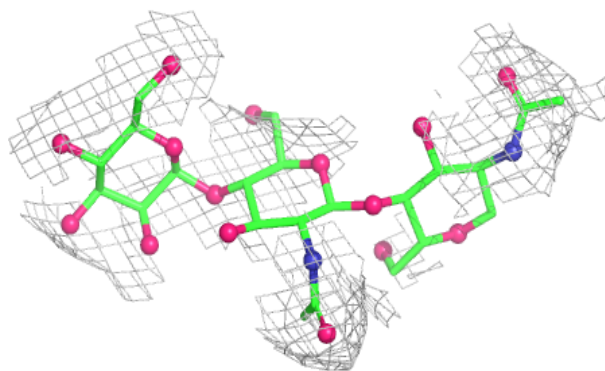
**Electron density around Chain Q:**

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

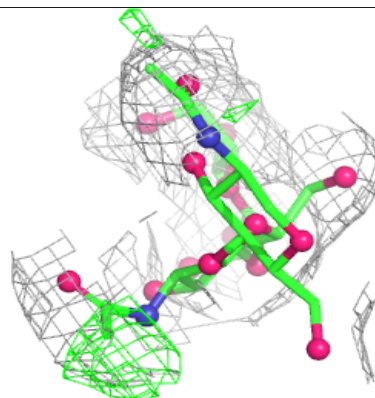
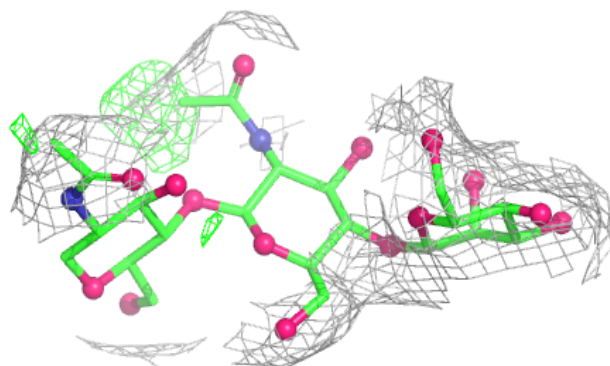
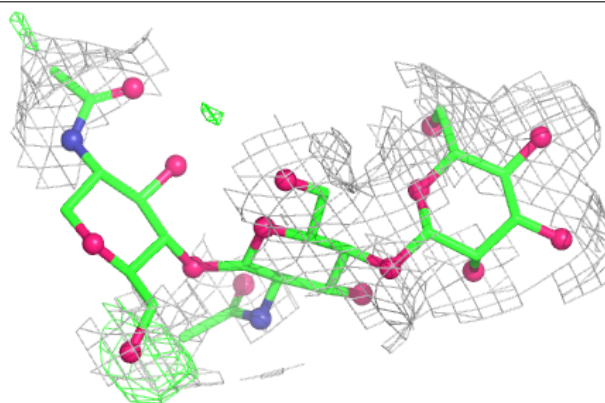


Electron density around Chain H:

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

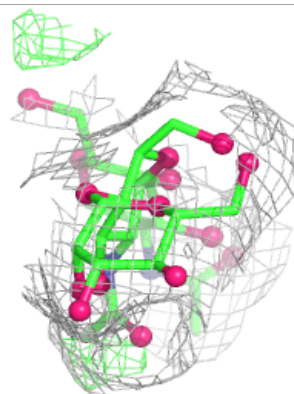
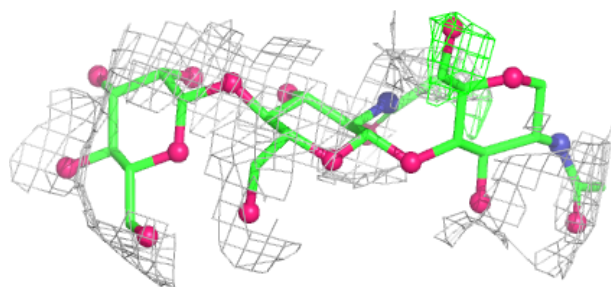
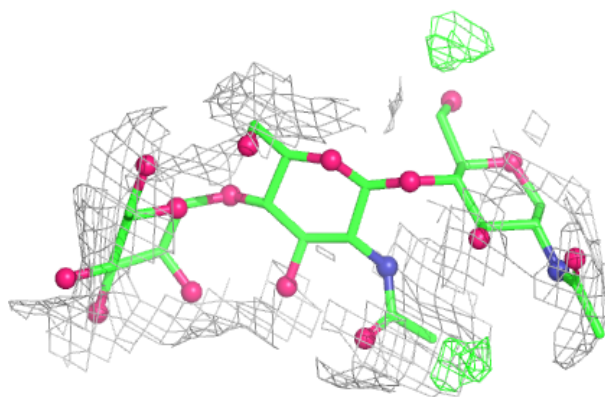
**Electron density around Chain N:**

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

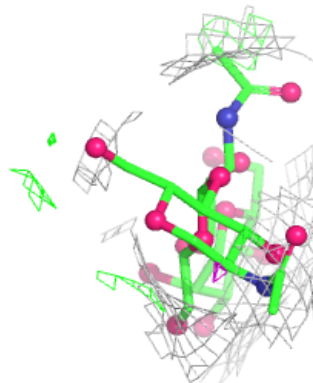
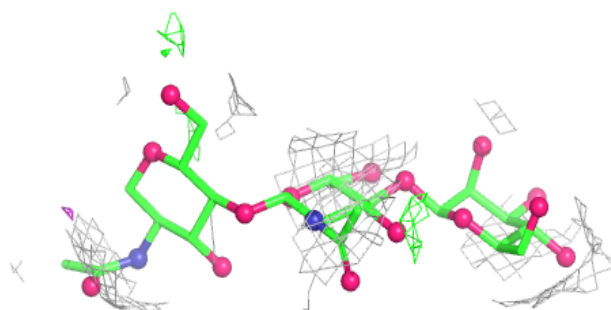
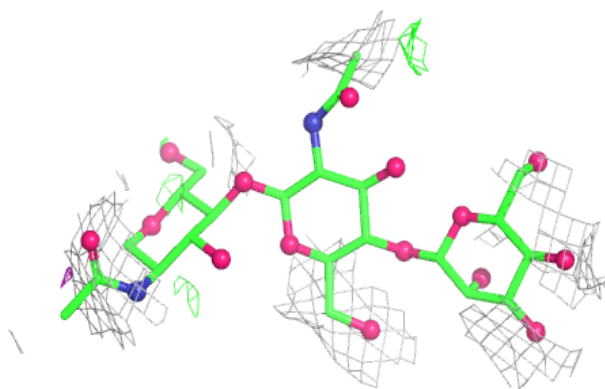


Electron density around Chain O:

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

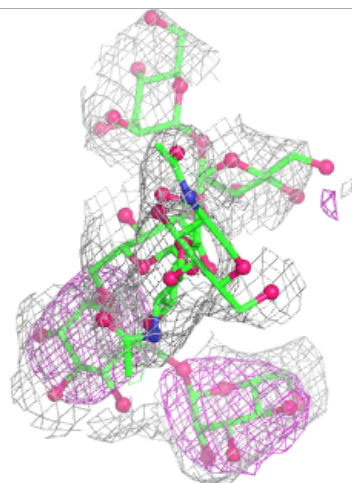
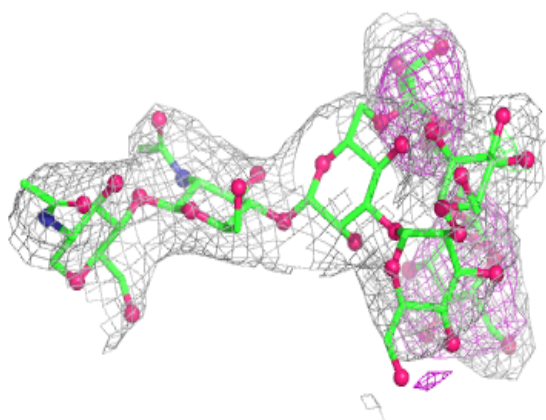
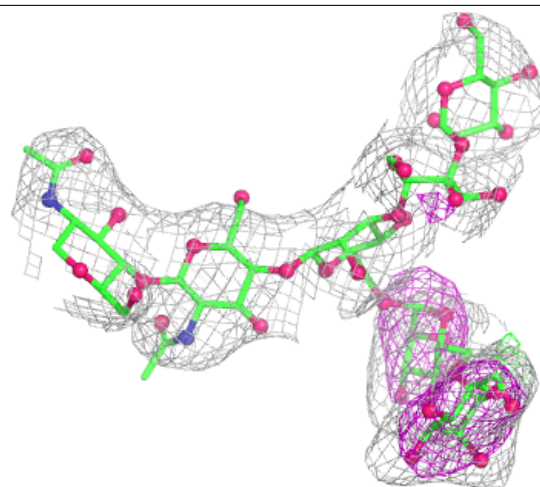
**Electron density around Chain R:**

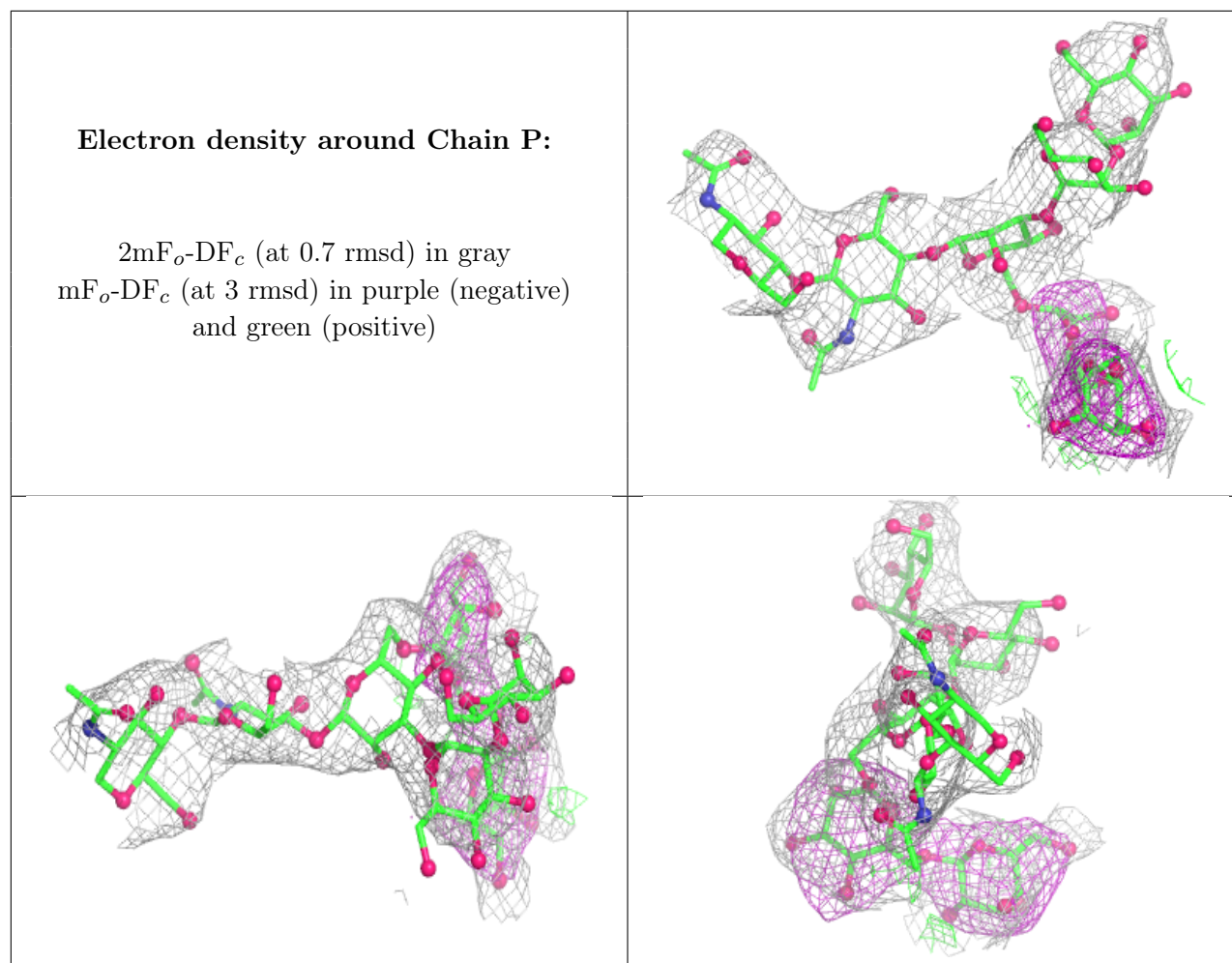
$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain I:

$2mF_o-DF_c$ (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($\text{\AA}^2$)	Q<0.9
7	NAG	D	1001	14/15	0.01	0.13	127,142,151,152	0
7	NAG	D	1003	14/15	0.04	0.12	167,179,186,189	0
7	NAG	D	1002	14/15	0.35	0.11	149,158,161,168	0
7	NAG	C	1003	14/15	0.62	0.09	141,154,157,160	0
7	NAG	C	1002	14/15	0.68	0.08	95,122,130,132	0
7	NAG	C	1001	14/15	0.72	0.09	99,116,123,127	0

6.5 Other polymers [i](#)

There are no such residues in this entry.