



Full wwPDB X-ray Structure Validation Report ⓘ

May 7, 2026 – 11:05 AM EDT

PDB ID : 6TAV / pdb_00006tav
Title : Crystal structure of endopeptidase-induced alpha2-macroglobulin
Authors : Gomis-Ruth, F.X.; Duquerroy, S.; Trapani, S.; Marrero, A.; Goulas, T.; Guevara, T.; Andersen, G.A.; Sottrup-Jensen, L.; Navaza, J.
Deposited on : 2019-10-30
Resolution : 4.20 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

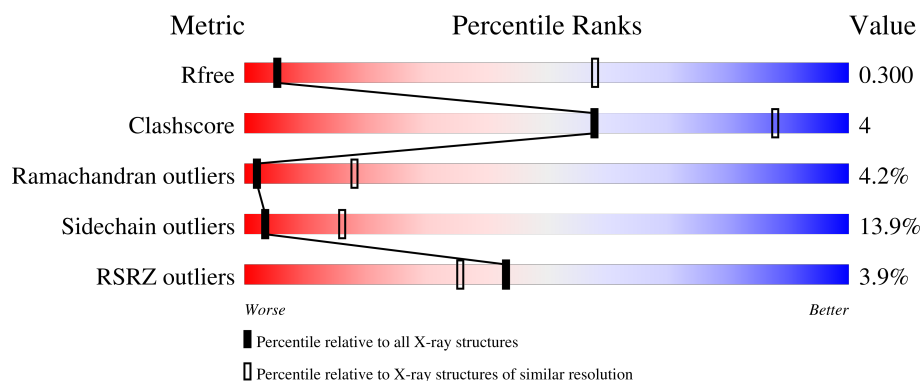
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.20 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.



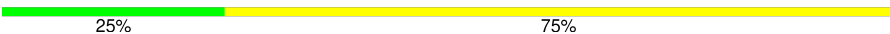
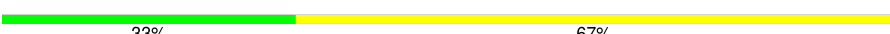
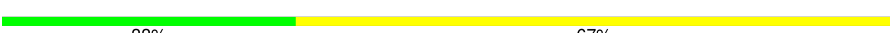
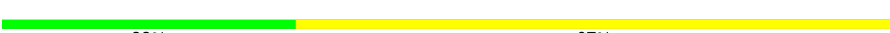
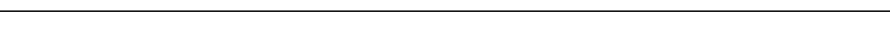
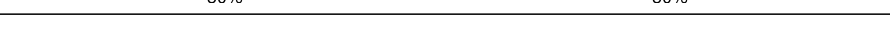
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1004 (4.52-3.88)
Clashscore	190562	1019 (4.50-3.90)
Ramachandran outliers	187476	1020 (4.56-3.84)
Sidechain outliers	187428	1006 (4.56-3.84)
RSRZ outliers	180081	1001 (4.52-3.88)

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	1474	
1	B	1474	
1	C	1474	
1	D	1474	
2	E	4	

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Mol	Chain	Length	Quality of chain
2	G	4	 50% 50%
2	J	4	 25% 75%
2	O	4	 50% 50%
2	V	4	 25% 75%
3	F	3	 33% 67%
3	I	3	 33% 67%
3	M	3	 33% 67%
3	R	3	 67% 33%
4	H	2	 50% 50%
4	K	2	 50% 50%
4	L	2	 100%
4	N	2	 100%
4	P	2	 50% 50%
4	Q	2	 50% 50%
4	S	2	 50% 50%
4	T	2	 50% 50%
4	U	2	 50% 50%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 82015 atoms, of which 40382 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 Alpha-2-macroglobulin.

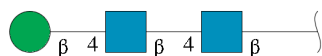
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	1416	Total	C	H	N	O	S	10926	0	0
			21976	7027	10926	1849	2125	49			
1	B	1273	Total	C	H	N	O	S	9812	0	0
			19741	6312	9812	1665	1909	43			
1	C	1274	Total	C	H	N	O	S	9834	0	0
			19770	6315	9834	1668	1910	43			
1	D	1271	Total	C	H	N	O	S	9810	0	0
			19716	6298	9810	1664	1901	43			

- Molecule 2 is an oligosaccharide called 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
2	E	4	Total	C	N	O	0	0	0
			50	28	2	20			
2	G	4	Total	C	N	O	0	0	0
			50	28	2	20			
2	J	4	Total	C	N	O	0	0	0
			50	28	2	20			
2	O	4	Total	C	N	O	0	0	0
			50	28	2	20			
2	V	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 3 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
3	F	3	Total	C	N	O	0	0	0
			39	22	2	15			
3	I	3	Total	C	N	O	0	0	0
			39	22	2	15			
3	M	3	Total	C	N	O	0	0	0
			39	22	2	15			
3	R	3	Total	C	N	O	0	0	0
			39	22	2	15			

- 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	H	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	L	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	N	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	P	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			
4	S	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	T	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	U	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).

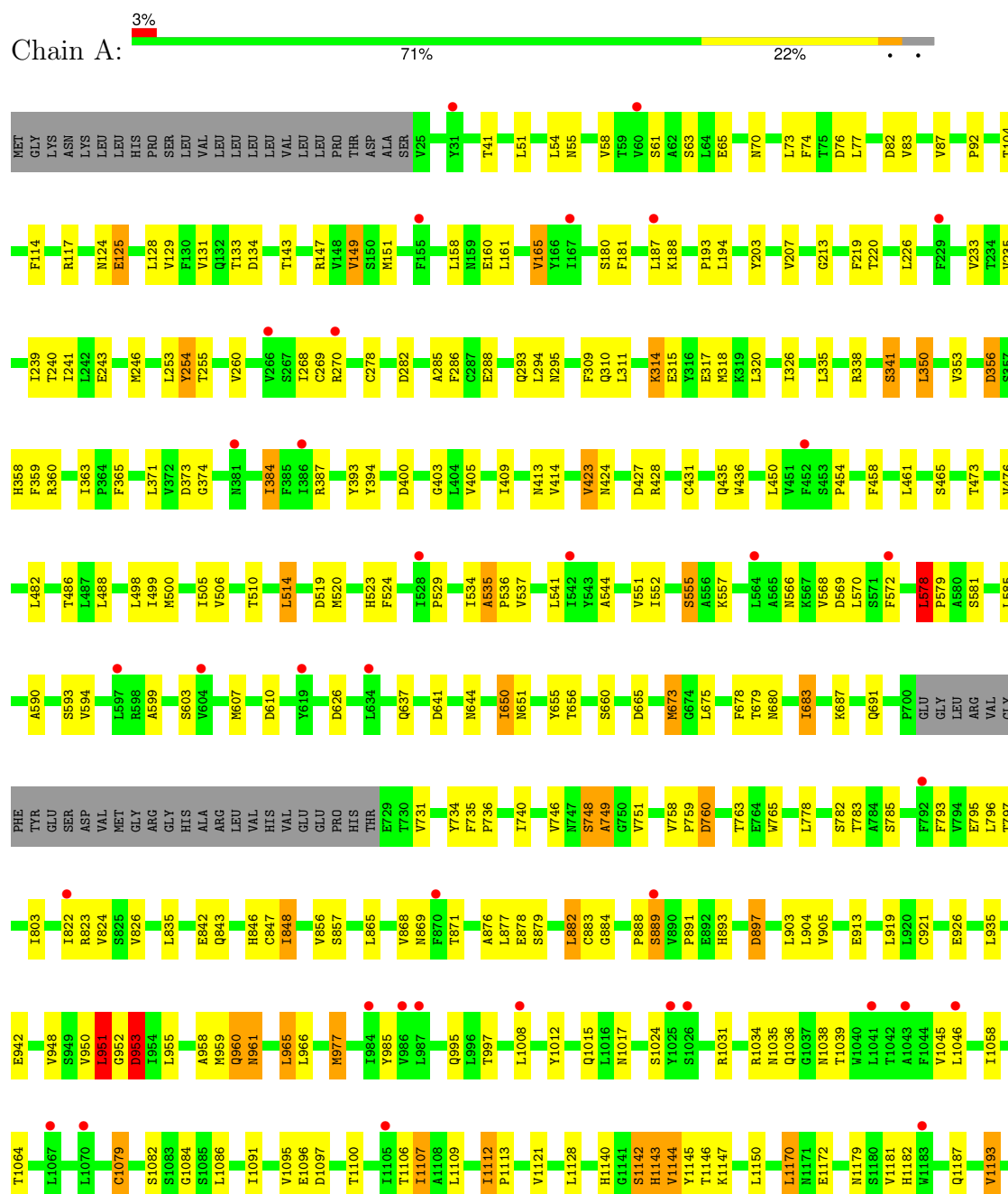


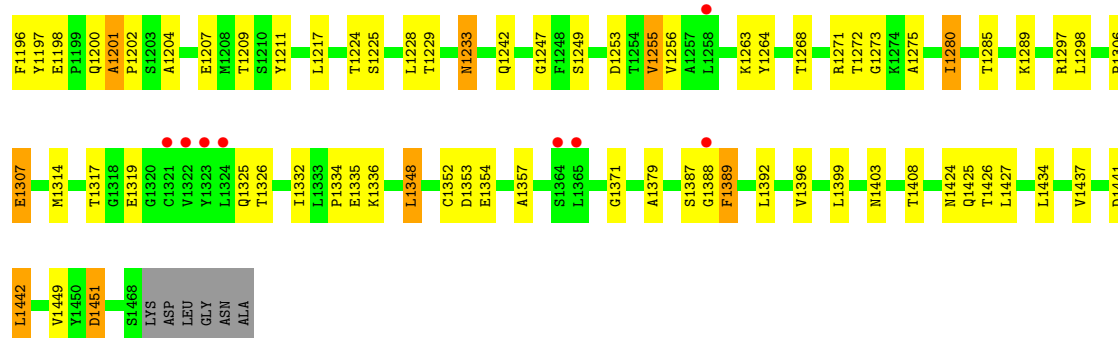
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	B	1	Total	C	N	O	0	0
			14	8	1	5		
5	C	1	Total	C	N	O	0	0
			14	8	1	5		
5	C	1	Total	C	N	O	0	0
			14	8	1	5		
5	C	1	Total	C	N	O	0	0
			14	8	1	5		
5	D	1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

3 Residue-property plots

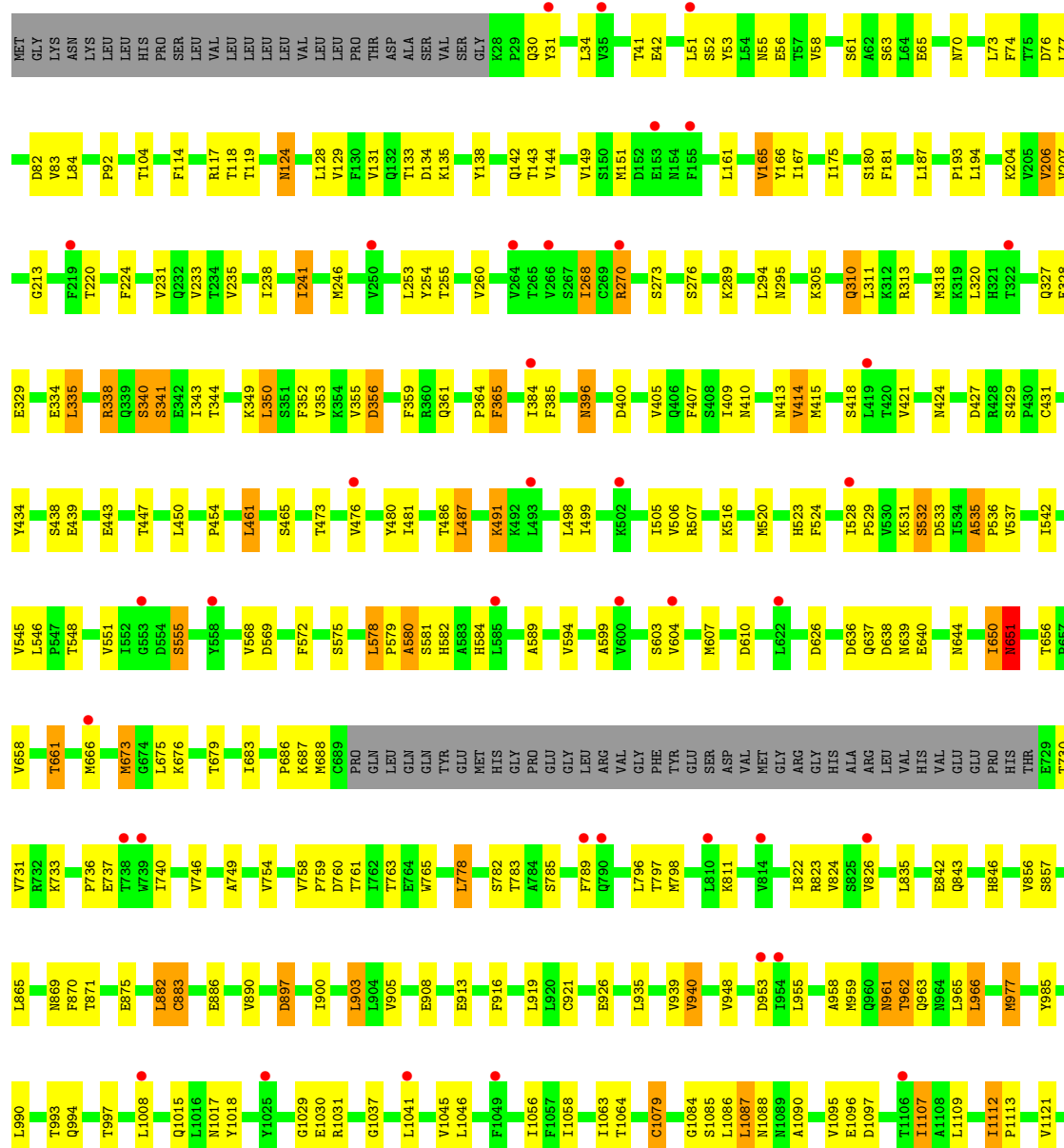
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

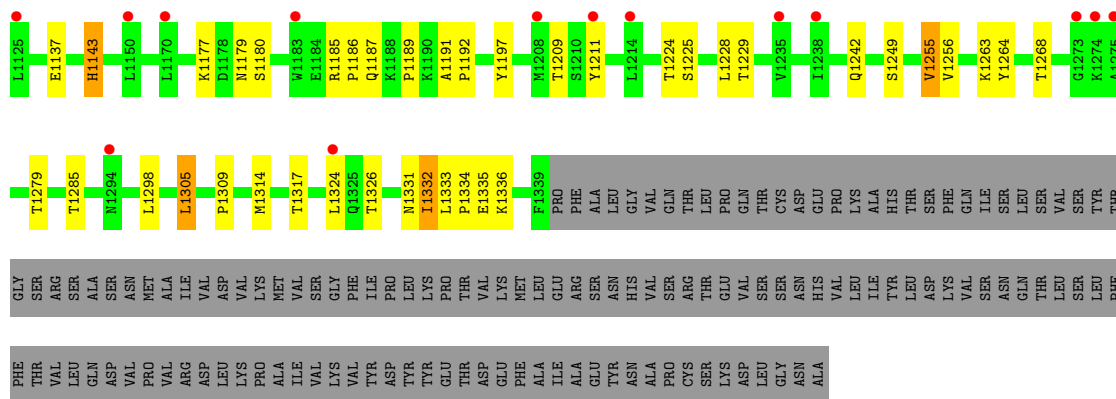
• Molecule 1: Alpha-2-macroglobulin



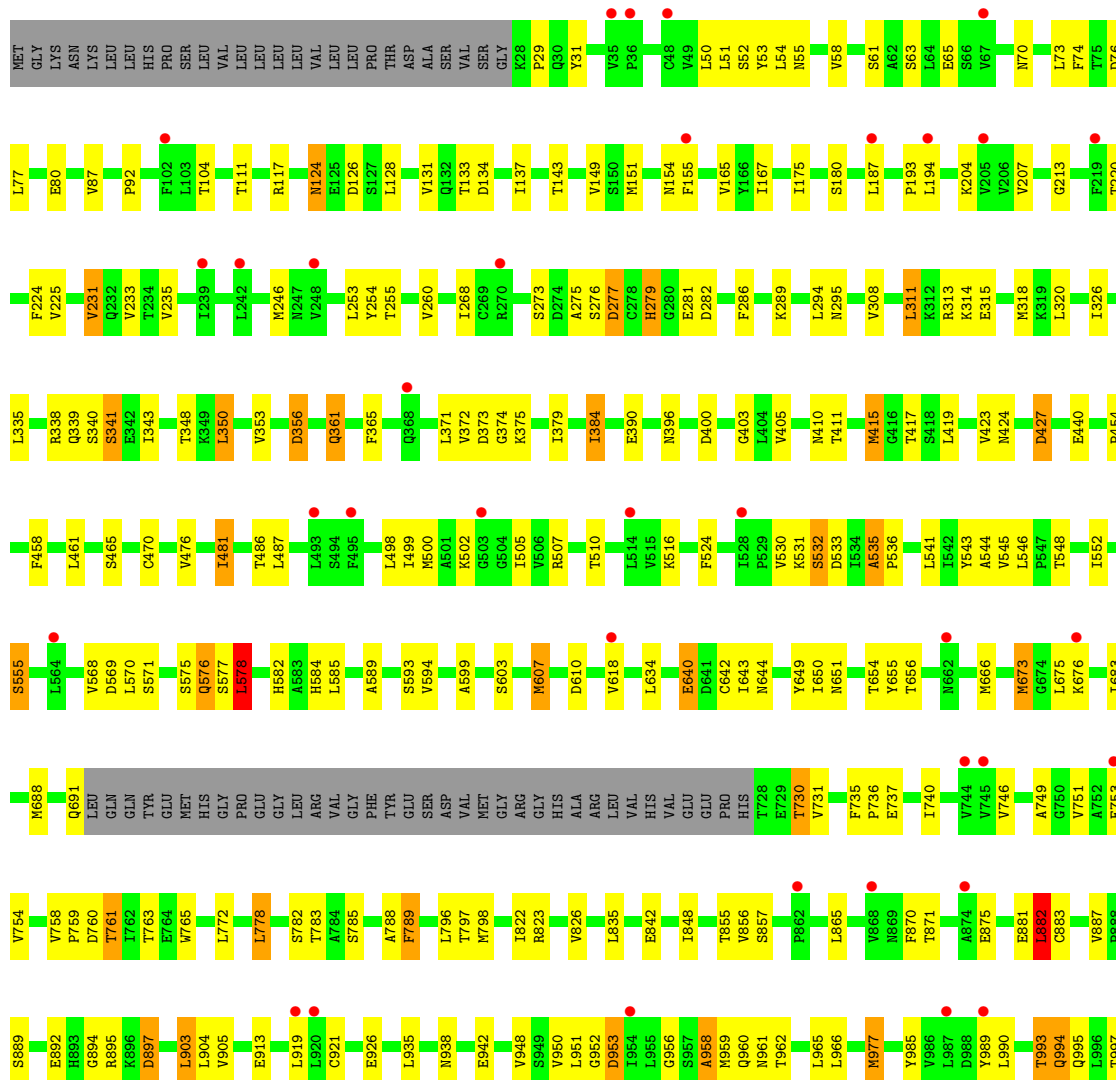


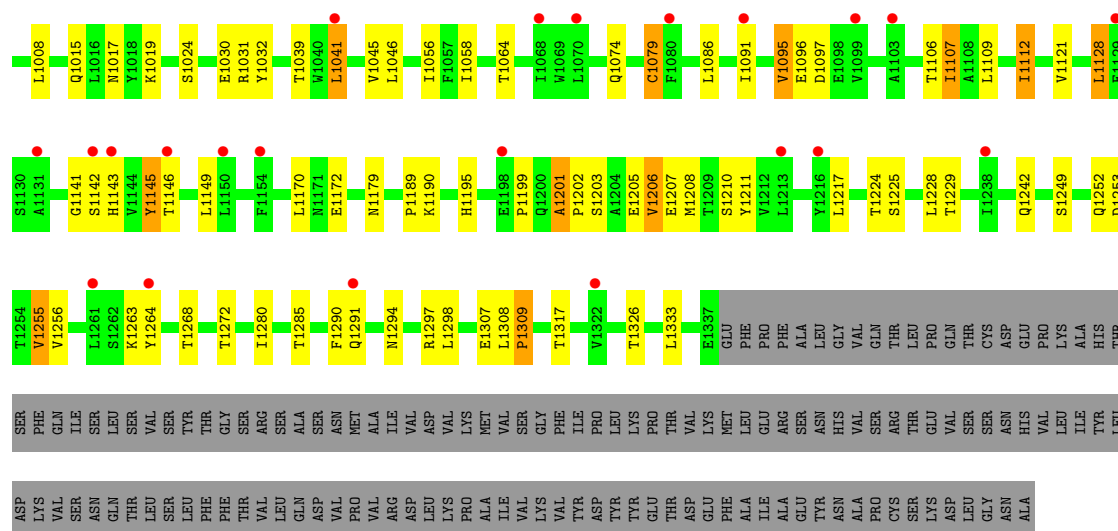
• Molecule 1: Alpha-2-macroglobulin



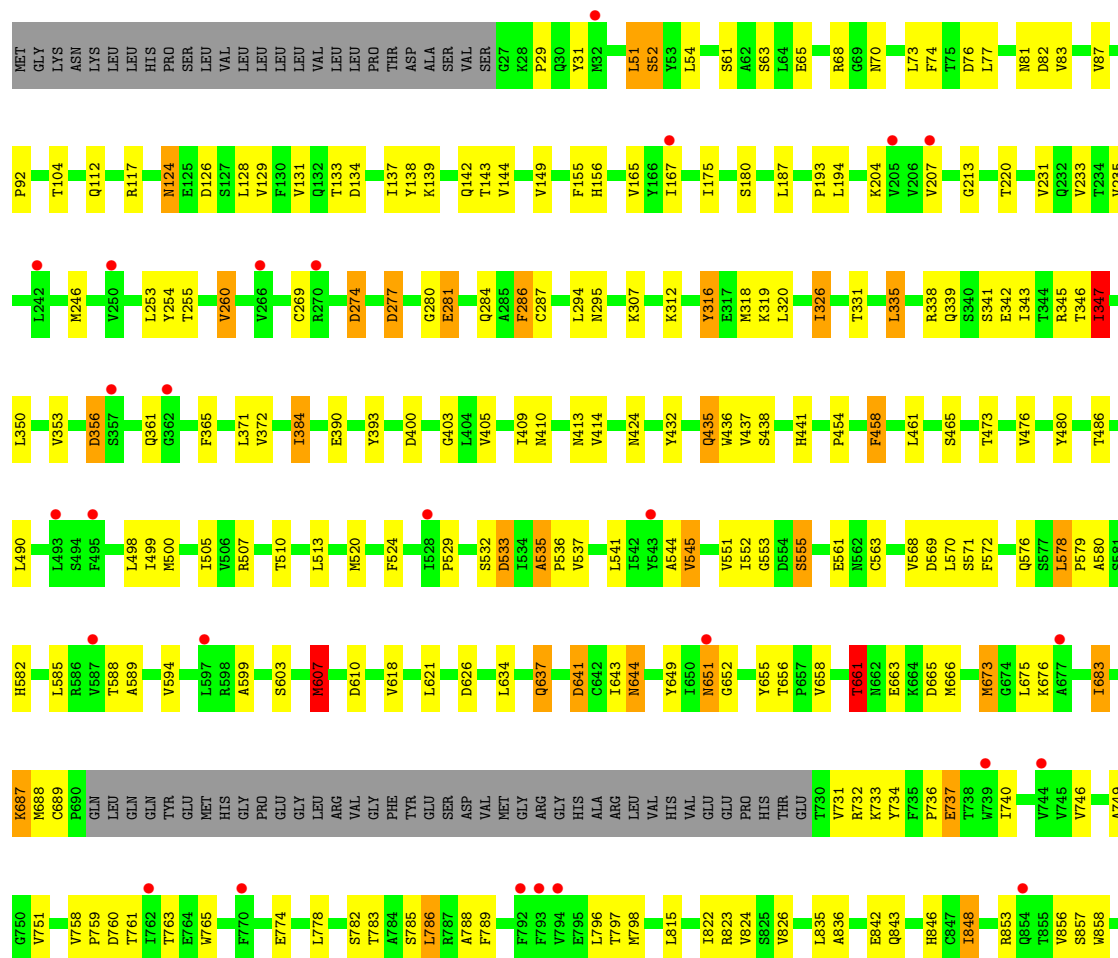


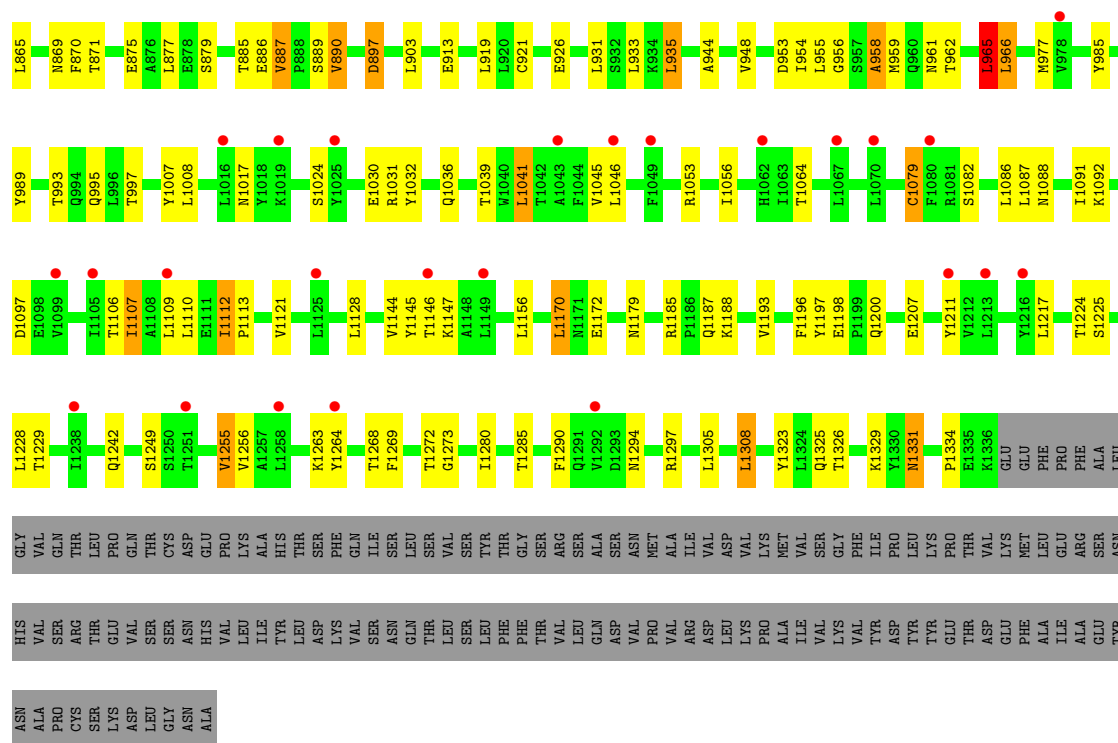
• Molecule 1: Alpha-2-macroglobulin





• Molecule 1: Alpha-2-macroglobulin





- Molecule 2: 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

Chain E:  50%

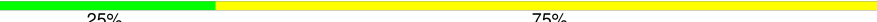


- Molecule 2: alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:  50%



- Molecule 2: 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

Chain J:  25%



- Molecule 2: 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

Chain O:  50%



- Molecule 2: 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

Chain V:



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

Chain F:



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

Chain I:



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

Chain M:



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

Chain R:



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

Chain H:

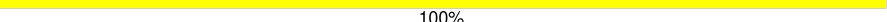


- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:  50% 50%

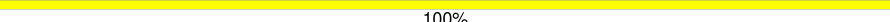
MAG1
MAG2

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

Chain L:  100%

MAG1
MAG2

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

Chain N:  100%

MAG1
MAG2

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

Chain P:  50% 50%

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

Chain S:  50% 50%

MAG1
MAG2

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

Chain T:  50% 50%

MAG1
MAG2

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

Chain U: 

MAG1
MAG2

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	130.80Å 260.30Å 281.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.24 – 4.20 34.24 – 4.20	Depositor EDS
% Data completeness (in resolution range)	99.2 (34.24-4.20) 99.0 (34.24-4.20)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.03 (at 4.15Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.235 , 0.282 0.263 , 0.300	Depositor DCC
R_{free} test set	834 reflections (1.19%)	wwPDB-VP
Wilson B-factor (Å ²)	221.9	Xtriage
Anisotropy	0.306	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 270.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	82015	wwPDB-VP
Average B, all atoms (Å ²)	256.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.43% 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: NAG, MAN, BMA

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	1.00	9/11297 (0.1%)	1.24	54/15352 (0.4%)
1	B	0.96	5/10149 (0.0%)	1.23	42/13786 (0.3%)
1	C	0.97	8/10156 (0.1%)	1.25	52/13798 (0.4%)
1	D	0.94	6/10126 (0.1%)	1.24	44/13757 (0.3%)
All	All	0.97	28/41728 (0.1%)	1.24	192/56693 (0.3%)

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	889	SER	CA-C	7.52	1.57	1.53
1	C	576	GLN	CA-C	7.12	1.59	1.53
1	C	642	CYS	CA-C	6.56	1.60	1.53
1	C	415	MET	CA-C	5.96	1.60	1.52
1	B	1143	HIS	CA-C	5.90	1.58	1.53
1	A	1348	LEU	CA-C	5.74	1.60	1.52
1	C	950	VAL	C-N	5.71	1.40	1.33
1	C	1195	HIS	CA-C	5.62	1.59	1.52
1	A	1193	VAL	CA-C	5.61	1.59	1.52
1	D	889	SER	C-N	5.57	1.38	1.33
1	A	1144	VAL	CA-C	5.57	1.59	1.52
1	A	1442	LEU	CA-C	5.56	1.59	1.53
1	D	435	GLN	CA-C	5.55	1.60	1.52
1	D	607	MET	SD-CE	-5.55	1.65	1.79
1	B	1335	GLU	CA-C	5.47	1.57	1.52
1	D	788	ALA	C-N	5.36	1.40	1.33
1	B	343	ILE	CG1-CD1	-5.33	1.30	1.51
1	C	977	MET	SD-CE	-5.28	1.66	1.79
1	A	977	MET	SD-CE	-5.15	1.66	1.79
1	B	656	THR	CA-C	5.12	1.56	1.52
1	D	887	VAL	CA-C	5.11	1.58	1.52
1	C	688	MET	CA-C	5.09	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1280	ILE	CG1-CD1	-5.08	1.31	1.51
1	C	761	THR	CA-C	-5.07	1.47	1.53
1	A	1353	ASP	CA-C	5.06	1.60	1.53
1	A	1201	ALA	C-N	5.03	1.39	1.34
1	B	977	MET	SD-CE	-5.02	1.67	1.79
1	A	961	ASN	CA-CB	5.01	1.61	1.53

All (192) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	1112	ILE	N-CA-C	-11.47	97.71	108.95
1	B	1112	ILE	N-CA-C	-11.16	98.01	108.95
1	C	1112	ILE	N-CA-C	-11.09	98.08	108.95
1	D	651	ASN	CA-CB-CG	10.61	123.21	112.60
1	C	1107	ILE	N-CA-CB	9.42	121.29	110.65
1	A	1107	ILE	N-CA-CB	9.24	121.09	110.65
1	D	1107	ILE	N-CA-CB	9.19	121.04	110.65
1	B	1107	ILE	N-CA-CB	9.18	121.03	110.65
1	C	952	GLY	CA-C-N	9.04	138.81	121.54
1	C	952	GLY	C-N-CA	9.04	138.81	121.54
1	D	953	ASP	N-CA-C	8.53	123.30	113.15
1	D	789	PHE	CA-CB-CG	8.25	122.05	113.80
1	B	940	VAL	N-CA-CB	7.77	119.44	110.82
1	C	651	ASN	CA-CB-CG	7.72	120.32	112.60
1	D	665	ASP	CA-CB-CG	7.58	120.18	112.60
1	C	789	PHE	CA-CB-CG	7.55	121.35	113.80
1	C	760	ASP	CA-CB-CG	7.43	120.03	112.60
1	A	952	GLY	CA-C-N	7.42	135.70	121.54
1	A	952	GLY	C-N-CA	7.42	135.70	121.54
1	C	953	ASP	N-CA-C	7.36	126.47	110.80
1	A	897	ASP	CA-CB-CG	7.29	119.89	112.60
1	D	644	ASN	CA-CB-CG	7.21	119.81	112.60
1	B	385	PHE	CA-CB-CG	7.20	121.00	113.80
1	D	1331	ASN	CA-CB-CG	7.18	119.78	112.60
1	C	134	ASP	CA-CB-CG	7.16	119.76	112.60
1	A	55	ASN	N-CA-C	-7.15	103.42	112.93
1	B	897	ASP	CA-CB-CG	7.11	119.71	112.60
1	D	134	ASP	CA-CB-CG	7.10	119.70	112.60
1	A	793	PHE	CA-CB-CG	7.10	120.90	113.80
1	D	897	ASP	CA-CB-CG	7.05	119.66	112.60
1	C	897	ASP	CA-CB-CG	7.03	119.63	112.60
1	B	134	ASP	CA-CB-CG	7.02	119.62	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	277	ASP	CA-CB-CG	6.99	119.58	112.60
1	D	410	ASN	OD1-CG-ND2	-6.88	115.72	122.60
1	A	427	ASP	CA-CB-CG	6.85	119.45	112.60
1	A	889	SER	N-CA-C	6.85	119.64	108.55
1	C	427	ASP	CA-CB-CG	6.84	119.44	112.60
1	A	134	ASP	CA-CB-CG	6.82	119.42	112.60
1	B	644	ASN	CA-CB-CG	6.82	119.42	112.60
1	D	286	PHE	CA-CB-CG	6.80	120.60	113.80
1	C	339	GLN	N-CA-C	-6.79	105.32	112.93
1	A	1196	PHE	CA-CB-CG	6.73	120.53	113.80
1	C	960	GLN	CA-C-N	6.71	129.60	120.54
1	C	960	GLN	C-N-CA	6.71	129.60	120.54
1	C	154	ASN	N-CA-C	-6.71	98.33	109.46
1	B	1335	GLU	N-CA-C	-6.70	104.14	112.72
1	D	641	ASP	CA-CB-CG	6.64	119.24	112.60
1	A	961	ASN	CA-CB-CG	6.61	119.21	112.60
1	C	643	ILE	CA-C-N	6.60	129.37	120.65
1	C	643	ILE	C-N-CA	6.60	129.37	120.65
1	D	533	ASP	N-CA-C	-6.57	104.75	112.89
1	C	953	ASP	CA-CB-CG	6.55	119.15	112.60
1	C	961	ASN	CA-C-N	6.55	129.95	120.38
1	C	961	ASN	C-N-CA	6.55	129.95	120.38
1	D	274	ASP	CA-CB-CG	6.55	119.15	112.60
1	D	661	THR	N-CA-C	6.50	118.73	108.79
1	A	1451	ASP	CA-CB-CG	6.49	119.09	112.60
1	B	241	ILE	N-CA-C	-6.45	104.87	110.74
1	D	458	PHE	CA-CB-CG	6.42	120.22	113.80
1	A	959	MET	CA-C-N	6.41	129.35	120.63
1	A	959	MET	C-N-CA	6.41	129.35	120.63
1	A	400	ASP	CA-CB-CG	6.36	118.96	112.60
1	A	1253	ASP	CA-CB-CG	6.36	118.95	112.60
1	D	400	ASP	CA-CB-CG	6.23	118.83	112.60
1	C	400	ASP	CA-CB-CG	6.22	118.82	112.60
1	A	1084	GLY	N-CA-C	6.11	120.02	111.10
1	D	869	ASN	OD1-CG-ND2	-6.08	116.52	122.60
1	B	400	ASP	CA-CB-CG	6.07	118.67	112.60
1	B	533	ASP	CA-CB-CG	6.02	118.62	112.60
1	C	1307	GLU	N-CA-C	6.01	118.98	109.96
1	D	760	ASP	CA-CB-CG	6.00	118.60	112.60
1	D	1196	PHE	CA-CB-CG	5.96	119.76	113.80
1	C	1145	TYR	CA-C-N	5.92	128.14	120.44
1	C	1145	TYR	C-N-CA	5.92	128.14	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	869	ASN	OD1-CG-ND2	-5.90	116.70	122.60
1	D	683	ILE	N-CA-CB	-5.89	106.81	111.64
1	C	282	ASP	CA-CB-CG	5.87	118.47	112.60
1	B	516	LYS	N-CA-C	-5.87	100.89	109.63
1	B	916	PHE	CA-CB-CG	5.84	119.64	113.80
1	A	55	ASN	OD1-CG-ND2	-5.83	116.77	122.60
1	A	486	THR	N-CA-C	-5.82	104.63	110.97
1	A	1371	GLY	CA-C-N	5.80	128.33	120.38
1	A	1371	GLY	C-N-CA	5.80	128.33	120.38
1	C	1290	PHE	CA-CB-CG	5.80	119.60	113.80
1	A	1233	ASN	CA-CB-CG	5.77	118.37	112.60
1	B	82	ASP	CA-CB-CG	5.77	118.37	112.60
1	B	55	ASN	OD1-CG-ND2	-5.73	116.87	122.60
1	C	1297	ARG	N-CA-C	-5.72	105.13	111.71
1	D	1087	LEU	N-CA-C	-5.70	100.95	109.96
1	D	959	MET	CA-C-N	5.70	128.39	120.29
1	D	959	MET	C-N-CA	5.70	128.39	120.29
1	B	1097	ASP	CA-CB-CG	5.70	118.30	112.60
1	D	1088	ASN	CA-CB-CG	5.69	118.29	112.60
1	D	890	VAL	N-CA-C	5.68	113.85	109.19
1	C	578	LEU	CA-C-O	-5.68	112.38	120.16
1	D	578	LEU	CA-C-O	-5.68	112.38	120.16
1	D	81	ASN	CA-C-N	5.67	130.19	122.07
1	D	81	ASN	C-N-CA	5.67	130.19	122.07
1	D	652	GLY	N-CA-C	-5.65	103.51	112.66
1	C	951	LEU	N-CA-C	5.63	116.79	107.73
1	C	126	ASP	CA-CB-CG	5.61	118.21	112.60
1	D	643	ILE	CA-C-N	5.61	128.59	120.79
1	D	643	ILE	C-N-CA	5.61	128.59	120.79
1	A	1396	VAL	CA-C-N	5.60	127.78	120.28
1	A	1396	VAL	C-N-CA	5.60	127.78	120.28
1	A	1097	ASP	CA-CB-CG	5.58	118.18	112.60
1	D	126	ASP	CA-CB-CG	5.58	118.18	112.60
1	C	533	ASP	CA-CB-CG	5.57	118.17	112.60
1	C	1112	ILE	N-CA-CB	5.57	115.26	110.08
1	B	760	ASP	CA-CB-CG	5.55	118.15	112.60
1	C	410	ASN	OD1-CG-ND2	5.55	128.15	122.60
1	B	70	ASN	CA-CB-CG	5.53	118.13	112.60
1	A	1271	ARG	N-CA-C	-5.51	102.37	110.52
1	A	951	LEU	N-CA-C	5.50	115.81	108.38
1	B	961	ASN	CA-CB-CG	5.50	118.10	112.60
1	B	953	ASP	N-CA-C	5.45	119.92	112.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	760	ASP	CA-CB-CG	5.45	118.05	112.60
1	B	661	THR	N-CA-C	5.42	117.64	109.41
1	C	70	ASN	CA-CB-CG	5.41	118.00	112.60
1	A	665	ASP	CA-CB-CG	5.40	118.00	112.60
1	C	51	LEU	N-CA-C	-5.39	100.39	109.07
1	A	356	ASP	CA-CB-CG	5.39	117.99	112.60
1	D	1200	GLN	N-CA-C	5.38	118.31	109.76
1	C	1097	ASP	CA-CB-CG	5.37	117.97	112.60
1	A	660	SER	N-CA-C	5.36	117.25	110.33
1	A	1403	ASN	CA-CB-CG	5.36	117.96	112.60
1	B	1087	LEU	CA-C-N	5.35	131.76	121.54
1	B	1087	LEU	C-N-CA	5.35	131.76	121.54
1	A	70	ASN	CA-CB-CG	5.33	117.93	112.60
1	A	735	PHE	CA-CB-CG	5.33	119.13	113.80
1	C	1031	ARG	N-CA-C	-5.32	98.33	108.17
1	B	359	PHE	CA-CB-CG	5.29	119.09	113.80
1	B	651	ASN	CA-CB-CG	5.28	117.88	112.60
1	A	578	LEU	CA-C-O	-5.28	112.92	120.16
1	D	70	ASN	CA-CB-CG	5.28	117.88	112.60
1	A	1143	HIS	CA-C-N	5.28	131.47	121.97
1	A	1143	HIS	C-N-CA	5.28	131.47	121.97
1	D	124	ASN	CA-CB-CG	5.27	117.87	112.60
1	B	310	GLN	CA-C-N	5.27	130.22	122.63
1	B	310	GLN	C-N-CA	5.27	130.22	122.63
1	C	894	GLY	CA-C-N	5.27	131.60	121.54
1	C	894	GLY	C-N-CA	5.27	131.60	121.54
1	A	965	LEU	CA-C-N	5.26	131.60	121.54
1	A	965	LEU	C-N-CA	5.26	131.60	121.54
1	B	1112	ILE	N-CA-CB	5.26	114.97	110.08
1	A	960	GLN	CA-C-N	5.26	127.64	120.54
1	A	960	GLN	C-N-CA	5.26	127.64	120.54
1	B	396	ASN	CA-CB-CG	5.26	117.86	112.60
1	B	789	PHE	N-CA-C	5.25	115.29	107.88
1	C	753	GLU	CA-C-N	5.22	126.55	121.65
1	C	753	GLU	C-N-CA	5.22	126.55	121.65
1	A	1389	PHE	CA-CB-CG	5.21	119.00	113.80
1	C	603	SER	N-CA-C	-5.19	106.07	112.72
1	A	869	ASN	OD1-CG-ND2	-5.19	117.41	122.60
1	A	678	PHE	N-CA-C	-5.18	100.79	109.24
1	A	953	ASP	N-CA-C	5.18	121.83	110.80
1	B	356	ASP	CA-CB-CG	5.17	117.77	112.60
1	A	680	ASN	CA-CB-CG	5.15	117.75	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	1112	ILE	CB-CA-C	-5.14	105.34	110.89
1	A	488	LEU	N-CA-C	-5.14	106.11	112.38
1	A	644	ASN	CA-CB-CG	5.13	117.73	112.60
1	D	356	ASP	CA-CB-CG	5.12	117.72	112.60
1	B	55	ASN	N-CA-C	-5.11	106.73	113.17
1	A	1112	ILE	N-CA-C	-5.11	97.84	108.88
1	A	1424	ASN	CA-CB-CG	5.11	117.71	112.60
1	D	139	LYS	N-CA-C	-5.10	103.10	110.40
1	A	1348	LEU	CA-C-O	-5.10	113.18	120.16
1	B	1090	ALA	CA-C-N	5.10	128.98	120.62
1	B	1090	ALA	C-N-CA	5.10	128.98	120.62
1	C	644	ASN	CA-CB-CG	5.08	117.68	112.60
1	B	1037	GLY	N-CA-C	5.07	118.44	111.54
1	B	603	SER	N-CA-C	-5.07	106.23	112.72
1	C	356	ASP	CA-CB-CG	5.07	117.67	112.60
1	B	1112	ILE	CB-CA-C	-5.06	105.42	110.89
1	B	55	ASN	CB-CG-ND2	5.06	123.99	116.40
1	B	427	ASP	CA-CB-CG	5.06	117.66	112.60
1	D	1297	ARG	N-CA-C	-5.06	105.85	111.36
1	D	51	LEU	N-CA-C	-5.05	98.35	107.75
1	C	396	ASN	CA-CB-CG	5.05	117.65	112.60
1	A	310	GLN	CA-C-N	5.04	130.45	122.78
1	A	310	GLN	C-N-CA	5.04	130.45	122.78
1	B	1096	GLU	CB-CG-CD	5.04	121.17	112.60
1	D	342	GLU	N-CA-C	5.04	118.33	110.32
1	C	882	LEU	CA-C-N	5.03	126.98	120.44
1	C	882	LEU	C-N-CA	5.03	126.98	120.44
1	C	959	MET	CA-C-N	5.03	129.11	120.71
1	C	959	MET	C-N-CA	5.03	129.11	120.71
1	D	603	SER	N-CA-C	-5.03	106.28	112.72
1	B	124	ASN	CA-CB-CG	5.03	117.62	112.60
1	C	124	ASN	CA-CB-CG	5.01	117.61	112.60
1	D	316	TYR	N-CA-C	5.01	119.02	111.96
1	A	603	SER	N-CA-C	-5.00	106.32	112.72

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	11050	10926	10934	93	0
1	B	9929	9812	9818	88	0
1	C	9936	9834	9836	96	0
1	D	9906	9810	9812	100	0
2	E	50	0	43	1	0
2	G	50	0	43	1	0
2	J	50	0	43	0	0
2	O	50	0	43	0	0
2	V	50	0	43	0	0
3	F	39	0	34	0	0
3	I	39	0	34	0	0
3	M	39	0	34	0	0
3	R	39	0	34	1	0
4	H	28	0	25	0	0
4	K	28	0	25	0	0
4	L	28	0	25	0	0
4	N	28	0	25	0	0
4	P	28	0	25	0	0
4	Q	28	0	25	0	0
4	S	28	0	25	1	0
4	T	28	0	25	0	0
4	U	28	0	25	0	0
5	A	42	0	39	0	0
5	B	14	0	13	0	0
5	C	56	0	52	0	0
5	D	42	0	39	0	0
All	All	41633	40382	41119	371	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 4.

All (371) 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:D:1147:LYS:HB3	1:D:1170:LEU:HD21	1.54	0.90
1:D:77:LEU:HD22	1:D:87:VAL:HG11	1.53	0.89
1:C:77:LEU:HD22	1:C:87:VAL:HG11	1.55	0.89
1:A:77:LEU:HD22	1:A:87:VAL:HG11	1.56	0.87
1:A:977:MET:HE3	1:A:1045:VAL:HG22	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:977:MET:HE3	1:B:1045:VAL:HG22	1.71	0.71
1:C:535:ALA:HB1	1:C:536:PRO:CD	2.20	0.71
1:D:977:MET:HE3	1:D:1045:VAL:HG22	1.72	0.71
1:C:977:MET:HE3	1:C:1045:VAL:HG22	1.71	0.70
1:B:679:THR:HG21	1:B:683:ILE:HD12	1.73	0.70
1:A:1399:LEU:HB2	1:A:1408:THR:HG21	1.73	0.70
1:A:1095:VAL:HG21	1:A:1145:TYR:CE2	2.27	0.69
1:C:165:VAL:HG22	1:C:207:VAL:HG12	1.73	0.69
1:C:384:ILE:CD1	1:C:405:VAL:HG21	2.23	0.69
1:D:384:ILE:CD1	1:D:405:VAL:HG21	2.24	0.68
1:D:165:VAL:HG22	1:D:207:VAL:HG12	1.76	0.68
1:A:384:ILE:CD1	1:A:405:VAL:HG21	2.24	0.67
1:D:935:LEU:HD11	1:D:1308:LEU:HD13	1.76	0.66
1:D:312:LYS:HD3	1:D:437:VAL:HG21	1.78	0.66
1:C:231:VAL:HG13	1:C:335:LEU:HB2	1.79	0.65
1:D:826:VAL:HG11	1:D:856:VAL:HG21	1.79	0.65
1:B:658:VAL:HG12	1:C:656:THR:CG2	2.27	0.64
1:B:658:VAL:HG12	1:C:656:THR:HG22	1.79	0.64
1:C:962:THR:HG22	1:C:990:LEU:HD21	1.80	0.64
1:C:1145:TYR:CE2	1:C:1149:LEU:HD11	2.32	0.64
1:A:1106:THR:HG21	1:A:1128:LEU:HD11	1.80	0.64
1:D:1106:THR:HG21	1:D:1128:LEU:HD11	1.80	0.63
1:D:962:THR:O	1:D:965:LEU:HD22	1.99	0.63
1:C:758:VAL:HG11	1:C:765:TRP:CZ2	2.33	0.63
1:D:758:VAL:HG11	1:D:765:TRP:CZ2	2.34	0.62
1:D:138:TYR:CZ	1:D:144:VAL:HG23	2.35	0.61
1:A:1100:THR:CG2	1:A:1146:THR:HG22	2.30	0.61
1:B:535:ALA:HB1	1:B:536:PRO:CD	2.30	0.61
1:B:499:ILE:HD11	1:B:507:ARG:HB2	1.83	0.61
1:D:535:ALA:HB1	1:D:536:PRO:CD	2.30	0.61
1:A:1211:TYR:CE2	1:A:1256:VAL:HG11	2.36	0.60
1:B:758:VAL:HG11	1:B:765:TRP:CZ2	2.36	0.60
1:A:656:THR:HG22	1:D:658:VAL:HG12	1.82	0.60
1:D:1211:TYR:CE2	1:D:1256:VAL:HG11	2.37	0.60
1:A:239:ILE:HD11	1:A:243:GLU:HG2	1.83	0.60
1:A:535:ALA:HB1	1:A:536:PRO:CD	2.31	0.60
1:D:1147:LYS:CB	1:D:1170:LEU:HD21	2.30	0.59
1:A:1100:THR:HG22	1:A:1146:THR:HG22	1.84	0.59
1:B:535:ALA:HB1	1:B:536:PRO:HD3	1.83	0.59
1:B:350:LEU:HD21	1:B:443:GLU:HA	1.83	0.59
1:B:365:PHE:CE1	1:B:409:ILE:HD13	2.38	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:656:THR:CG2	1:D:658:VAL:HG12	2.33	0.59
1:B:551:VAL:HG11	1:B:666:MET:HE2	1.83	0.59
1:A:826:VAL:HG11	1:A:856:VAL:HG21	1.84	0.58
1:C:1211:TYR:CE2	1:C:1256:VAL:HG11	2.37	0.58
1:B:166:TYR:CE1	1:B:206:VAL:HG13	2.38	0.58
1:B:1211:TYR:CE2	1:B:1256:VAL:HG11	2.39	0.58
1:B:268:ILE:HD12	1:B:320:LEU:HD21	1.86	0.58
1:A:498:LEU:HD22	1:A:505:ILE:HD11	1.84	0.58
1:A:535:ALA:HB1	1:A:536:PRO:HD3	1.84	0.58
1:A:537:VAL:HG21	1:A:626:ASP:CG	2.29	0.58
1:D:578:LEU:O	1:D:580:ALA:N	2.36	0.58
1:B:151:MET:HE2	1:B:778:LEU:HD13	1.85	0.57
1:B:537:VAL:HG21	1:B:626:ASP:CG	2.28	0.57
1:D:535:ALA:HB1	1:D:536:PRO:HD3	1.84	0.57
1:D:572:PHE:CZ	1:D:786:LEU:HD22	2.39	0.57
1:D:836:ALA:HB1	1:D:858:TRP:CE3	2.39	0.57
1:C:498:LEU:HD22	1:C:505:ILE:HD11	1.86	0.57
1:D:1046:LEU:HG	1:D:1112:ILE:HD11	1.87	0.57
1:A:977:MET:CE	1:A:1045:VAL:HG22	2.34	0.57
1:C:73:LEU:HD11	1:C:92:PRO:CD	2.34	0.57
1:C:977:MET:CE	1:C:1045:VAL:HG22	2.34	0.57
1:D:537:VAL:HG21	1:D:626:ASP:CG	2.29	0.57
1:B:151:MET:CE	1:B:778:LEU:HD13	2.35	0.57
1:C:371:LEU:HD22	1:C:379:ILE:HG22	1.85	0.57
1:D:977:MET:CE	1:D:1045:VAL:HG22	2.35	0.57
1:D:498:LEU:HD22	1:D:505:ILE:HD11	1.86	0.57
1:C:870:PHE:CE1	1:C:903:LEU:HD21	2.39	0.57
1:B:498:LEU:HD22	1:B:505:ILE:HD11	1.87	0.57
1:B:73:LEU:HD11	1:B:92:PRO:CD	2.35	0.57
1:C:958:ALA:HB2	1:C:989:TYR:OH	2.05	0.57
1:B:599:ALA:HB3	1:B:740:ILE:HG22	1.87	0.56
1:D:966:LEU:HD13	1:D:1007:TYR:CD2	2.39	0.56
1:A:73:LEU:HD11	1:A:92:PRO:CD	2.35	0.56
1:B:824:VAL:HG23	1:B:875:GLU:C	2.30	0.56
1:B:977:MET:CE	1:B:1045:VAL:HG22	2.34	0.56
1:D:73:LEU:HD11	1:D:92:PRO:CD	2.35	0.56
1:C:1046:LEU:HG	1:C:1112:ILE:HD11	1.87	0.56
1:D:260:VAL:HB	1:D:326:ILE:HD11	1.87	0.56
1:A:824:VAL:HG12	1:A:848:ILE:HD11	1.88	0.56
1:D:870:PHE:CE1	1:D:903:LEU:HD21	2.40	0.56
1:B:1046:LEU:HG	1:B:1112:ILE:HD11	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:129:VAL:HG23	1:A:149:VAL:O	2.06	0.55
1:C:546:LEU:HB3	1:C:548:THR:HG22	1.88	0.55
1:C:650:ILE:HD12	1:C:655:TYR:CD2	2.41	0.55
1:A:1095:VAL:HG21	1:A:1145:TYR:CD2	2.41	0.55
1:C:570:LEU:HD21	1:C:585:LEU:HD21	1.88	0.55
1:A:578:LEU:HD13	1:A:579:PRO:HD2	1.89	0.55
1:A:1182:HIS:HB2	1:A:1209:THR:HG21	1.87	0.55
1:A:551:VAL:HG21	1:A:683:ILE:HD11	1.89	0.54
1:A:1046:LEU:HG	1:A:1112:ILE:HD11	1.88	0.54
1:A:235:VAL:HG21	1:A:320:LEU:HD22	1.89	0.54
1:C:350:LEU:HD11	1:C:423:VAL:HG12	1.88	0.54
1:A:1012:TYR:CE1	1:A:1058:ILE:HG23	2.43	0.54
1:C:235:VAL:HG21	1:C:320:LEU:HD22	1.89	0.54
1:D:318:MET:HE2	1:D:320:LEU:HD11	1.90	0.54
1:B:235:VAL:HG21	1:B:320:LEU:HD22	1.90	0.54
1:A:1147:LYS:HB3	1:A:1170:LEU:HD21	1.89	0.53
1:B:1063:ILE:HD12	1:D:68:ARG:NH2	2.23	0.53
1:C:589:ALA:HB3	1:C:746:VAL:HG21	1.90	0.53
1:D:931:LEU:HD11	1:D:933:LEU:HD21	1.90	0.53
1:D:746:VAL:HG22	1:D:751:VAL:HG12	1.90	0.53
1:B:340:SER:O	1:B:341:SER:C	2.51	0.53
1:B:962:THR:HG22	1:B:990:LEU:HD21	1.90	0.53
1:C:882:LEU:HD13	1:C:887:VAL:HG13	1.90	0.53
1:C:584:HIS:NE2	1:C:754:VAL:HG22	2.23	0.53
1:C:458:PHE:CZ	1:C:481:ILE:HD12	2.44	0.53
1:C:224:PHE:CD2	1:C:607:MET:CE	2.92	0.52
1:D:848:ILE:N	1:D:848:ILE:HD12	2.25	0.52
2:E:1:NAG:H3	2:E:2:NAG:N2	2.25	0.52
1:A:371:LEU:HD12	1:A:423:VAL:HG21	1.90	0.52
1:D:919:LEU:HD22	1:D:1228:LEU:CD1	2.40	0.52
1:D:758:VAL:HG13	1:D:761:THR:CG2	2.40	0.52
1:C:1206:VAL:CG1	1:C:1253:ASP:OD2	2.57	0.52
1:C:151:MET:CE	1:C:778:LEU:HD13	2.39	0.51
1:A:965:LEU:HD11	1:A:1247:GLY:CA	2.40	0.51
1:B:1314:MET:HG2	1:B:1324:LEU:HD13	1.92	0.51
1:A:254:TYR:CD2	1:A:255:THR:HG22	2.45	0.51
1:C:52:SER:OG	1:C:545:VAL:HG21	2.10	0.51
1:C:318:MET:SD	1:C:318:MET:N	2.84	0.51
1:C:104:THR:HG22	1:C:117:ARG:CB	2.41	0.51
1:C:361:GLN:HA	1:C:411:THR:HB	1.92	0.51
1:B:241:ILE:HD11	1:B:344:THR:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1095:VAL:HG12	1:B:1095:VAL:O	2.11	0.51
1:D:104:THR:HG22	1:D:117:ARG:CB	2.40	0.51
1:C:570:LEU:HD23	1:C:571:SER:N	2.27	0.50
1:C:746:VAL:HG22	1:C:751:VAL:HG12	1.94	0.50
1:A:919:LEU:HD22	1:A:1228:LEU:CD1	2.42	0.50
1:B:758:VAL:HG13	1:B:761:THR:HG22	1.93	0.50
1:B:104:THR:HG22	1:B:117:ARG:CB	2.41	0.50
1:D:961:ASN:O	1:D:965:LEU:HB2	2.11	0.50
1:C:758:VAL:HG13	1:C:761:THR:CG2	2.41	0.50
1:A:823:ARG:O	1:A:876:ALA:HA	2.11	0.50
1:B:231:VAL:O	1:B:335:LEU:HD22	2.12	0.50
1:C:1205:GLU:HA	1:C:1208:MET:HE2	1.94	0.50
1:D:661:THR:HG21	1:D:663:GLU:CD	2.36	0.50
1:B:555:SER:OG	1:B:673:MET:HE1	2.11	0.50
1:A:104:THR:HG22	1:A:117:ARG:HB2	1.93	0.49
1:C:578:LEU:HD23	1:C:578:LEU:N	2.27	0.49
1:C:499:ILE:HD11	1:C:507:ARG:HB2	1.94	0.49
1:B:1191:ALA:HB3	1:B:1192:PRO:HD3	1.95	0.49
1:C:535:ALA:HB1	1:C:536:PRO:HD3	1.94	0.49
1:D:138:TYR:CE2	1:D:144:VAL:HG23	2.47	0.49
1:B:919:LEU:HD22	1:B:1228:LEU:CD1	2.41	0.49
1:C:1207:GLU:HB3	1:C:1253:ASP:HB3	1.93	0.49
1:D:589:ALA:HB3	1:D:746:VAL:HG21	1.95	0.49
1:A:360:ARG:HB2	1:A:363:ILE:CG2	2.43	0.49
1:D:499:ILE:HD11	1:D:507:ARG:HB2	1.94	0.49
1:D:570:LEU:HD21	1:D:585:LEU:HD21	1.95	0.49
1:D:1308:LEU:O	1:D:1308:LEU:HD12	2.12	0.49
1:A:977:MET:HE2	1:A:1015:GLN:CD	2.38	0.48
1:B:823:ARG:HD3	1:B:846:HIS:N	2.28	0.48
1:B:661:THR:CG2	1:C:655:TYR:HB2	2.44	0.48
1:D:962:THR:HA	1:D:965:LEU:HD13	1.96	0.48
1:C:155:PHE:CE1	1:C:618:VAL:HG12	2.49	0.48
1:A:203:TYR:HB2	1:A:219:PHE:CE1	2.48	0.48
1:A:270:ARG:NH2	1:A:318:MET:HE2	2.28	0.48
1:A:359:PHE:CZ	1:A:450:LEU:HB3	2.48	0.48
1:A:268:ILE:HD12	1:A:320:LEU:HD21	1.95	0.48
1:A:384:ILE:HD13	1:A:405:VAL:HG21	1.96	0.48
1:D:568:VAL:HG23	1:D:588:THR:O	2.13	0.48
1:C:977:MET:HE2	1:C:1015:GLN:CD	2.39	0.48
1:D:384:ILE:HD13	1:D:405:VAL:HG21	1.95	0.48
1:C:384:ILE:HD13	1:C:405:VAL:HG21	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1145:TYR:CD2	1:A:1146:THR:HG23	2.49	0.48
1:B:461:LEU:HD12	1:B:542:ILE:HG22	1.95	0.48
1:D:231:VAL:HB	1:D:335:LEU:HB2	1.96	0.47
1:B:985:TYR:CE1	1:B:1255:VAL:HG13	2.49	0.47
1:B:165:VAL:HB	1:B:207:VAL:HG12	1.96	0.47
1:D:235:VAL:HG21	1:D:320:LEU:HD22	1.96	0.47
1:A:578:LEU:HD13	1:A:579:PRO:CD	2.44	0.47
1:B:823:ARG:HH22	1:B:843:GLN:NE2	2.13	0.47
1:D:551:VAL:HG12	1:D:666:MET:HE2	1.95	0.47
1:D:585:LEU:C	1:D:585:LEU:HD23	2.39	0.47
1:A:950:VAL:C	1:A:951:LEU:HD23	2.39	0.47
1:D:985:TYR:CE1	1:D:1255:VAL:HG13	2.49	0.47
1:A:241:ILE:HA	1:A:311:LEU:HD11	1.96	0.47
1:C:919:LEU:HD22	1:C:1228:LEU:CD1	2.44	0.47
1:A:514:LEU:O	1:A:514:LEU:HD23	2.14	0.47
1:A:882:LEU:HD23	1:A:884:GLY:O	2.14	0.47
1:A:985:TYR:CE1	1:A:1255:VAL:HG13	2.50	0.47
1:B:104:THR:HG22	1:B:117:ARG:HB2	1.96	0.47
1:B:798:MET:SD	1:B:903:LEU:HD22	2.54	0.47
1:C:985:TYR:CE1	1:C:1255:VAL:HG13	2.49	0.47
1:C:1199:PRO:O	1:C:1203:SER:HB3	2.15	0.47
1:D:326:ILE:HG22	1:D:331:THR:HB	1.97	0.47
1:D:758:VAL:HG13	1:D:761:THR:HG22	1.96	0.47
1:A:544:ALA:HB3	1:A:552:ILE:HG13	1.97	0.47
1:B:977:MET:HE2	1:B:1015:GLN:CD	2.39	0.47
1:B:1109:LEU:HA	1:B:1112:ILE:HD12	1.96	0.47
1:B:758:VAL:HG13	1:B:761:THR:CG2	2.45	0.47
1:D:561:GLU:HG3	1:D:563:CYS:SG	2.54	0.47
1:D:958:ALA:HB1	1:D:995:GLN:OE1	2.15	0.47
1:D:798:MET:SD	1:D:903:LEU:HD22	2.55	0.46
1:D:1041:LEU:O	1:D:1045:VAL:HG23	2.15	0.46
1:C:675:LEU:HD12	1:C:675:LEU:O	2.16	0.46
1:C:761:THR:HB	1:C:788:ALA:HB3	1.96	0.46
1:C:231:VAL:HG13	1:C:335:LEU:CB	2.45	0.46
1:C:772:LEU:CD2	1:C:778:LEU:HD12	2.45	0.46
1:C:1225:SER:O	1:C:1229:THR:HG23	2.15	0.46
1:A:758:VAL:HG11	1:A:765:TRP:CH2	2.51	0.46
1:C:165:VAL:CG2	1:C:207:VAL:HG12	2.45	0.46
1:C:350:LEU:N	1:C:350:LEU:HD12	2.31	0.46
1:A:350:LEU:N	1:A:350:LEU:HD12	2.31	0.46
1:C:50:LEU:HD21	1:C:52:SER:OG	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1308:LEU:HD12	1:D:1308:LEU:C	2.41	0.46
2:G:1:NAG:H4	2:G:2:NAG:N2	2.31	0.46
1:B:407:PHE:CE2	1:B:409:ILE:HD11	2.51	0.45
1:A:104:THR:HG22	1:A:117:ARG:CB	2.46	0.45
1:B:531:LYS:O	1:B:532:SER:CB	2.63	0.45
1:C:1109:LEU:HA	1:C:1112:ILE:HD12	1.98	0.45
1:C:1203:SER:HA	1:C:1206:VAL:HG12	1.97	0.45
1:C:798:MET:SD	1:C:903:LEU:HD22	2.56	0.45
1:D:1225:SER:O	1:D:1229:THR:HG23	2.15	0.45
1:B:409:ILE:HD12	1:B:409:ILE:N	2.32	0.45
1:D:155:PHE:CE1	1:D:618:VAL:HG12	2.52	0.45
1:D:347:ILE:HG22	1:D:441:HIS:CE1	2.50	0.45
1:A:748:SER:O	1:A:749:ALA:HB2	2.17	0.45
1:C:535:ALA:HB1	1:C:536:PRO:HD2	1.98	0.45
1:B:268:ILE:HD11	1:B:270:ARG:NH2	2.32	0.45
1:B:589:ALA:HB3	1:B:746:VAL:HG21	1.99	0.45
1:C:531:LYS:O	1:C:532:SER:CB	2.65	0.45
1:D:1110:LEU:HB3	1:D:1156:LEU:HG	1.98	0.45
1:B:919:LEU:HD23	1:B:919:LEU:C	2.42	0.45
1:C:29:PRO:HA	1:C:53:TYR:HB2	1.98	0.45
1:A:270:ARG:HD3	1:A:309:PHE:CG	2.53	0.45
1:A:826:VAL:HG23	1:A:826:VAL:O	2.16	0.45
1:B:584:HIS:CE1	1:B:754:VAL:HG22	2.52	0.45
1:B:870:PHE:O	1:B:900:ILE:HG23	2.17	0.45
1:B:962:THR:O	1:B:963:GLN:C	2.59	0.45
1:D:961:ASN:O	1:D:965:LEU:CB	2.65	0.45
1:D:1109:LEU:HA	1:D:1112:ILE:HD12	1.98	0.45
1:C:599:ALA:HB3	1:C:740:ILE:HG22	1.99	0.44
1:A:423:VAL:HG22	1:A:424:ASN:H	1.81	0.44
1:A:1200:GLN:O	1:A:1204:ALA:HB2	2.17	0.44
1:B:939:VAL:HG12	1:B:1332:ILE:HG22	2.00	0.44
1:C:384:ILE:HD12	1:C:405:VAL:HG21	1.99	0.44
1:C:535:ALA:CB	1:C:536:PRO:CD	2.95	0.44
1:D:231:VAL:HB	1:D:335:LEU:CB	2.47	0.44
1:D:544:ALA:HB3	1:D:552:ILE:HG13	1.99	0.44
1:A:1225:SER:O	1:A:1229:THR:HG23	2.18	0.44
1:D:143:THR:HG22	1:D:193:PRO:HA	1.99	0.44
1:C:1201:ALA:HB3	1:C:1202:PRO:CD	2.47	0.44
1:D:1106:THR:HG21	1:D:1128:LEU:CD1	2.47	0.44
1:D:281:GLU:CB	1:D:284:GLN:HB3	2.48	0.44
1:A:254:TYR:CE2	1:A:255:THR:HG22	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1041:LEU:O	1:C:1045:VAL:HG23	2.18	0.44
3:R:1:NAG:H62	3:R:2:NAG:C7	2.47	0.44
1:A:555:SER:HB2	1:A:673:MET:HE1	1.99	0.44
1:C:143:THR:HG22	1:C:193:PRO:HA	2.00	0.44
1:D:269:CYS:HA	1:D:287:CYS:HB3	2.00	0.44
1:D:824:VAL:HG23	1:D:875:GLU:O	2.17	0.44
1:D:826:VAL:HG23	1:D:826:VAL:O	2.17	0.44
1:D:958:ALA:HB2	1:D:989:TYR:OH	2.17	0.44
1:A:1264:TYR:CE2	1:A:1268:THR:HG21	2.53	0.43
1:C:61:SER:HB2	1:C:74:PHE:CE1	2.53	0.43
1:C:919:LEU:C	1:C:919:LEU:HD23	2.42	0.43
1:C:1211:TYR:CZ	1:C:1256:VAL:HG11	2.53	0.43
1:B:658:VAL:HG12	1:C:656:THR:HG21	2.00	0.43
1:A:147:ARG:HB2	1:A:187:LEU:HD11	2.00	0.43
1:A:384:ILE:HD12	1:A:405:VAL:HG21	2.00	0.43
1:C:1106:THR:HG21	1:C:1128:LEU:HD21	2.00	0.43
1:D:167:ILE:O	1:D:175:ILE:HG22	2.18	0.43
1:C:543:TYR:HB3	1:C:666:MET:HE1	2.00	0.43
1:D:52:SER:HB3	1:D:545:VAL:HG21	2.00	0.43
1:B:650:ILE:HG23	1:B:651:ASN:N	2.33	0.43
1:A:599:ALA:HB3	1:A:740:ILE:HG22	2.01	0.43
1:A:746:VAL:HA	1:A:751:VAL:HB	2.01	0.43
1:C:1264:TYR:CE2	1:C:1268:THR:HG21	2.53	0.43
1:A:1211:TYR:CZ	1:A:1256:VAL:HG11	2.54	0.43
1:D:599:ALA:HB3	1:D:740:ILE:HG22	2.00	0.43
1:A:143:THR:HG22	1:A:193:PRO:HA	2.00	0.43
1:A:822:ILE:HG22	1:A:889:SER:CB	2.49	0.43
1:A:1106:THR:HG21	1:A:1128:LEU:CD1	2.46	0.43
1:A:1399:LEU:CB	1:A:1408:THR:HG21	2.46	0.43
1:B:34:LEU:HB3	1:B:675:LEU:HD13	2.00	0.43
1:B:119:THR:O	1:B:676:LYS:NZ	2.51	0.43
1:B:1225:SER:O	1:B:1229:THR:HG23	2.18	0.43
1:C:371:LEU:HD23	1:C:372:VAL:N	2.33	0.43
1:C:544:ALA:HB3	1:C:552:ILE:HG13	2.01	0.43
1:C:758:VAL:HG13	1:C:761:THR:HG22	1.99	0.43
1:C:826:VAL:O	1:C:826:VAL:HG23	2.18	0.43
1:D:1211:TYR:CZ	1:D:1256:VAL:HG11	2.54	0.43
1:A:269:CYS:O	1:A:318:MET:HB2	2.19	0.43
1:A:570:LEU:HD21	1:A:585:LEU:HD21	1.99	0.43
1:A:1095:VAL:HG23	1:A:1100:THR:HG21	2.01	0.43
1:B:338:ARG:HD3	1:B:340:SER:HB2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:826:VAL:HG23	1:B:826:VAL:O	2.17	0.43
1:D:553:GLY:HA3	1:D:666:MET:HE1	2.00	0.43
1:D:966:LEU:HD13	1:D:1007:TYR:HD2	1.84	0.43
1:D:1264:TYR:CE2	1:D:1268:THR:HG21	2.53	0.43
1:B:1264:TYR:CE2	1:B:1268:THR:HG21	2.54	0.43
1:D:61:SER:HB2	1:D:74:PHE:CE1	2.54	0.43
1:D:480:TYR:CE2	1:D:513:LEU:HD21	2.53	0.43
1:D:965:LEU:O	1:D:966:LEU:O	2.37	0.43
1:B:1185:ARG:HB3	1:B:1186:PRO:CD	2.49	0.42
1:A:948:VAL:HG12	1:A:1326:THR:HG23	2.01	0.42
1:B:61:SER:HB2	1:B:74:PHE:CE1	2.54	0.42
1:A:650:ILE:O	1:A:655:TYR:CD2	2.72	0.42
1:C:167:ILE:O	1:C:175:ILE:HG22	2.19	0.42
1:B:349:LYS:C	1:B:350:LEU:HD23	2.44	0.42
1:B:882:LEU:HB3	1:B:886:GLU:O	2.20	0.42
1:A:270:ARG:CZ	1:A:318:MET:HE2	2.49	0.42
1:A:482:LEU:HD22	1:A:482:LEU:N	2.34	0.42
1:A:919:LEU:C	1:A:919:LEU:HD23	2.44	0.42
1:B:138:TYR:CZ	1:B:144:VAL:HG23	2.55	0.42
1:B:143:THR:HG22	1:B:193:PRO:HA	2.01	0.42
1:B:364:PRO:HB3	1:B:410:ASN:HA	2.01	0.42
1:D:919:LEU:HD23	1:D:919:LEU:C	2.44	0.42
1:D:555:SER:HB2	1:D:673:MET:HE1	2.02	0.42
1:D:944:ALA:HA	1:D:1329:LYS:O	2.20	0.42
1:C:502:LYS:CG	1:C:535:ALA:HB2	2.49	0.42
1:D:1323:TYR:CE2	1:D:1325:GLN:HB2	2.54	0.42
1:A:566:ASN:OD1	1:A:590:ALA:HB2	2.20	0.42
1:C:948:VAL:HG12	1:C:1326:THR:HG23	2.01	0.42
1:D:948:VAL:HG12	1:D:1326:THR:HG23	2.02	0.42
1:B:352:PHE:CD1	1:B:355:VAL:HG11	2.54	0.42
1:D:473:THR:HG22	1:D:529:PRO:HB3	2.02	0.42
1:A:535:ALA:CB	1:A:536:PRO:CD	2.98	0.42
1:A:61:SER:HB2	1:A:74:PHE:CE1	2.54	0.41
1:B:167:ILE:O	1:B:175:ILE:HG22	2.19	0.41
1:B:1018:TYR:HB3	1:B:1029:GLY:HA2	2.01	0.41
1:C:286:PHE:CD2	1:C:308:VAL:O	2.73	0.41
1:A:77:LEU:HD22	1:A:87:VAL:CG1	2.37	0.41
1:B:329:GLU:HA	1:B:811:LYS:HE2	2.02	0.41
1:C:1308:LEU:HB3	1:C:1309:PRO:HD3	2.02	0.41
1:D:129:VAL:O	1:D:621:LEU:HD21	2.20	0.41
1:A:165:VAL:HB	1:A:207:VAL:HG12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1041:LEU:O	1:B:1045:VAL:HG23	2.21	0.41
1:B:1191:ALA:HB3	1:B:1192:PRO:CD	2.51	0.41
1:A:235:VAL:CG2	1:A:320:LEU:HD22	2.51	0.41
1:A:393:TYR:CG	1:A:409:ILE:HG22	2.55	0.41
1:D:29:PRO:HD3	4:S:1:NAG:HN2	1.84	0.41
1:A:1201:ALA:HB3	1:A:1202:PRO:HD3	2.02	0.41
1:B:473:THR:HG22	1:B:529:PRO:HB3	2.03	0.41
1:C:338:ARG:C	1:C:340:SER:H	2.28	0.41
1:A:387:ARG:HD3	1:A:394:TYR:CE1	2.56	0.41
1:B:350:LEU:HD23	1:B:350:LEU:N	2.36	0.41
1:B:1211:TYR:CZ	1:B:1256:VAL:HG11	2.56	0.41
1:B:135:LYS:CE	1:B:604:VAL:HG11	2.51	0.41
1:B:666:MET:CG	1:B:683:ILE:HG23	2.51	0.41
1:C:958:ALA:HB1	1:C:995:GLN:OE1	2.21	0.41
1:D:137:ILE:CD1	1:D:607:MET:HG2	2.51	0.41
1:D:384:ILE:HD12	1:D:405:VAL:HG21	1.99	0.41
1:D:535:ALA:CB	1:D:536:PRO:CD	2.98	0.41
1:D:954:ILE:HD12	1:D:1269:PHE:CE2	2.56	0.41
1:C:137:ILE:CD1	1:C:607:MET:HG2	2.51	0.41
1:C:555:SER:HB2	1:C:673:MET:HE1	2.02	0.41
1:A:679:THR:HG21	1:A:683:ILE:HD13	2.03	0.40
1:B:418:SER:HA	1:B:447:THR:HG22	2.03	0.40
1:A:239:ILE:HD12	1:A:240:THR:N	2.37	0.40
1:A:1379:ALA:HA	1:A:1451:ASP:HA	2.03	0.40
1:B:578:LEU:O	1:B:580:ALA:N	2.54	0.40
1:B:948:VAL:HG12	1:B:1326:THR:HG23	2.02	0.40
1:D:903:LEU:HD23	1:D:903:LEU:N	2.36	0.40
1:C:275:ALA:HB3	1:D:436:TRP:HE1	1.85	0.40
1:C:318:MET:SD	1:C:341:SER:O	2.80	0.40
1:D:393:TYR:CG	1:D:409:ILE:HG22	2.57	0.40
1:A:655:TYR:H	1:D:661:THR:HG23	1.87	0.40
1:B:551:VAL:CG1	1:B:666:MET:HE2	2.50	0.40
1:C:470:CYS:HA	1:C:530:VAL:HG12	2.01	0.40
1:C:993:THR:O	1:C:994:GLN:HB2	2.21	0.40
1:A:473:THR:HG22	1:A:529:PRO:HB3	2.03	0.40
1:B:1333:LEU:N	1:B:1334:PRO:CD	2.84	0.40
1:C:1095:VAL:O	1:C:1095:VAL:HG12	2.22	0.40
1:C:1128:LEU:N	1:C:1128:LEU:HD13	2.37	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	1412/1474 (96%)	1184 (84%)	168 (12%)	60 (4%)	2	18
1	B	1269/1474 (86%)	1064 (84%)	146 (12%)	59 (5%)	2	17
1	C	1270/1474 (86%)	1082 (85%)	141 (11%)	47 (4%)	2	20
1	D	1267/1474 (86%)	1068 (84%)	145 (11%)	54 (4%)	2	18
All	All	5218/5896 (88%)	4398 (84%)	600 (12%)	220 (4%)	2	18

All (220) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	125	GLU
1	A	282	ASP
1	A	286	PHE
1	A	374	GLY
1	A	535	ALA
1	A	578	LEU
1	A	749	ALA
1	A	953	ASP
1	A	966	LEU
1	A	1079	CYS
1	A	1144	VAL
1	A	1348	LEU
1	A	1387	SER
1	B	328	GLU
1	B	340	SER
1	B	413	ASN
1	B	424	ASN
1	B	535	ALA
1	B	736	PRO
1	B	749	ALA
1	B	959	MET
1	B	966	LEU

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Mol	Chain	Res	Type
1	B	1079	CYS
1	B	1088	ASN
1	B	1187	GLN
1	C	311	LEU
1	C	424	ASN
1	C	578	LEU
1	C	730	THR
1	C	736	PRO
1	C	749	ALA
1	C	895	ARG
1	C	1032	TYR
1	C	1201	ALA
1	D	286	PHE
1	D	435	GLN
1	D	532	SER
1	D	535	ALA
1	D	582	HIS
1	D	736	PRO
1	D	749	ALA
1	D	965	LEU
1	D	966	LEU
1	D	1079	CYS
1	D	1193	VAL
1	D	1294	ASN
1	A	213	GLY
1	A	314	LYS
1	A	338	ARG
1	A	651	ASN
1	A	687	LYS
1	A	748	SER
1	A	891	PRO
1	A	1038	ASN
1	A	1140	HIS
1	A	1193	VAL
1	A	1249	SER
1	A	1273	GLY
1	A	1334	PRO
1	A	1357	ALA
1	B	56	GLU
1	B	213	GLY
1	B	310	GLN
1	B	313	ARG

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Mol	Chain	Res	Type
1	B	341	SER
1	B	414	VAL
1	B	438	SER
1	B	439	GLU
1	B	491	LYS
1	B	532	SER
1	B	582	HIS
1	B	638	ASP
1	B	639	ASN
1	B	688	MET
1	B	883	CYS
1	B	961	ASN
1	B	962	THR
1	B	1031	ARG
1	B	1249	SER
1	B	1285	THR
1	C	180	SER
1	C	213	GLY
1	C	374	GLY
1	C	516	LYS
1	C	532	SER
1	C	582	HIS
1	C	892	GLU
1	C	953	ASP
1	C	958	ALA
1	C	966	LEU
1	C	1079	CYS
1	C	1096	GLU
1	C	1249	SER
1	C	1285	THR
1	D	180	SER
1	D	213	GLY
1	D	338	ARG
1	D	390	GLU
1	D	579	PRO
1	D	842	GLU
1	D	955	LEU
1	D	956	GLY
1	D	958	ALA
1	D	1031	ARG
1	D	1144	VAL
1	D	1249	SER

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Mol	Chain	Res	Type
1	D	1273	GLY
1	D	1285	THR
1	A	180	SER
1	A	285	ALA
1	A	423	VAL
1	A	454	PRO
1	A	581	SER
1	A	641	ASP
1	A	783	THR
1	A	842	GLU
1	A	888	PRO
1	A	893	HIS
1	A	1298	LEU
1	B	338	ARG
1	B	454	PRO
1	B	581	SER
1	B	640	GLU
1	B	730	THR
1	B	783	THR
1	B	1197	TYR
1	C	55	ASN
1	C	454	PRO
1	C	783	THR
1	C	1294	ASN
1	D	274	ASP
1	D	414	VAL
1	D	424	ASN
1	D	454	PRO
1	D	637	GLN
1	D	641	ASP
1	D	651	ASN
1	D	655	TYR
1	D	689	CYS
1	D	783	THR
1	A	254	TYR
1	A	341	SER
1	A	403	GLY
1	A	1031	ARG
1	A	1272	THR
1	A	1285	THR
1	A	1297	ARG
1	A	1307	GLU

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Mol	Chain	Res	Type
1	A	1352	CYS
1	B	180	SER
1	B	254	TYR
1	B	429	SER
1	B	487	LEU
1	B	580	ALA
1	B	958	ALA
1	B	1336	LYS
1	C	279	HIS
1	C	390	GLU
1	C	403	GLY
1	C	535	ALA
1	C	640	GLU
1	C	994	GLN
1	C	1141	GLY
1	D	281	GLU
1	D	687	LYS
1	D	759	PRO
1	D	885	THR
1	D	1032	TYR
1	D	1053	ARG
1	D	1097	ASP
1	D	1334	PRO
1	A	607	MET
1	A	736	PRO
1	A	1034	ARG
1	A	1142	SER
1	A	1275	ALA
1	A	1335	GLU
1	B	53	TYR
1	B	520	MET
1	B	607	MET
1	B	686	PRO
1	B	759	PRO
1	B	994	GLN
1	B	1309	PRO
1	C	254	TYR
1	C	415	MET
1	C	607	MET
1	C	649	TYR
1	C	735	PHE
1	C	1309	PRO

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Mol	Chain	Res	Type
1	D	403	GLY
1	D	607	MET
1	D	1198	GLU
1	A	414	VAL
1	A	759	PRO
1	A	958	ALA
1	B	579	PRO
1	B	1305	LEU
1	C	487	LEU
1	D	254	TYR
1	D	277	ASP
1	D	737	GLU
1	D	1197	TYR
1	A	1306	PRO
1	B	1084	GLY
1	C	1189	PRO
1	A	1388	GLY
1	B	1189	PRO
1	C	1091	ILE
1	C	1095	VAL
1	D	1113	PRO
1	A	1113	PRO
1	A	1449	VAL
1	B	1113	PRO
1	C	956	GLY
1	C	1333	LEU
1	D	280	GLY
1	D	347	ILE
1	B	268	ILE
1	C	759	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	1241/1290 (96%)	1066 (86%)	175 (14%)	3 16

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	1110/1290 (86%)	957 (86%)	153 (14%)	3	16
1	C	1112/1290 (86%)	959 (86%)	153 (14%)	3	16
1	D	1108/1290 (86%)	953 (86%)	155 (14%)	3	16
All	All	4571/5160 (89%)	3935 (86%)	636 (14%)	3	16

All (636) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	THR
1	A	51	LEU
1	A	54	LEU
1	A	58	VAL
1	A	63	SER
1	A	65	GLU
1	A	76	ASP
1	A	82	ASP
1	A	83	VAL
1	A	114	PHE
1	A	124	ASN
1	A	125	GLU
1	A	128	LEU
1	A	131	VAL
1	A	133	THR
1	A	149	VAL
1	A	151	MET
1	A	158	LEU
1	A	160	GLU
1	A	161	LEU
1	A	165	VAL
1	A	181	PHE
1	A	188	LYS
1	A	194	LEU
1	A	220	THR
1	A	226	LEU
1	A	233	VAL
1	A	246	MET
1	A	253	LEU
1	A	260	VAL
1	A	278	CYS
1	A	288	GLU
1	A	293	GLN

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Mol	Chain	Res	Type
1	A	294	LEU
1	A	295	ASN
1	A	314	LYS
1	A	315	GLU
1	A	317	GLU
1	A	326	ILE
1	A	335	LEU
1	A	341	SER
1	A	350	LEU
1	A	353	VAL
1	A	356	ASP
1	A	358	HIS
1	A	365	PHE
1	A	373	ASP
1	A	384	ILE
1	A	413	ASN
1	A	428	ARG
1	A	431	CYS
1	A	435	GLN
1	A	436	TRP
1	A	458	PHE
1	A	461	LEU
1	A	465	SER
1	A	476	VAL
1	A	499	ILE
1	A	500	MET
1	A	506	VAL
1	A	510	THR
1	A	514	LEU
1	A	519	ASP
1	A	520	MET
1	A	523	HIS
1	A	524	PHE
1	A	534	ILE
1	A	541	LEU
1	A	555	SER
1	A	557	LYS
1	A	568	VAL
1	A	569	ASP
1	A	572	PHE
1	A	578	LEU
1	A	593	SER

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Mol	Chain	Res	Type
1	A	594	VAL
1	A	610	ASP
1	A	637	GLN
1	A	650	ILE
1	A	673	MET
1	A	675	LEU
1	A	683	ILE
1	A	691	GLN
1	A	731	VAL
1	A	734	TYR
1	A	760	ASP
1	A	763	THR
1	A	778	LEU
1	A	782	SER
1	A	785	SER
1	A	795	GLU
1	A	796	LEU
1	A	797	THR
1	A	803	ILE
1	A	835	LEU
1	A	843	GLN
1	A	846	HIS
1	A	847	CYS
1	A	848	ILE
1	A	857	SER
1	A	865	LEU
1	A	868	VAL
1	A	871	THR
1	A	877	LEU
1	A	878	GLU
1	A	879	SER
1	A	882	LEU
1	A	883	CYS
1	A	897	ASP
1	A	903	LEU
1	A	904	LEU
1	A	905	VAL
1	A	913	GLU
1	A	921	CYS
1	A	926	GLU
1	A	935	LEU
1	A	942	GLU

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Mol	Chain	Res	Type
1	A	951	LEU
1	A	953	ASP
1	A	955	LEU
1	A	960	GLN
1	A	961	ASN
1	A	995	GLN
1	A	997	THR
1	A	1008	LEU
1	A	1017	ASN
1	A	1024	SER
1	A	1035	ASN
1	A	1036	GLN
1	A	1039	THR
1	A	1064	THR
1	A	1079	CYS
1	A	1082	SER
1	A	1086	LEU
1	A	1091	ILE
1	A	1096	GLU
1	A	1107	ILE
1	A	1109	LEU
1	A	1121	VAL
1	A	1142	SER
1	A	1143	HIS
1	A	1150	LEU
1	A	1170	LEU
1	A	1172	GLU
1	A	1179	ASN
1	A	1181	VAL
1	A	1187	GLN
1	A	1197	TYR
1	A	1198	GLU
1	A	1207	GLU
1	A	1217	LEU
1	A	1224	THR
1	A	1233	ASN
1	A	1242	GLN
1	A	1255	VAL
1	A	1263	LYS
1	A	1280	ILE
1	A	1289	LYS
1	A	1307	GLU

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Mol	Chain	Res	Type
1	A	1314	MET
1	A	1317	THR
1	A	1319	GLU
1	A	1325	GLN
1	A	1332	ILE
1	A	1336	LYS
1	A	1354	GLU
1	A	1389	PHE
1	A	1392	LEU
1	A	1425	GLN
1	A	1426	THR
1	A	1427	LEU
1	A	1434	LEU
1	A	1437	VAL
1	A	1441	ASP
1	A	1442	LEU
1	B	30	GLN
1	B	31	TYR
1	B	41	THR
1	B	42	GLU
1	B	51	LEU
1	B	52	SER
1	B	58	VAL
1	B	63	SER
1	B	65	GLU
1	B	76	ASP
1	B	77	LEU
1	B	83	VAL
1	B	84	LEU
1	B	114	PHE
1	B	118	THR
1	B	124	ASN
1	B	128	LEU
1	B	129	VAL
1	B	131	VAL
1	B	133	THR
1	B	142	GLN
1	B	149	VAL
1	B	161	LEU
1	B	165	VAL
1	B	181	PHE
1	B	187	LEU

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Mol	Chain	Res	Type
1	B	194	LEU
1	B	204	LYS
1	B	206	VAL
1	B	220	THR
1	B	224	PHE
1	B	233	VAL
1	B	238	ILE
1	B	246	MET
1	B	253	LEU
1	B	255	THR
1	B	260	VAL
1	B	270	ARG
1	B	273	SER
1	B	276	SER
1	B	289	LYS
1	B	294	LEU
1	B	295	ASN
1	B	305	LYS
1	B	311	LEU
1	B	318	MET
1	B	327	GLN
1	B	334	GLU
1	B	335	LEU
1	B	350	LEU
1	B	353	VAL
1	B	356	ASP
1	B	361	GLN
1	B	365	PHE
1	B	384	ILE
1	B	396	ASN
1	B	405	VAL
1	B	414	VAL
1	B	415	MET
1	B	421	VAL
1	B	431	CYS
1	B	434	TYR
1	B	450	LEU
1	B	461	LEU
1	B	465	SER
1	B	476	VAL
1	B	480	TYR
1	B	481	ILE

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Mol	Chain	Res	Type
1	B	486	THR
1	B	487	LEU
1	B	491	LYS
1	B	506	VAL
1	B	523	HIS
1	B	524	PHE
1	B	528	ILE
1	B	545	VAL
1	B	546	LEU
1	B	548	THR
1	B	555	SER
1	B	568	VAL
1	B	569	ASP
1	B	572	PHE
1	B	575	SER
1	B	578	LEU
1	B	594	VAL
1	B	610	ASP
1	B	636	ASP
1	B	637	GLN
1	B	650	ILE
1	B	651	ASN
1	B	673	MET
1	B	687	LYS
1	B	731	VAL
1	B	733	LYS
1	B	737	GLU
1	B	763	THR
1	B	778	LEU
1	B	782	SER
1	B	785	SER
1	B	796	LEU
1	B	797	THR
1	B	822	ILE
1	B	835	LEU
1	B	842	GLU
1	B	856	VAL
1	B	857	SER
1	B	865	LEU
1	B	871	THR
1	B	882	LEU
1	B	883	CYS

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Mol	Chain	Res	Type
1	B	890	VAL
1	B	897	ASP
1	B	903	LEU
1	B	905	VAL
1	B	908	GLU
1	B	913	GLU
1	B	921	CYS
1	B	926	GLU
1	B	935	LEU
1	B	940	VAL
1	B	955	LEU
1	B	965	LEU
1	B	966	LEU
1	B	993	THR
1	B	997	THR
1	B	1008	LEU
1	B	1017	ASN
1	B	1030	GLU
1	B	1056	ILE
1	B	1058	ILE
1	B	1064	THR
1	B	1079	CYS
1	B	1085	SER
1	B	1086	LEU
1	B	1087	LEU
1	B	1107	ILE
1	B	1121	VAL
1	B	1137	GLU
1	B	1143	HIS
1	B	1177	LYS
1	B	1179	ASN
1	B	1180	SER
1	B	1209	THR
1	B	1224	THR
1	B	1242	GLN
1	B	1255	VAL
1	B	1263	LYS
1	B	1279	THR
1	B	1298	LEU
1	B	1305	LEU
1	B	1317	THR
1	B	1331	ASN

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Mol	Chain	Res	Type
1	B	1332	ILE
1	C	31	TYR
1	C	54	LEU
1	C	58	VAL
1	C	63	SER
1	C	65	GLU
1	C	76	ASP
1	C	80	GLU
1	C	111	THR
1	C	124	ASN
1	C	128	LEU
1	C	131	VAL
1	C	133	THR
1	C	149	VAL
1	C	187	LEU
1	C	194	LEU
1	C	204	LYS
1	C	220	THR
1	C	225	VAL
1	C	231	VAL
1	C	233	VAL
1	C	246	MET
1	C	253	LEU
1	C	255	THR
1	C	260	VAL
1	C	268	ILE
1	C	273	SER
1	C	276	SER
1	C	277	ASP
1	C	279	HIS
1	C	281	GLU
1	C	289	LYS
1	C	294	LEU
1	C	295	ASN
1	C	311	LEU
1	C	313	ARG
1	C	314	LYS
1	C	315	GLU
1	C	326	ILE
1	C	341	SER
1	C	343	ILE
1	C	348	THR

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Mol	Chain	Res	Type
1	C	350	LEU
1	C	353	VAL
1	C	356	ASP
1	C	361	GLN
1	C	365	PHE
1	C	373	ASP
1	C	375	LYS
1	C	384	ILE
1	C	417	THR
1	C	419	LEU
1	C	427	ASP
1	C	440	GLU
1	C	461	LEU
1	C	465	SER
1	C	476	VAL
1	C	481	ILE
1	C	486	THR
1	C	500	MET
1	C	510	THR
1	C	524	PHE
1	C	541	LEU
1	C	555	SER
1	C	568	VAL
1	C	569	ASP
1	C	575	SER
1	C	576	GLN
1	C	577	SER
1	C	578	LEU
1	C	593	SER
1	C	594	VAL
1	C	610	ASP
1	C	634	LEU
1	C	640	GLU
1	C	654	THR
1	C	673	MET
1	C	676	LYS
1	C	683	ILE
1	C	691	GLN
1	C	730	THR
1	C	731	VAL
1	C	737	GLU
1	C	763	THR

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Mol	Chain	Res	Type
1	C	778	LEU
1	C	782	SER
1	C	785	SER
1	C	789	PHE
1	C	796	LEU
1	C	797	THR
1	C	822	ILE
1	C	823	ARG
1	C	835	LEU
1	C	842	GLU
1	C	848	ILE
1	C	855	THR
1	C	856	VAL
1	C	857	SER
1	C	865	LEU
1	C	871	THR
1	C	875	GLU
1	C	881	GLU
1	C	882	LEU
1	C	883	CYS
1	C	889	SER
1	C	897	ASP
1	C	903	LEU
1	C	904	LEU
1	C	905	VAL
1	C	913	GLU
1	C	921	CYS
1	C	926	GLU
1	C	935	LEU
1	C	938	ASN
1	C	942	GLU
1	C	965	LEU
1	C	993	THR
1	C	997	THR
1	C	1008	LEU
1	C	1017	ASN
1	C	1019	LYS
1	C	1024	SER
1	C	1030	GLU
1	C	1039	THR
1	C	1041	LEU
1	C	1056	ILE

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Mol	Chain	Res	Type
1	C	1058	ILE
1	C	1064	THR
1	C	1074	GLN
1	C	1079	CYS
1	C	1086	LEU
1	C	1107	ILE
1	C	1121	VAL
1	C	1128	LEU
1	C	1142	SER
1	C	1143	HIS
1	C	1146	THR
1	C	1170	LEU
1	C	1172	GLU
1	C	1179	ASN
1	C	1190	LYS
1	C	1206	VAL
1	C	1210	SER
1	C	1217	LEU
1	C	1224	THR
1	C	1242	GLN
1	C	1252	GLN
1	C	1255	VAL
1	C	1263	LYS
1	C	1272	THR
1	C	1280	ILE
1	C	1291	GLN
1	C	1298	LEU
1	C	1317	THR
1	D	31	TYR
1	D	51	LEU
1	D	52	SER
1	D	54	LEU
1	D	63	SER
1	D	65	GLU
1	D	76	ASP
1	D	82	ASP
1	D	83	VAL
1	D	112	GLN
1	D	124	ASN
1	D	128	LEU
1	D	131	VAL
1	D	133	THR

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Mol	Chain	Res	Type
1	D	142	GLN
1	D	149	VAL
1	D	156	HIS
1	D	187	LEU
1	D	194	LEU
1	D	204	LYS
1	D	220	THR
1	D	233	VAL
1	D	246	MET
1	D	253	LEU
1	D	255	THR
1	D	260	VAL
1	D	277	ASP
1	D	294	LEU
1	D	295	ASN
1	D	307	LYS
1	D	316	TYR
1	D	319	LYS
1	D	326	ILE
1	D	335	LEU
1	D	339	GLN
1	D	341	SER
1	D	343	ILE
1	D	345	ARG
1	D	346	THR
1	D	347	ILE
1	D	350	LEU
1	D	353	VAL
1	D	356	ASP
1	D	361	GLN
1	D	365	PHE
1	D	371	LEU
1	D	372	VAL
1	D	384	ILE
1	D	413	ASN
1	D	432	TYR
1	D	438	SER
1	D	458	PHE
1	D	461	LEU
1	D	465	SER
1	D	476	VAL
1	D	486	THR

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Mol	Chain	Res	Type
1	D	490	LEU
1	D	500	MET
1	D	510	THR
1	D	520	MET
1	D	524	PHE
1	D	533	ASP
1	D	541	LEU
1	D	545	VAL
1	D	555	SER
1	D	569	ASP
1	D	571	SER
1	D	576	GLN
1	D	594	VAL
1	D	610	ASP
1	D	634	LEU
1	D	637	GLN
1	D	644	ASN
1	D	649	TYR
1	D	656	THR
1	D	661	THR
1	D	673	MET
1	D	675	LEU
1	D	676	LYS
1	D	683	ILE
1	D	687	LYS
1	D	688	MET
1	D	731	VAL
1	D	732	ARG
1	D	733	LYS
1	D	734	TYR
1	D	737	GLU
1	D	763	THR
1	D	774	GLU
1	D	778	LEU
1	D	782	SER
1	D	785	SER
1	D	786	LEU
1	D	796	LEU
1	D	797	THR
1	D	815	LEU
1	D	822	ILE
1	D	823	ARG

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Mol	Chain	Res	Type
1	D	835	LEU
1	D	843	GLN
1	D	846	HIS
1	D	848	ILE
1	D	853	ARG
1	D	857	SER
1	D	865	LEU
1	D	871	THR
1	D	877	LEU
1	D	879	SER
1	D	886	GLU
1	D	887	VAL
1	D	890	VAL
1	D	897	ASP
1	D	913	GLU
1	D	921	CYS
1	D	926	GLU
1	D	935	LEU
1	D	965	LEU
1	D	993	THR
1	D	997	THR
1	D	1008	LEU
1	D	1017	ASN
1	D	1024	SER
1	D	1030	GLU
1	D	1036	GLN
1	D	1039	THR
1	D	1041	LEU
1	D	1056	ILE
1	D	1064	THR
1	D	1079	CYS
1	D	1082	SER
1	D	1086	LEU
1	D	1091	ILE
1	D	1092	LYS
1	D	1107	ILE
1	D	1121	VAL
1	D	1145	TYR
1	D	1146	THR
1	D	1170	LEU
1	D	1172	GLU
1	D	1179	ASN

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Mol	Chain	Res	Type
1	D	1185	ARG
1	D	1187	GLN
1	D	1188	LYS
1	D	1207	GLU
1	D	1217	LEU
1	D	1224	THR
1	D	1242	GLN
1	D	1255	VAL
1	D	1263	LYS
1	D	1272	THR
1	D	1280	ILE
1	D	1290	PHE
1	D	1305	LEU
1	D	1308	LEU
1	D	1331	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (79) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	85	HIS
1	A	97	ASN
1	A	112	GLN
1	A	208	GLN
1	A	279	HIS
1	A	284	GLN
1	A	321	HIS
1	A	361	GLN
1	A	424	ASN
1	A	474	GLN
1	A	511	HIS
1	A	562	ASN
1	A	584	HIS
1	A	637	GLN
1	A	651	ASN
1	A	693	GLN
1	A	747	ASN
1	A	790	GLN
1	A	816	ASN
1	A	1013	GLN
1	A	1241	GLN
1	A	1259	HIS
1	A	1295	ASN

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Mol	Chain	Res	Type
1	A	1413	ASN
1	B	40	HIS
1	B	97	ASN
1	B	295	ASN
1	B	321	HIS
1	B	358	HIS
1	B	361	GLN
1	B	474	GLN
1	B	479	HIS
1	B	511	HIS
1	B	584	HIS
1	B	592	GLN
1	B	602	GLN
1	B	843	GLN
1	B	967	GLN
1	B	1036	GLN
1	B	1136	GLN
1	B	1195	HIS
1	B	1233	ASN
1	B	1241	GLN
1	C	97	ASN
1	C	112	GLN
1	C	208	GLN
1	C	321	HIS
1	C	339	GLN
1	C	389	ASN
1	C	474	GLN
1	C	511	HIS
1	C	517	GLN
1	C	592	GLN
1	C	639	ASN
1	C	843	GLN
1	C	967	GLN
1	C	1036	GLN
1	C	1325	GLN
1	D	97	ASN
1	D	112	GLN
1	D	208	GLN
1	D	321	HIS
1	D	389	ASN
1	D	435	GLN
1	D	474	GLN

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Mol	Chain	Res	Type
1	D	511	HIS
1	D	584	HIS
1	D	651	ASN
1	D	747	ASN
1	D	854	GLN
1	D	967	GLN
1	D	976	ASN
1	D	1015	GLN
1	D	1035	ASN
1	D	1036	GLN
1	D	1088	ASN
1	D	1136	GLN
1	D	1241	GLN
1	D	1295	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 ⓘ

50 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	NAG	E	1	2,1	14,14,15	0.43	0	17,19,21	1.27	3 (17%)
2	NAG	E	2	2	14,14,15	0.48	0	17,19,21	1.55	2 (11%)
2	BMA	E	3	2	11,11,12	0.51	0	15,15,17	1.12	1 (6%)
2	MAN	E	4	2	11,11,12	0.57	0	15,15,17	1.00	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	F	1	1,3	14,14,15	0.47	0	17,19,21	0.98	1 (5%)
3	NAG	F	2	3	14,14,15	0.43	0	17,19,21	0.93	1 (5%)
3	BMA	F	3	3	11,11,12	0.38	0	15,15,17	0.70	0
2	NAG	G	1	2,1	14,14,15	0.40	0	17,19,21	0.85	1 (5%)
2	NAG	G	2	2	14,14,15	0.49	0	17,19,21	1.00	2 (11%)
2	BMA	G	3	2	11,11,12	0.59	0	15,15,17	0.96	1 (6%)
2	MAN	G	4	2	11,11,12	0.69	0	15,15,17	1.47	2 (13%)
4	NAG	H	1	4,1	14,14,15	0.41	0	17,19,21	1.05	1 (5%)
4	NAG	H	2	4	14,14,15	0.39	0	17,19,21	0.58	0
3	NAG	I	1	1,3	14,14,15	0.33	0	17,19,21	0.69	0
3	NAG	I	2	3	14,14,15	0.42	0	17,19,21	0.93	2 (11%)
3	BMA	I	3	3	11,11,12	0.49	0	15,15,17	0.69	1 (6%)
2	NAG	J	1	2,1	14,14,15	0.55	0	17,19,21	1.22	1 (5%)
2	NAG	J	2	2	14,14,15	0.47	0	17,19,21	1.18	2 (11%)
2	BMA	J	3	2	11,11,12	0.47	0	15,15,17	0.70	0
2	MAN	J	4	2	11,11,12	0.53	0	15,15,17	1.06	2 (13%)
4	NAG	K	1	4,1	14,14,15	0.46	0	17,19,21	0.89	1 (5%)
4	NAG	K	2	4	14,14,15	0.43	0	17,19,21	0.65	0
4	NAG	L	1	4,1	14,14,15	0.46	0	17,19,21	1.20	2 (11%)
4	NAG	L	2	4	14,14,15	0.49	0	17,19,21	0.81	1 (5%)
3	NAG	M	1	1,3	14,14,15	0.40	0	17,19,21	0.87	1 (5%)
3	NAG	M	2	3	14,14,15	0.47	0	17,19,21	1.11	2 (11%)
3	BMA	M	3	3	11,11,12	0.38	0	15,15,17	0.54	0
4	NAG	N	1	4,1	14,14,15	0.42	0	17,19,21	1.07	2 (11%)
4	NAG	N	2	4	14,14,15	0.48	0	17,19,21	1.69	3 (17%)
2	NAG	O	1	2,1	14,14,15	0.40	0	17,19,21	0.79	0
2	NAG	O	2	2	14,14,15	0.47	0	17,19,21	1.22	3 (17%)
2	BMA	O	3	2	11,11,12	0.57	0	15,15,17	0.72	0
2	MAN	O	4	2	11,11,12	0.43	0	15,15,17	0.83	1 (6%)
4	NAG	P	1	4,1	14,14,15	0.43	0	17,19,21	0.61	0
4	NAG	P	2	4	14,14,15	0.52	0	17,19,21	1.04	2 (11%)
4	NAG	Q	1	4,1	14,14,15	0.41	0	17,19,21	1.06	2 (11%)
4	NAG	Q	2	4	14,14,15	0.44	0	17,19,21	0.59	0
3	NAG	R	1	1,3	14,14,15	0.30	0	17,19,21	0.72	0
3	NAG	R	2	3	14,14,15	0.48	0	17,19,21	1.58	3 (17%)
3	BMA	R	3	3	11,11,12	0.49	0	15,15,17	0.91	1 (6%)
4	NAG	S	1	4,1	14,14,15	0.42	0	17,19,21	0.82	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	S	2	4	14,14,15	0.44	0	17,19,21	1.21	3 (17%)
4	NAG	T	1	4,1	14,14,15	0.41	0	17,19,21	0.80	0
4	NAG	T	2	4	14,14,15	0.44	0	17,19,21	1.21	3 (17%)
4	NAG	U	1	4,1	14,14,15	0.40	0	17,19,21	1.05	2 (11%)
4	NAG	U	2	4	14,14,15	0.39	0	17,19,21	0.71	0
2	NAG	V	1	2,1	14,14,15	0.42	0	17,19,21	1.44	4 (23%)
2	NAG	V	2	2	14,14,15	0.49	0	17,19,21	1.55	2 (11%)
2	BMA	V	3	2	11,11,12	0.48	0	15,15,17	0.84	0
2	MAN	V	4	2	11,11,12	0.45	0	15,15,17	0.98	1 (6%)

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

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	M	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	M	2	3	-	1/6/23/26	0/1/1/1
3	BMA	M	3	3	-	0/2/19/22	0/1/1/1
4	NAG	N	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	N	2	4	-	2/6/23/26	0/1/1/1
2	NAG	O	1	2,1	-	1/6/23/26	0/1/1/1
2	NAG	O	2	2	-	3/6/23/26	0/1/1/1
2	BMA	O	3	2	-	2/2/19/22	0/1/1/1
2	MAN	O	4	2	-	0/2/19/22	0/1/1/1
4	NAG	P	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	P	2	4	-	0/6/23/26	0/1/1/1
4	NAG	Q	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	Q	2	4	-	1/6/23/26	0/1/1/1
3	NAG	R	1	1,3	-	1/6/23/26	0/1/1/1
3	NAG	R	2	3	-	2/6/23/26	0/1/1/1
3	BMA	R	3	3	-	0/2/19/22	0/1/1/1
4	NAG	S	1	4,1	-	1/6/23/26	0/1/1/1
4	NAG	S	2	4	-	1/6/23/26	0/1/1/1
4	NAG	T	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	T	2	4	-	1/6/23/26	0/1/1/1
4	NAG	U	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	U	2	4	-	2/6/23/26	0/1/1/1
2	NAG	V	1	2,1	-	1/6/23/26	0/1/1/1
2	NAG	V	2	2	-	0/6/23/26	0/1/1/1
2	BMA	V	3	2	-	2/2/19/22	0/1/1/1
2	MAN	V	4	2	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (65) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	N	2	NAG	C1-C2-N2	5.35	118.87	110.43
2	G	4	MAN	C1-O5-C5	4.78	118.59	112.19
2	V	2	NAG	C1-C2-N2	4.43	117.42	110.43
2	E	2	NAG	C1-O5-C5	4.10	117.69	112.19
2	E	2	NAG	C1-C2-N2	4.08	116.86	110.43
2	J	1	NAG	C1-O5-C5	3.77	117.24	112.19
3	R	2	NAG	C1-O5-C5	3.71	117.16	112.19
3	R	2	NAG	C1-C2-N2	3.55	116.02	110.43
4	N	1	NAG	O5-C1-C2	-3.34	106.13	111.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	M	1	NAG	C1-O5-C5	3.21	116.49	112.19
2	V	1	NAG	C1-O5-C5	3.19	116.47	112.19
4	P	2	NAG	C1-O5-C5	3.17	116.44	112.19
3	R	2	NAG	C2-N2-C7	3.15	127.12	122.90
3	M	2	NAG	C2-N2-C7	3.10	127.05	122.90
2	E	1	NAG	C1-O5-C5	3.07	116.29	112.19
3	R	3	BMA	C1-O5-C5	3.03	116.25	112.19
4	H	1	NAG	O5-C1-C2	-3.02	106.62	111.29
4	S	2	NAG	C2-N2-C7	3.00	126.93	122.90
4	T	2	NAG	C1-O5-C5	2.98	116.18	112.19
4	Q	1	NAG	O5-C1-C2	-2.96	106.71	111.29
2	V	1	NAG	C2-N2-C7	2.96	126.86	122.90
4	N	2	NAG	C1-O5-C5	2.95	116.14	112.19
4	L	1	NAG	O5-C1-C2	-2.95	106.73	111.29
2	G	2	NAG	C1-C2-N2	2.91	115.03	110.43
2	G	3	BMA	C1-O5-C5	2.90	116.07	112.19
4	N	2	NAG	C2-N2-C7	2.88	126.76	122.90
4	U	1	NAG	O5-C1-C2	-2.79	106.98	111.29
4	U	1	NAG	C1-O5-C5	2.78	115.91	112.19
4	S	2	NAG	C1-C2-N2	2.78	114.81	110.43
2	J	4	MAN	C1-O5-C5	2.77	115.90	112.19
2	E	3	BMA	C1-O5-C5	2.75	115.87	112.19
4	T	2	NAG	C2-N2-C7	2.74	126.58	122.90
2	O	2	NAG	C1-C2-N2	2.70	114.68	110.43
2	J	2	NAG	O5-C1-C2	2.69	115.46	111.29
2	O	2	NAG	O5-C1-C2	-2.68	107.14	111.29
4	L	1	NAG	C1-O5-C5	2.64	115.72	112.19
2	E	4	MAN	C1-O5-C5	2.63	115.71	112.19
4	S	2	NAG	C1-O5-C5	2.53	115.58	112.19
2	O	2	NAG	C2-N2-C7	2.52	126.28	122.90
4	N	1	NAG	C1-O5-C5	2.48	115.50	112.19
4	K	1	NAG	O4-C4-C3	2.46	116.18	110.38
2	J	4	MAN	C1-C2-C3	2.46	113.23	109.64
2	V	1	NAG	O5-C1-C2	2.44	115.06	111.29
2	V	1	NAG	C1-C2-N2	2.43	114.26	110.43
4	S	1	NAG	C2-N2-C7	2.41	126.13	122.90
2	V	2	NAG	C1-O5-C5	2.39	115.39	112.19
2	E	1	NAG	C3-C4-C5	2.32	114.44	110.23
3	F	1	NAG	C3-C4-C5	2.32	114.44	110.23
2	V	4	MAN	C1-O5-C5	2.29	115.25	112.19
4	Q	1	NAG	C1-O5-C5	2.27	115.22	112.19
2	J	2	NAG	C1-C2-N2	-2.25	106.89	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	1	NAG	O5-C1-C2	-2.21	107.87	111.29
2	G	4	MAN	C1-C2-C3	2.20	112.85	109.64
3	F	2	NAG	O5-C1-C2	-2.18	107.91	111.29
4	P	2	NAG	C1-C2-N2	2.17	113.86	110.43
2	E	1	NAG	C1-C2-N2	2.17	113.85	110.43
3	M	2	NAG	C1-O5-C5	2.16	115.09	112.19
3	I	2	NAG	C1-O5-C5	2.16	115.08	112.19
3	I	3	BMA	C1-O5-C5	2.13	115.04	112.19
2	E	4	MAN	C1-C2-C3	2.09	112.69	109.64
4	L	2	NAG	C2-N2-C7	2.09	125.70	122.90
3	I	2	NAG	O5-C1-C2	-2.05	108.12	111.29
2	G	2	NAG	C1-O5-C5	2.03	114.90	112.19
2	O	4	MAN	C1-O5-C5	2.02	114.90	112.19
4	T	2	NAG	C1-C2-N2	2.02	113.61	110.43

There are no chirality outliers.

All (43) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	O	1	NAG	C1-C2-N2-C7
3	I	1	NAG	C1-C2-N2-C7
3	M	2	NAG	C1-C2-N2-C7
3	R	1	NAG	C1-C2-N2-C7
3	R	2	NAG	C1-C2-N2-C7
4	N	2	NAG	C1-C2-N2-C7
4	S	2	NAG	C1-C2-N2-C7
4	T	2	NAG	C1-C2-N2-C7
2	V	3	BMA	O5-C5-C6-O6
2	O	2	NAG	O5-C5-C6-O6
4	P	1	NAG	O5-C5-C6-O6
4	P	1	NAG	C4-C5-C6-O6
2	O	3	BMA	O5-C5-C6-O6
2	O	3	BMA	C4-C5-C6-O6
2	O	2	NAG	C4-C5-C6-O6
4	H	2	NAG	O5-C5-C6-O6
4	U	2	NAG	O5-C5-C6-O6
3	F	2	NAG	C4-C5-C6-O6
4	T	1	NAG	C4-C5-C6-O6
2	G	3	BMA	C4-C5-C6-O6
2	V	3	BMA	C4-C5-C6-O6
2	G	3	BMA	O5-C5-C6-O6
2	G	4	MAN	O5-C5-C6-O6

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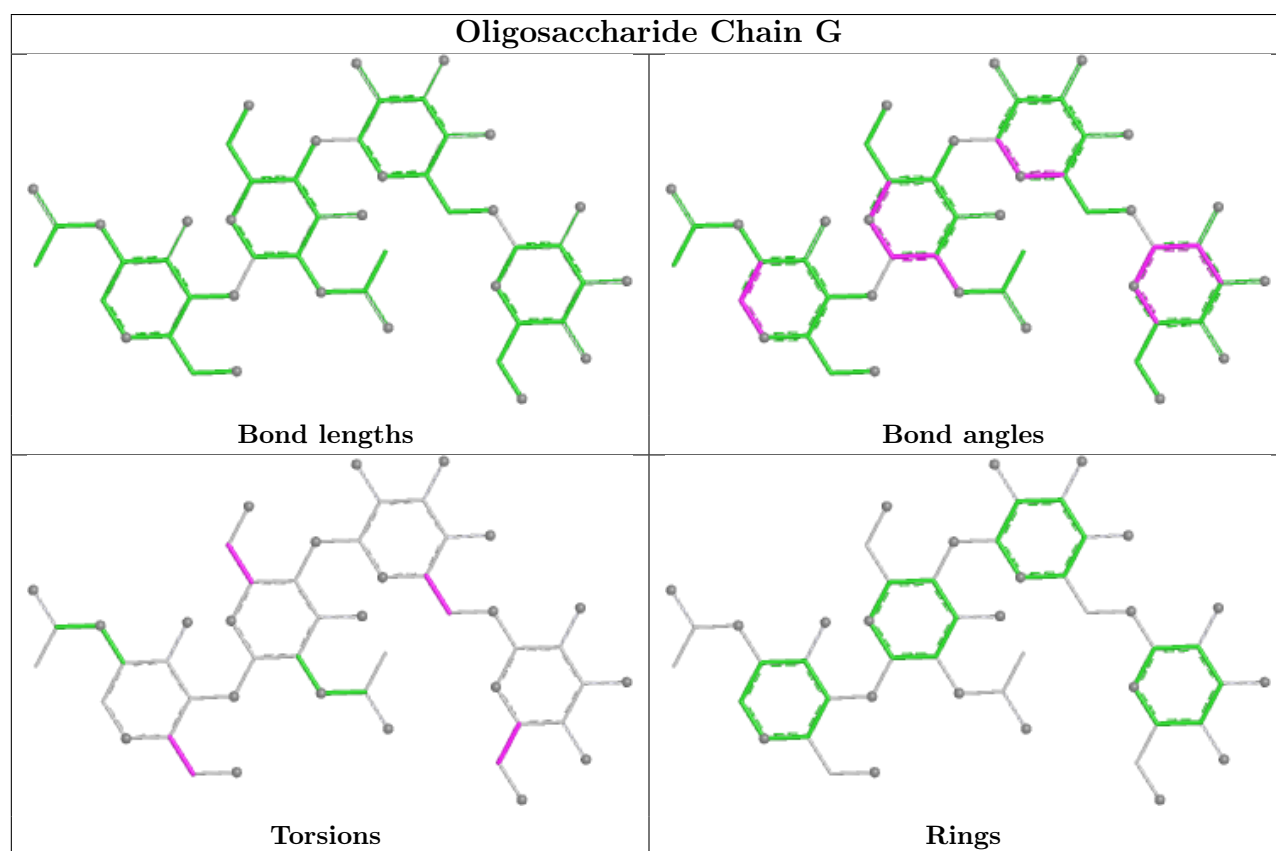
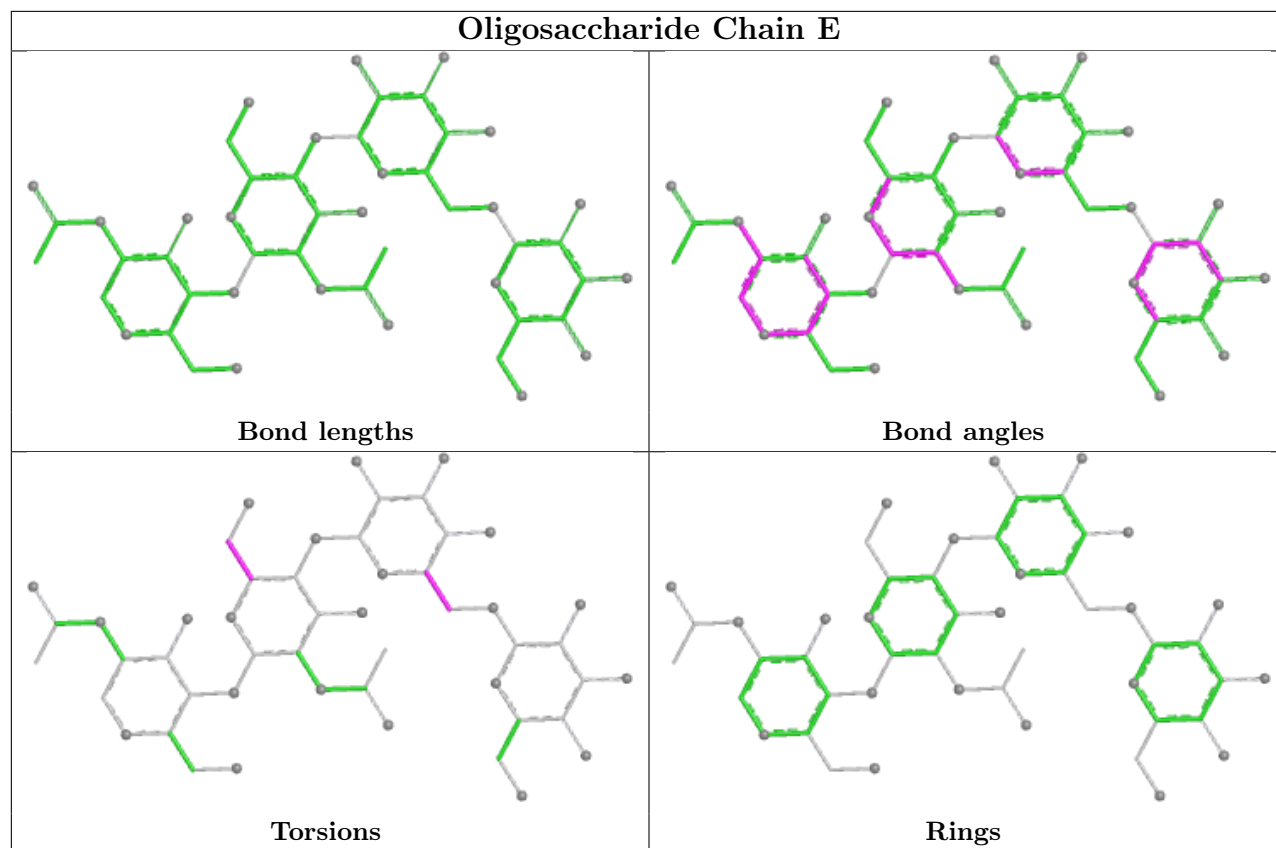
Mol	Chain	Res	Type	Atoms
2	E	3	BMA	O5-C5-C6-O6
4	Q	2	NAG	O5-C5-C6-O6
4	N	2	NAG	O5-C5-C6-O6
2	V	1	NAG	C3-C2-N2-C7
4	K	2	NAG	O5-C5-C6-O6
4	L	2	NAG	O5-C5-C6-O6
4	T	1	NAG	O5-C5-C6-O6
3	F	2	NAG	O5-C5-C6-O6
2	G	2	NAG	C4-C5-C6-O6
2	G	1	NAG	C4-C5-C6-O6
2	O	2	NAG	C3-C2-N2-C7
2	G	2	NAG	O5-C5-C6-O6
4	H	2	NAG	C4-C5-C6-O6
4	U	2	NAG	C4-C5-C6-O6
2	E	2	NAG	O5-C5-C6-O6
3	R	2	NAG	C3-C2-N2-C7
4	S	1	NAG	C3-C2-N2-C7
2	J	3	BMA	C4-C5-C6-O6
2	G	1	NAG	O5-C5-C6-O6
2	J	1	NAG	C4-C5-C6-O6

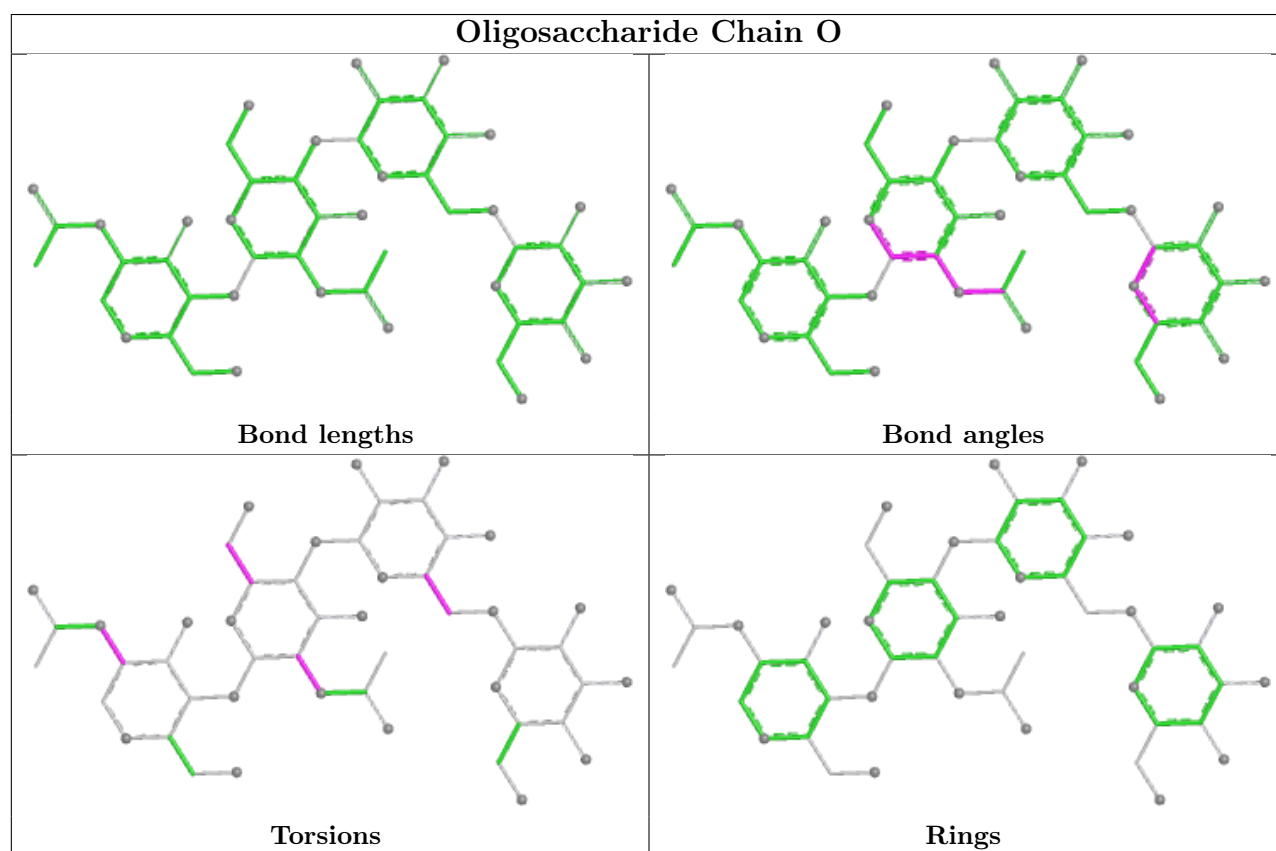
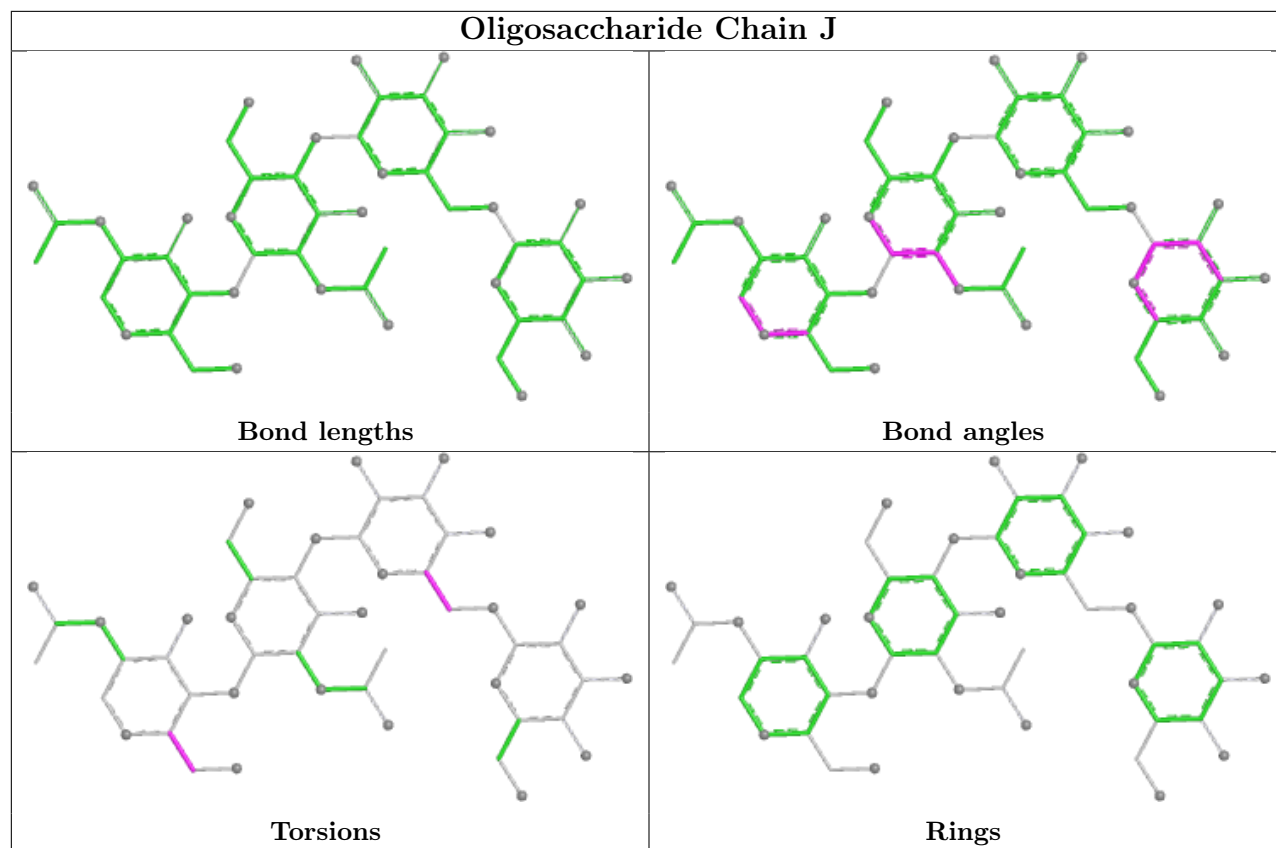
There are no ring outliers.

7 monomers are involved in 4 short contacts:

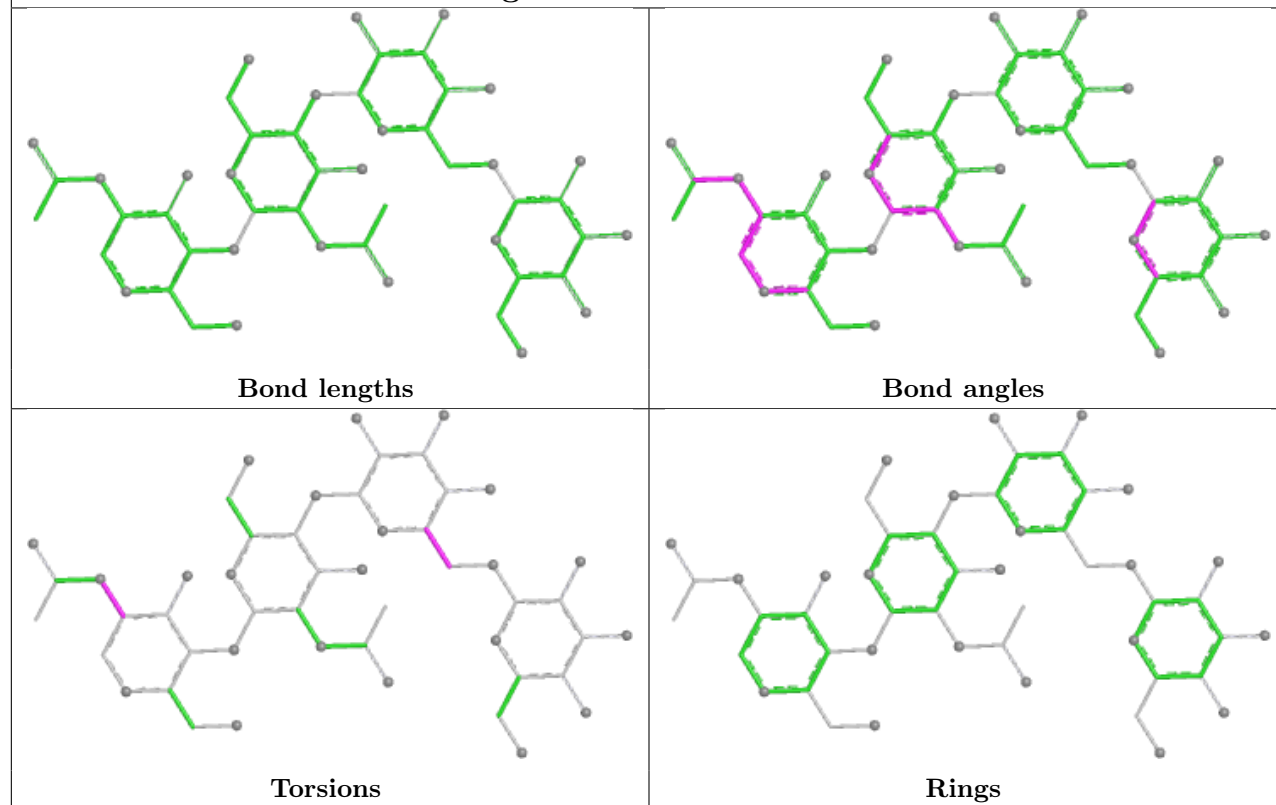
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	R	2	NAG	1	0
3	R	1	NAG	1	0
2	E	2	NAG	1	0
2	E	1	NAG	1	0
4	S	1	NAG	1	0
2	G	1	NAG	1	0
2	G	2	NAG	1	0

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

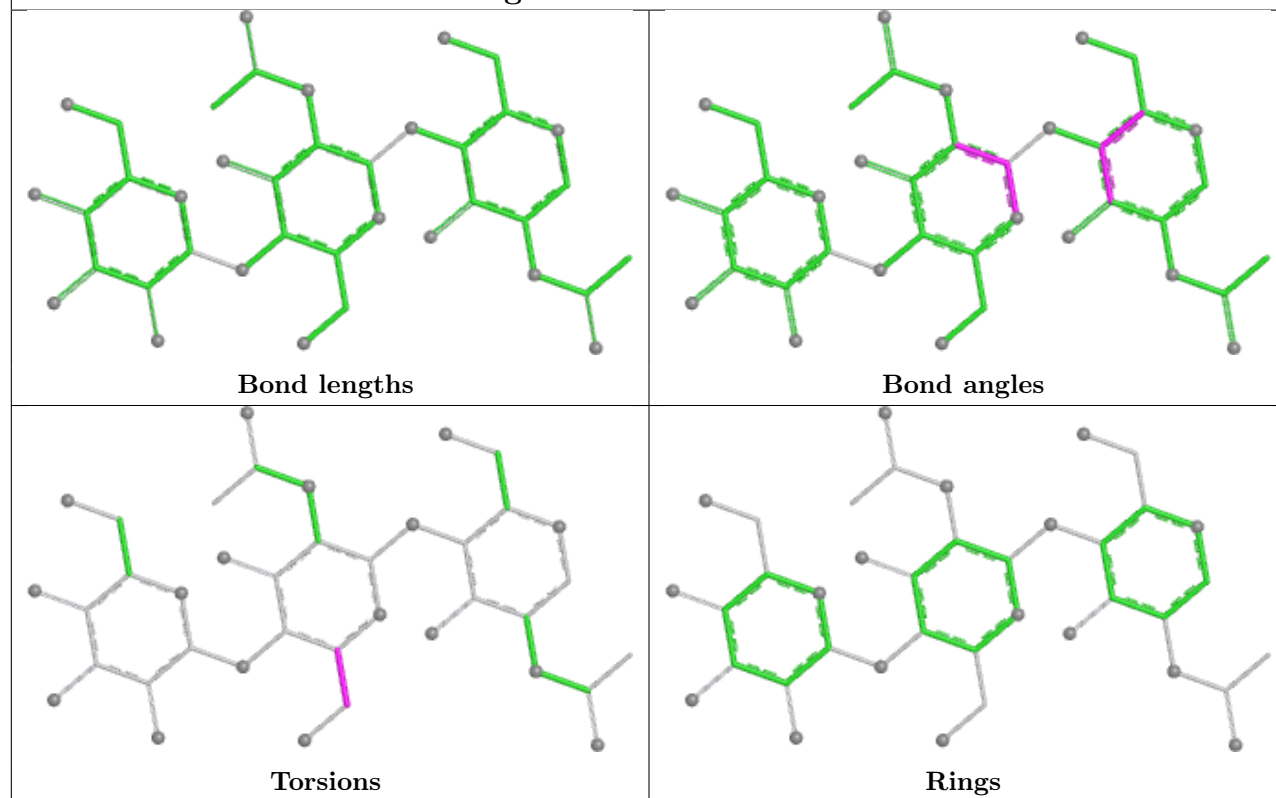


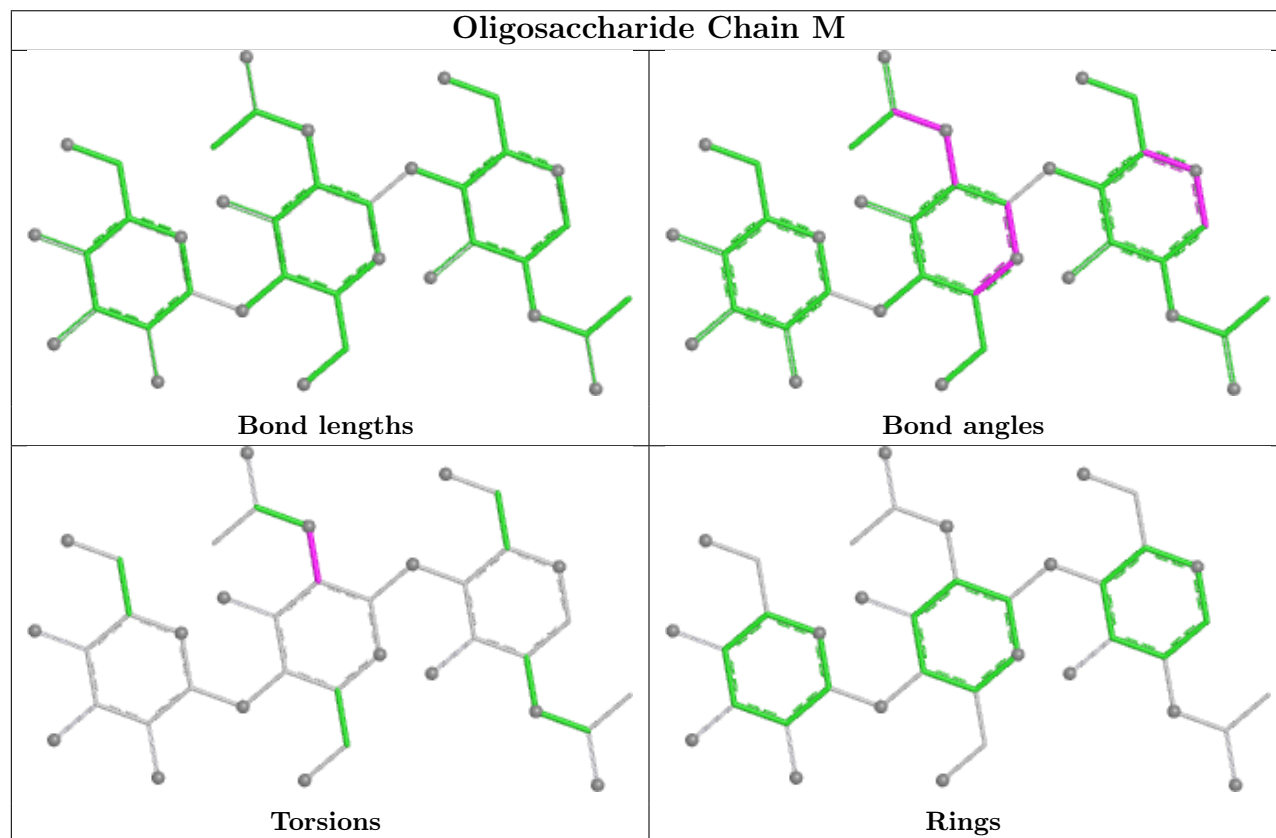
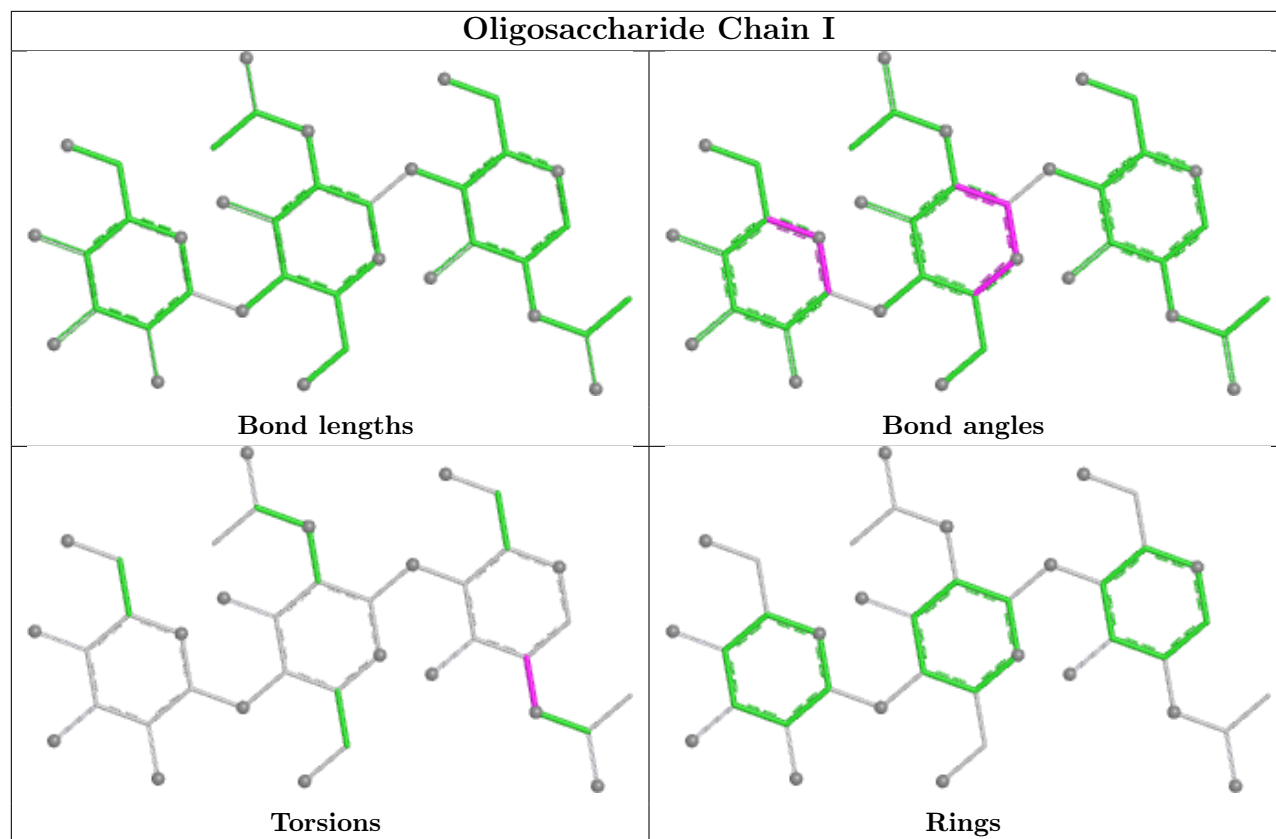


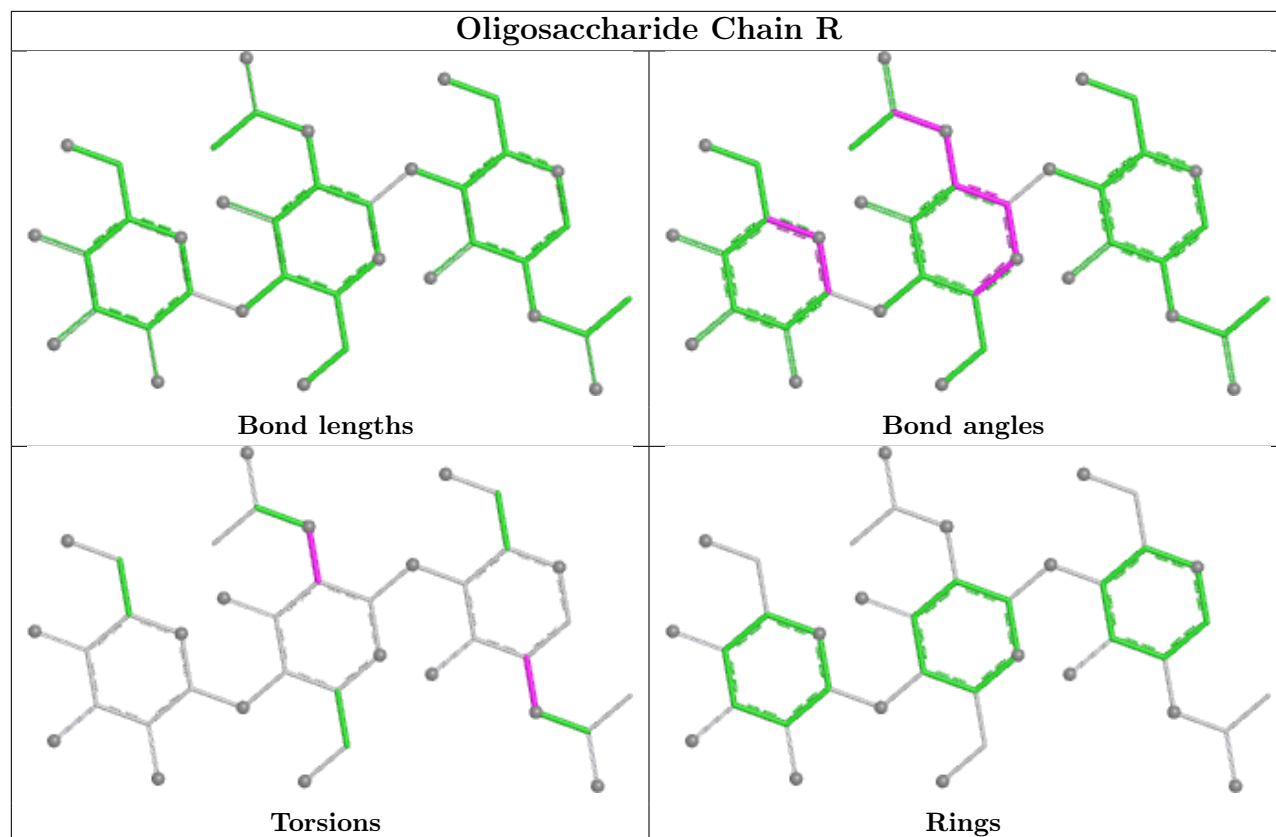
Oligosaccharide Chain V

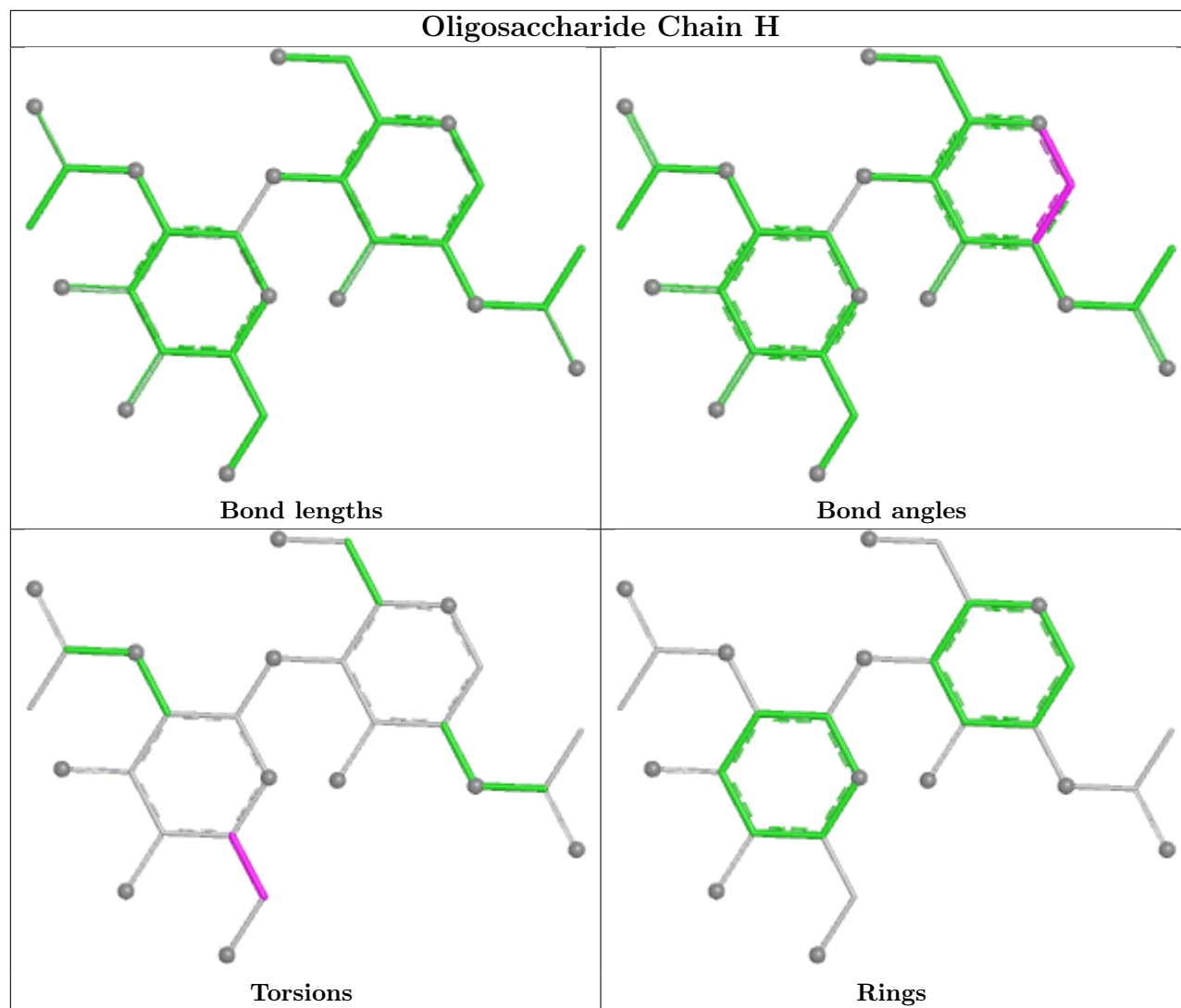


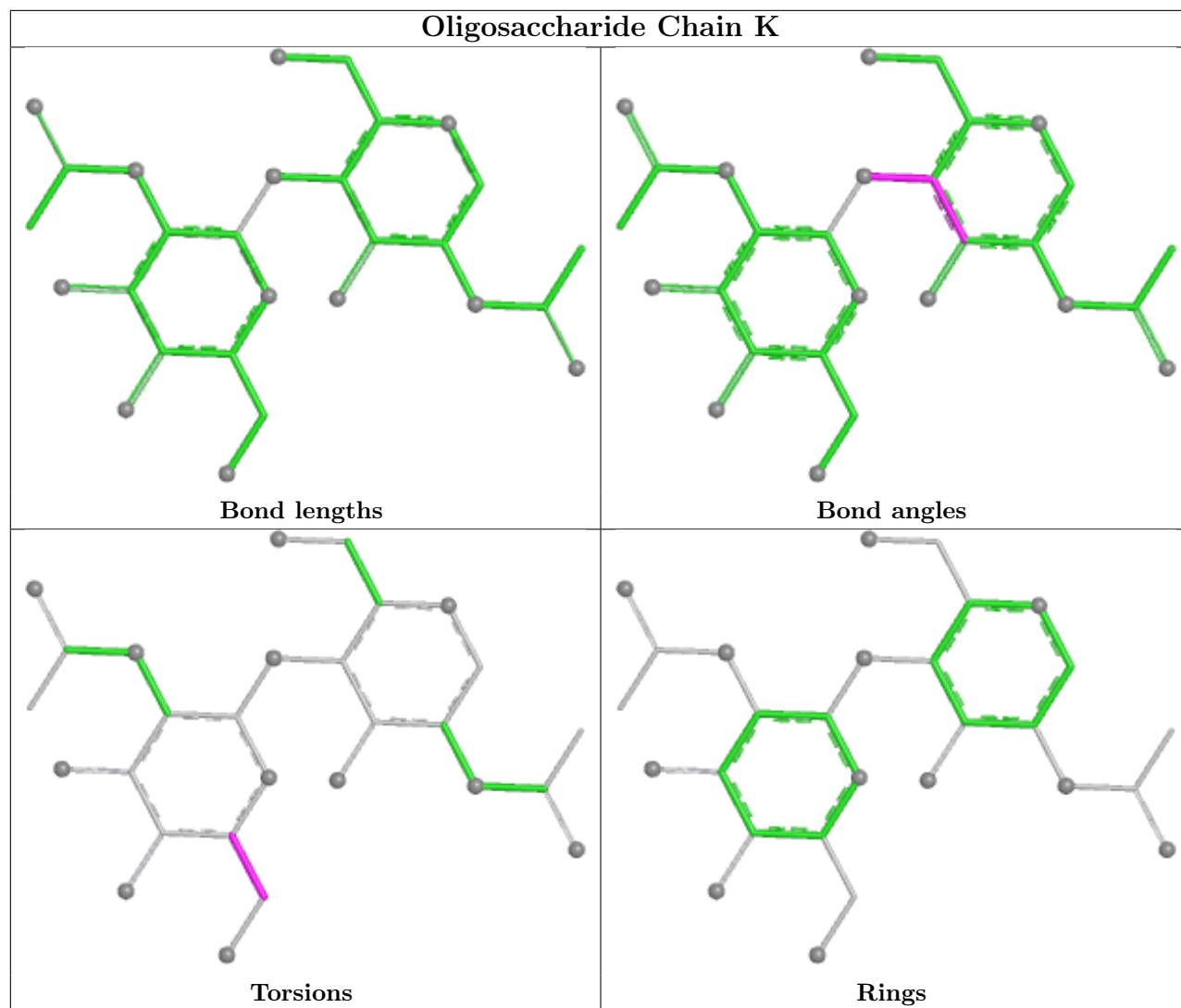
Oligosaccharide Chain F

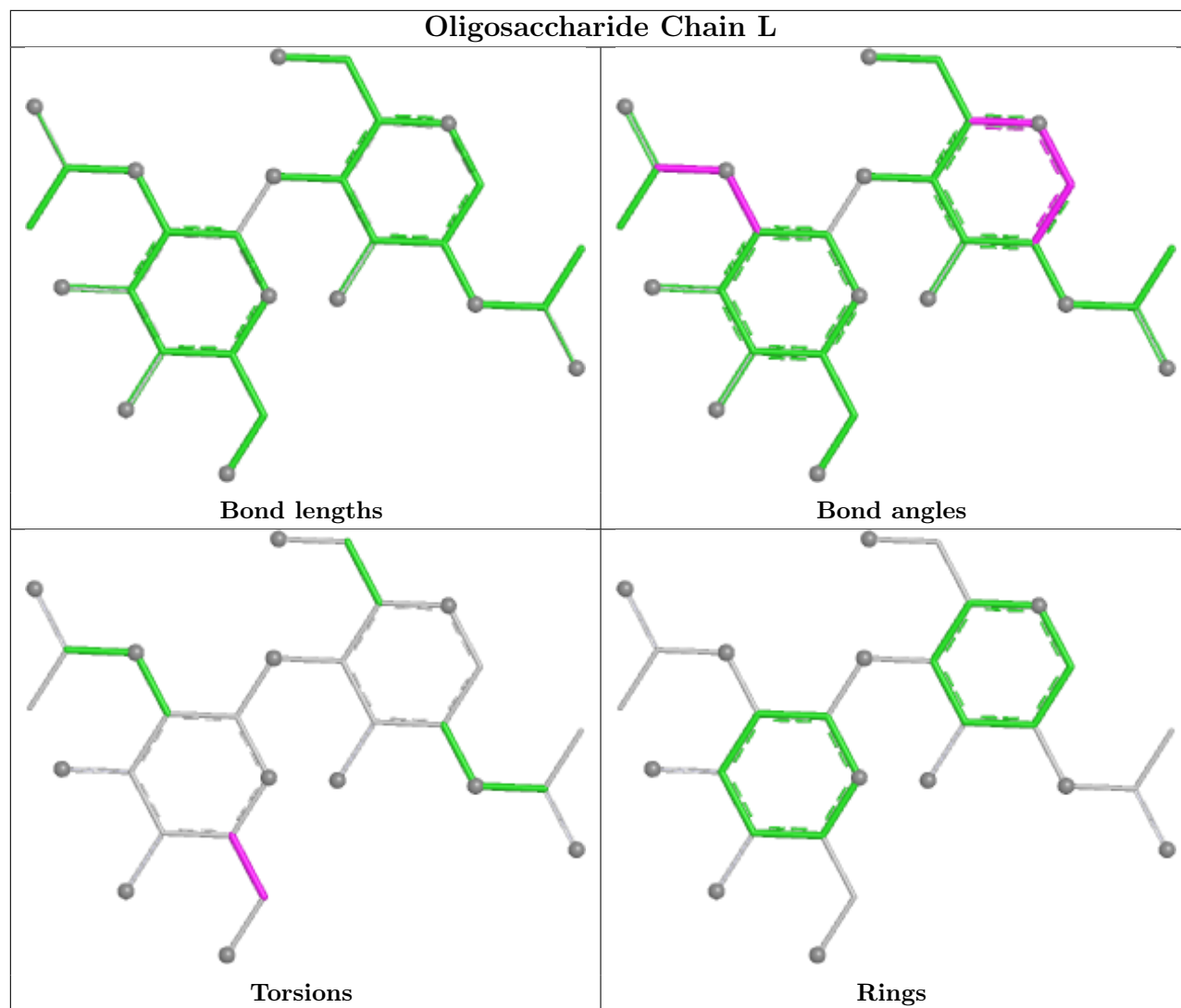


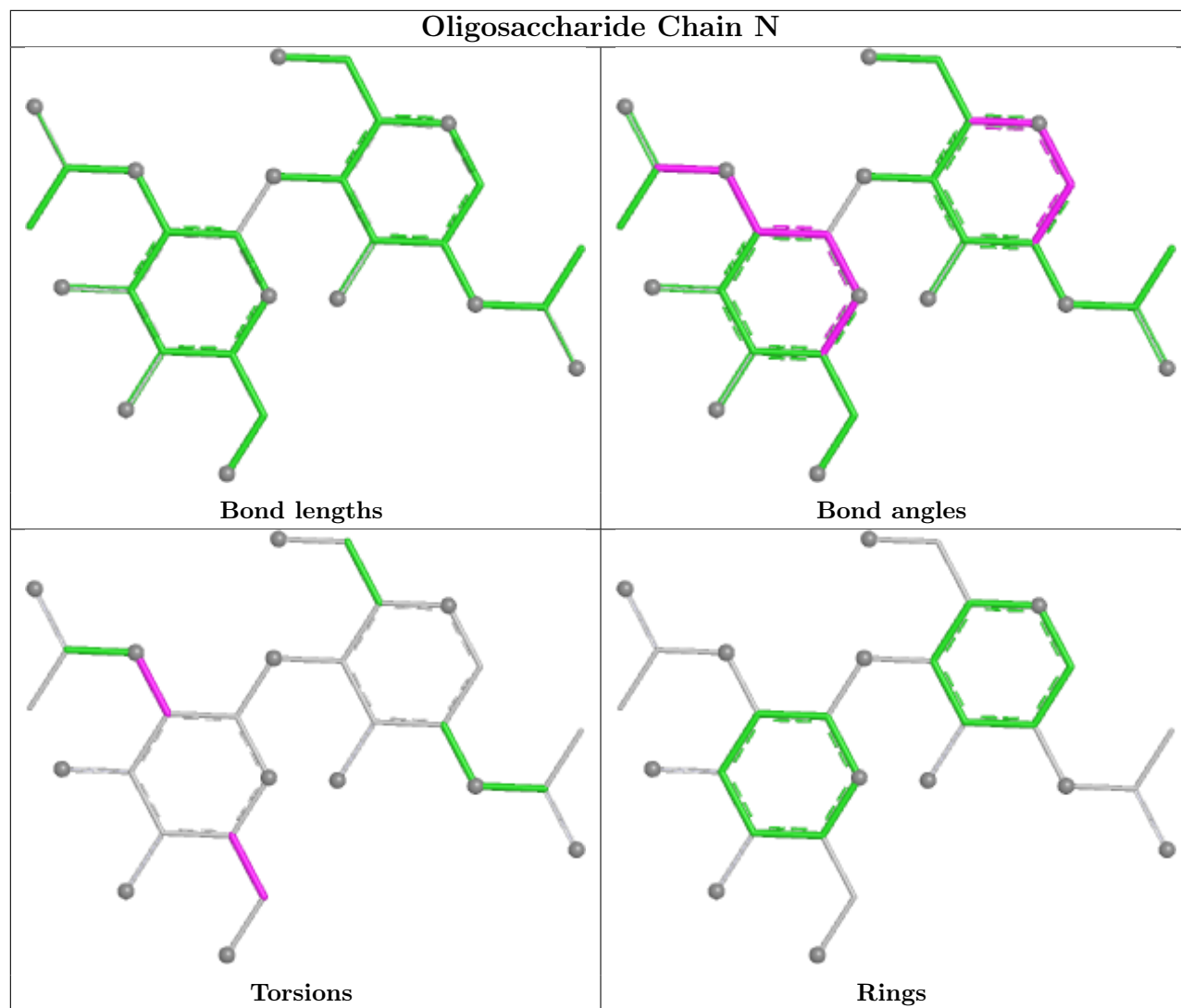


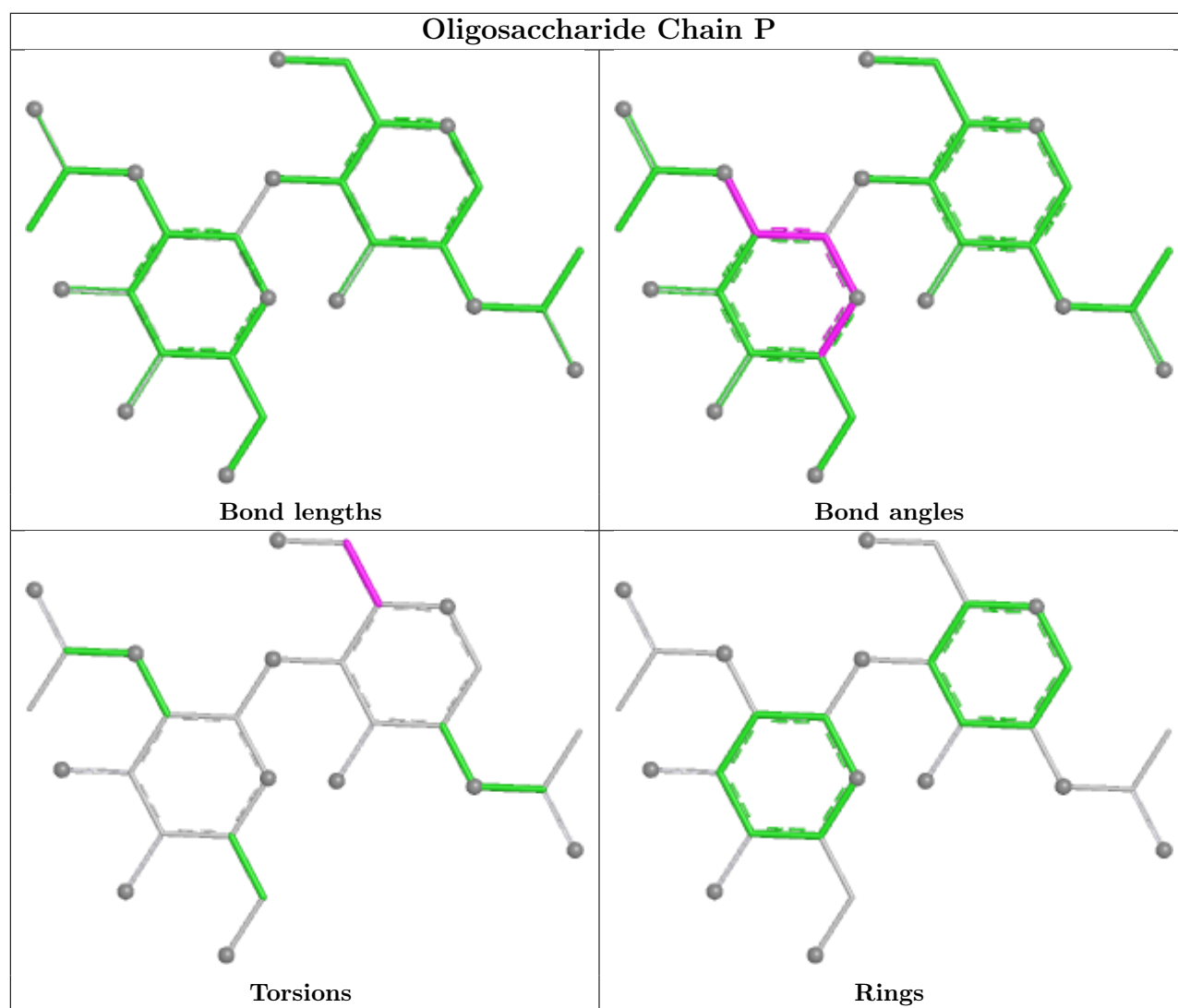


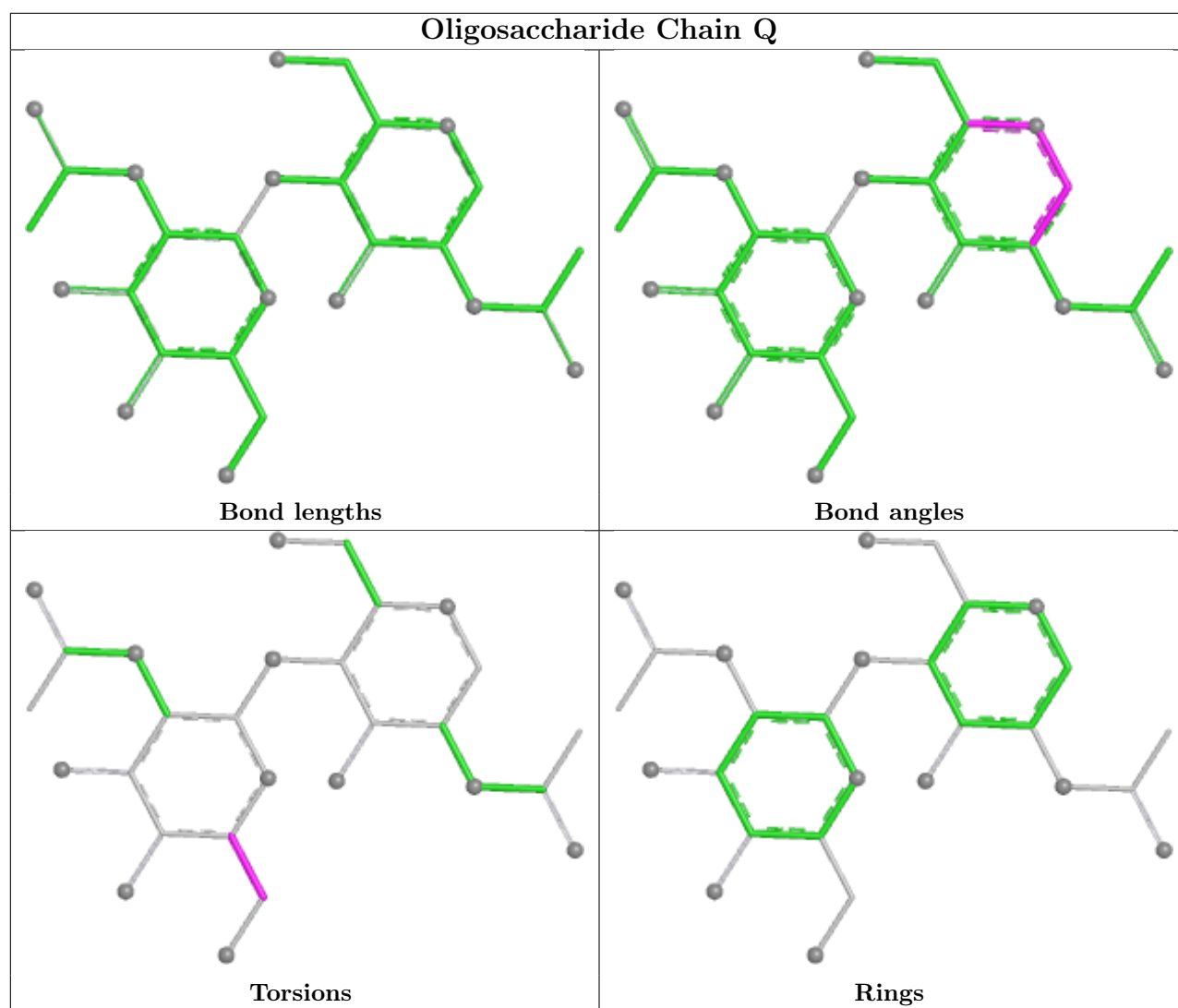


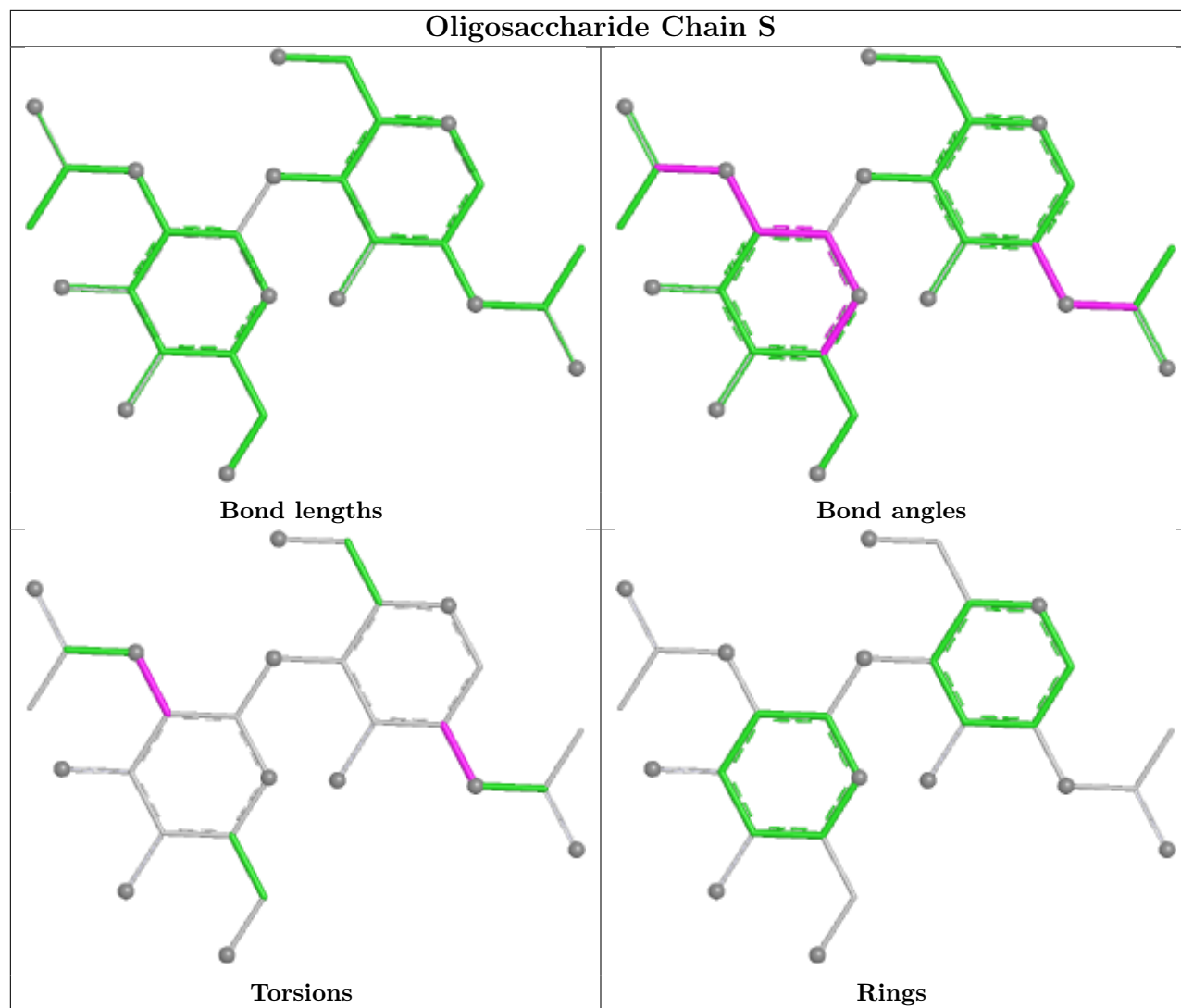


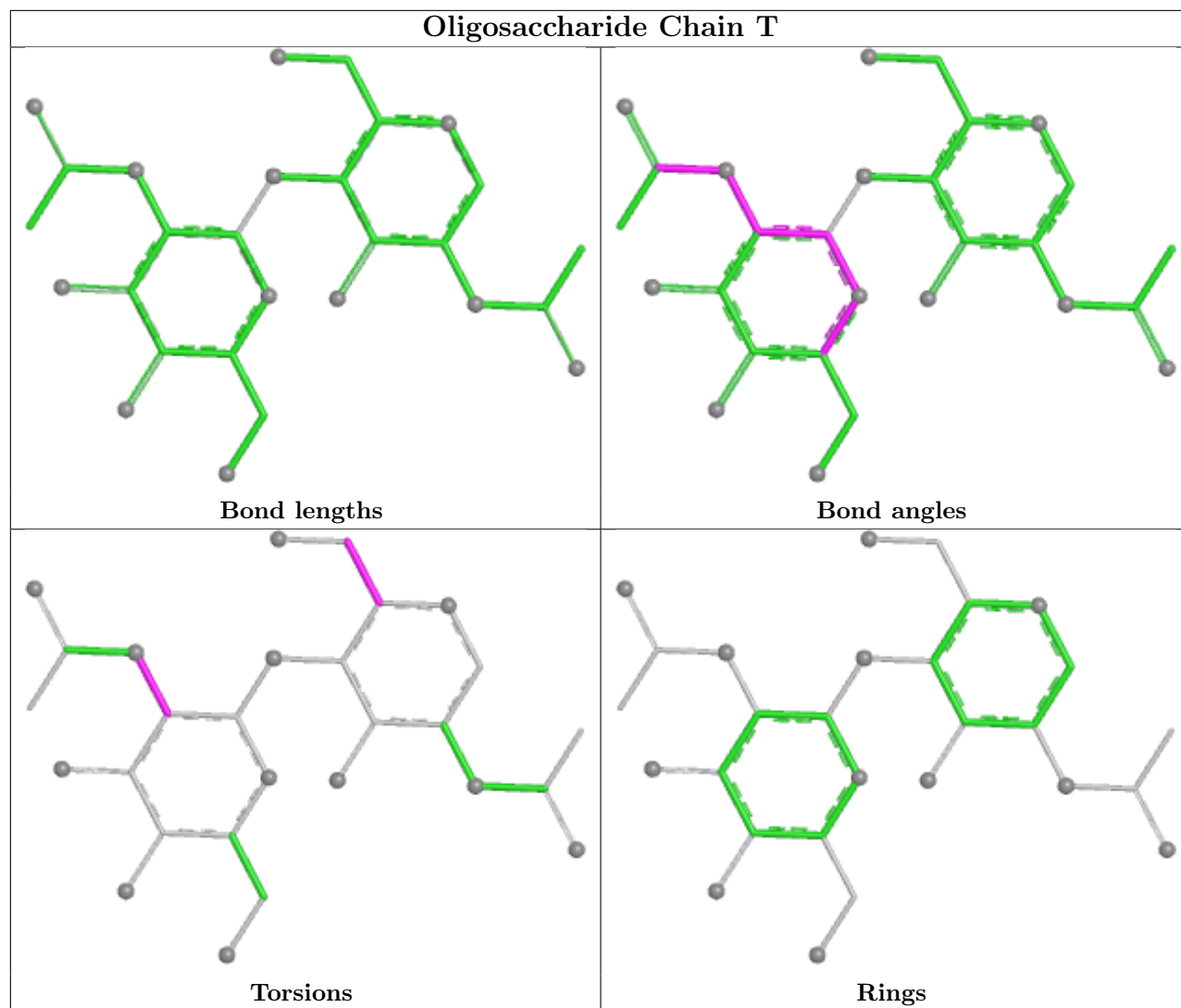


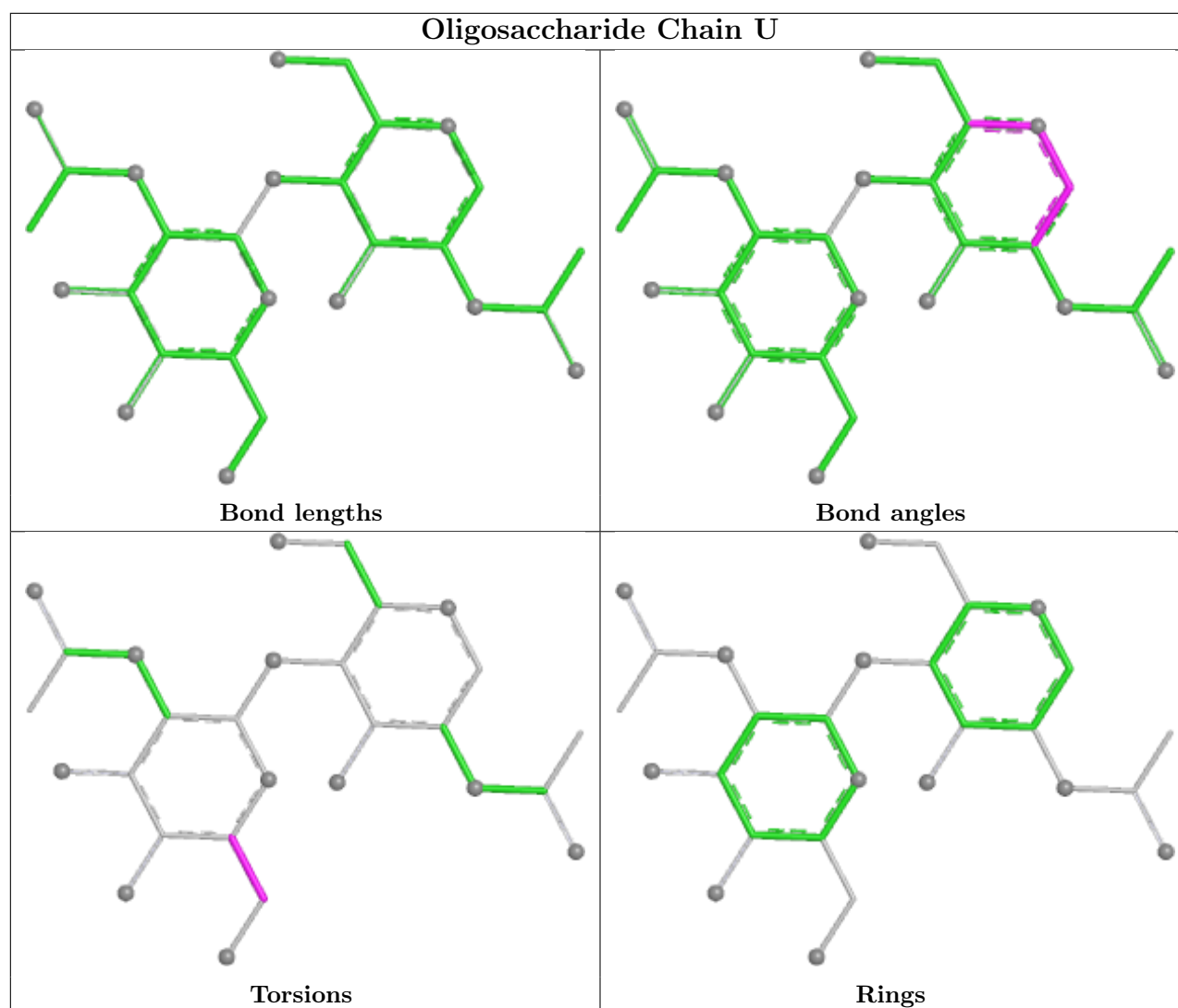












5.6 Ligand geometry [i](#)

11 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	$\# Z > 2$
5	NAG	B	2012	1	14,14,15	0.50	0	17,19,21	1.31	3 (17%)
5	NAG	D	2007	1	14,14,15	0.38	0	17,19,21	0.56	0
5	NAG	A	2013	1	14,14,15	0.41	0	17,19,21	0.50	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	C	2003	1	14,14,15	0.35	0	17,19,21	0.59	0
5	NAG	A	2019	1	14,14,15	0.52	0	17,19,21	1.48	3 (17%)
5	NAG	C	2004	1	14,14,15	0.43	0	17,19,21	0.76	0
5	NAG	D	2003	1	14,14,15	0.47	0	17,19,21	0.86	0
5	NAG	C	2002	1	14,14,15	0.40	0	17,19,21	0.72	0
5	NAG	D	2004	1	14,14,15	0.47	0	17,19,21	1.11	3 (17%)
5	NAG	A	2008	1	14,14,15	0.38	0	17,19,21	0.72	0
5	NAG	C	2001	1	14,14,15	0.45	0	17,19,21	1.59	3 (17%)

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
5	NAG	B	2012	1	-	2/6/23/26	0/1/1/1
5	NAG	D	2007	1	-	2/6/23/26	0/1/1/1
5	NAG	A	2013	1	-	2/6/23/26	0/1/1/1
5	NAG	C	2003	1	-	0/6/23/26	0/1/1/1
5	NAG	A	2019	1	-	1/6/23/26	0/1/1/1
5	NAG	C	2004	1	-	2/6/23/26	0/1/1/1
5	NAG	D	2003	1	-	2/6/23/26	0/1/1/1
5	NAG	C	2002	1	-	0/6/23/26	0/1/1/1
5	NAG	D	2004	1	-	1/6/23/26	0/1/1/1
5	NAG	A	2008	1	-	0/6/23/26	0/1/1/1
5	NAG	C	2001	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	2019	NAG	C1-O5-C5	4.75	118.55	112.19
5	C	2001	NAG	C1-C2-N2	3.99	116.73	110.43
5	C	2001	NAG	O5-C1-C2	-3.49	105.90	111.29
5	C	2001	NAG	C2-N2-C7	3.26	127.27	122.90
5	B	2012	NAG	C1-C2-N2	3.17	115.43	110.43
5	B	2012	NAG	C2-N2-C7	3.10	127.05	122.90
5	A	2019	NAG	C2-N2-C7	2.87	126.74	122.90
5	D	2004	NAG	O5-C1-C2	-2.64	107.20	111.29
5	D	2004	NAG	C1-O5-C5	2.55	115.61	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	2012	NAG	O5-C1-C2	-2.29	107.74	111.29
5	D	2004	NAG	C1-C2-N2	2.23	113.95	110.43
5	A	2019	NAG	C1-C2-N2	2.11	113.76	110.43

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	D	2007	NAG	O5-C5-C6-O6
5	A	2013	NAG	O5-C5-C6-O6
5	D	2003	NAG	C4-C5-C6-O6
5	D	2007	NAG	C4-C5-C6-O6
5	D	2003	NAG	O5-C5-C6-O6
5	C	2004	NAG	C4-C5-C6-O6
5	D	2004	NAG	O5-C5-C6-O6
5	A	2019	NAG	C3-C2-N2-C7
5	A	2013	NAG	C4-C5-C6-O6
5	C	2004	NAG	O5-C5-C6-O6
5	B	2012	NAG	C1-C2-N2-C7
5	C	2001	NAG	C1-C2-N2-C7
5	C	2001	NAG	C3-C2-N2-C7
5	B	2012	NAG	C3-C2-N2-C7

There are no ring outliers.

No monomer is involved in short contacts.

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	1416/1474 (96%)	0.13	44 (3%)	51	39	75, 135, 176, 200	0
1	B	1273/1474 (86%)	0.19	52 (4%)	41	35	89, 147, 180, 214	0
1	C	1274/1474 (86%)	0.24	57 (4%)	38	33	78, 130, 175, 200	0
1	D	1271/1474 (86%)	0.16	51 (4%)	42	35	84, 139, 177, 200	0
All	All	5234/5896 (88%)	0.18	204 (3%)	43	36	75, 138, 178, 214	0

All (204) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	270	ARG	7.8
1	B	1275	ALA	6.0
1	D	1211	TYR	5.3
1	C	744	VAL	5.2
1	D	1025	TYR	4.8
1	B	1025	TYR	4.7
1	A	270	ARG	4.7
1	D	1016	LEU	4.5
1	B	493	LEU	4.4
1	A	1008	LEU	4.3
1	C	493	LEU	4.3
1	D	739	TRP	4.2
1	C	270	ARG	4.2
1	B	953	ASP	4.0
1	C	242	LEU	4.0
1	D	493	LEU	3.9
1	B	622	LEU	3.9
1	A	870	PHE	3.8
1	D	1251	THR	3.8
1	C	1099	VAL	3.8
1	D	1105	ILE	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	987	LEU	3.7
1	B	153	GLU	3.7
1	D	242	LEU	3.7
1	C	495	PHE	3.6
1	D	1049	PHE	3.6
1	B	810	LEU	3.6
1	D	1062	HIS	3.6
1	C	1291	GLN	3.6
1	D	528	ILE	3.5
1	A	1322	VAL	3.5
1	A	229	PHE	3.5
1	B	1183	TRP	3.4
1	A	1321	CYS	3.4
1	D	1046	LEU	3.4
1	D	1216	TYR	3.4
1	A	634	LEU	3.3
1	C	954	ILE	3.3
1	D	1146	THR	3.3
1	C	745	VAL	3.3
1	C	1150	LEU	3.3
1	B	266	VAL	3.3
1	D	543	TYR	3.3
1	A	889	SER	3.3
1	B	1208	MET	3.2
1	C	1131	ALA	3.2
1	C	1041	LEU	3.2
1	B	31	TYR	3.2
1	D	587	VAL	3.2
1	B	1274	LYS	3.1
1	A	155	PHE	3.1
1	B	250	VAL	3.1
1	D	495	PHE	3.1
1	C	248	VAL	3.1
1	A	1070	LEU	3.0
1	C	219	PHE	3.0
1	A	822	ILE	3.0
1	C	1091	ILE	2.9
1	B	600	VAL	2.9
1	D	978	VAL	2.9
1	D	1099	VAL	2.9
1	C	1154	PHE	2.9
1	D	266	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	1026	SER	2.9
1	B	954	ILE	2.8
1	B	1238	ILE	2.8
1	A	266	VAL	2.8
1	C	1068	ILE	2.8
1	B	1211	TYR	2.8
1	D	1149	LEU	2.8
1	D	205	VAL	2.8
1	D	250	VAL	2.8
1	A	528	ILE	2.8
1	C	205	VAL	2.8
1	D	1019	LYS	2.7
1	A	1025	TYR	2.7
1	C	662	ASN	2.7
1	B	558	TYR	2.7
1	B	219	PHE	2.7
1	B	789	PHE	2.7
1	D	1080	PHE	2.7
1	B	790	GLN	2.7
1	A	564	LEU	2.7
1	D	1125	LEU	2.7
1	A	984	ILE	2.7
1	A	1105	ILE	2.7
1	C	862	PRO	2.7
1	C	919	LEU	2.7
1	D	1213	LEU	2.7
1	A	986	VAL	2.7
1	B	1049	PHE	2.7
1	B	1150	LEU	2.6
1	C	514	LEU	2.6
1	C	989	TYR	2.6
1	D	167	ILE	2.6
1	C	1322	VAL	2.6
1	D	793	PHE	2.6
1	B	1125	LEU	2.6
1	A	1388	GLY	2.6
1	B	35	VAL	2.6
1	D	207	VAL	2.6
1	D	597	LEU	2.6
1	A	381	ASN	2.6
1	C	67	VAL	2.6
1	A	1323	TYR	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	1106	THR	2.6
1	C	676	LYS	2.5
1	C	874	ALA	2.5
1	A	619	TYR	2.5
1	A	187	LEU	2.5
1	A	604	VAL	2.5
1	D	794	VAL	2.5
1	B	155	PHE	2.5
1	B	384	ILE	2.5
1	C	239	ILE	2.5
1	D	357	SER	2.5
1	C	1213	LEU	2.5
1	B	476	VAL	2.5
1	B	738	THR	2.4
1	C	503	GLY	2.4
1	D	1067	LEU	2.4
1	D	792	PHE	2.4
1	B	502	LYS	2.4
1	C	1261	LEU	2.4
1	D	677	ALA	2.4
1	D	651	ASN	2.4
1	C	1080	PHE	2.4
1	D	1292	VAL	2.4
1	C	1143	HIS	2.4
1	A	1258	LEU	2.4
1	D	1070	LEU	2.4
1	B	264	VAL	2.4
1	D	1109	LEU	2.4
1	B	322	THR	2.3
1	D	270	ARG	2.3
1	B	528	ILE	2.3
1	B	604	VAL	2.3
1	B	1008	LEU	2.3
1	B	1273	GLY	2.3
1	C	102	PHE	2.3
1	C	618	VAL	2.3
1	C	155	PHE	2.3
1	D	854	GLN	2.3
1	A	452	PHE	2.3
1	B	585	LEU	2.3
1	D	32	MET	2.3
1	A	572	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	386	ILE	2.3
1	C	1146	THR	2.3
1	B	814	VAL	2.3
1	C	35	VAL	2.3
1	C	1070	LEU	2.3
1	C	1238	ILE	2.2
1	A	1046	LEU	2.2
1	D	1264	TYR	2.2
1	A	1067	LEU	2.2
1	B	51	LEU	2.2
1	C	36	PRO	2.2
1	C	753	GLU	2.2
1	B	1235	VAL	2.2
1	B	666	MET	2.2
1	B	419	LEU	2.2
1	C	187	LEU	2.2
1	C	868	VAL	2.2
1	A	1364	SER	2.2
1	B	1041	LEU	2.2
1	B	1170	LEU	2.2
1	C	194	LEU	2.2
1	C	1264	TYR	2.2
1	C	1129	GLU	2.2
1	C	1198	GLU	2.2
1	B	553	GLY	2.1
1	A	167	ILE	2.1
1	A	1041	LEU	2.1
1	A	1365	LEU	2.1
1	C	1103	ALA	2.1
1	A	792	PHE	2.1
1	C	528	ILE	2.1
1	C	920	LEU	2.1
1	D	770	PHE	2.1
1	B	1294	ASN	2.1
1	D	744	VAL	2.1
1	C	368	GLN	2.1
1	A	1043	ALA	2.1
1	D	1258	LEU	2.1
1	A	597	LEU	2.1
1	A	1324	LEU	2.1
1	B	1214	LEU	2.1
1	B	1324	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	542	ILE	2.1
1	A	1183	TRP	2.1
1	A	31	TYR	2.1
1	D	362	GLY	2.1
1	D	1043	ALA	2.0
1	C	48	CYS	2.0
1	C	1142	SER	2.0
1	C	564	LEU	2.0
1	D	1238	ILE	2.0
1	A	60	VAL	2.0
1	B	739	TRP	2.0
1	C	1216	TYR	2.0
1	D	762	ILE	2.0
1	B	826	VAL	2.0
1	C	987	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	BMA	R	3	11/12	-0.04	0.14	300,300,300,300	0
2	BMA	O	3	11/12	0.05	0.12	300,300,300,300	0
2	BMA	V	3	11/12	0.13	0.10	295,297,298,298	0
3	NAG	M	2	14/15	0.20	0.12	300,300,300,300	0
4	NAG	Q	2	14/15	0.20	0.13	292,295,297,297	0
2	MAN	E	4	11/12	0.22	0.10	293,294,294,294	0
2	MAN	J	4	11/12	0.23	0.09	300,300,300,300	0
4	NAG	L	2	14/15	0.29	0.14	300,300,300,300	0
2	BMA	G	3	11/12	0.32	0.11	292,292,293,294	0
2	BMA	E	3	11/12	0.36	0.09	294,295,295,295	0
2	BMA	J	3	11/12	0.36	0.08	300,300,300,300	0
3	BMA	M	3	11/12	0.36	0.12	300,300,300,300	0
4	NAG	P	2	14/15	0.37	0.11	300,300,300,300	0

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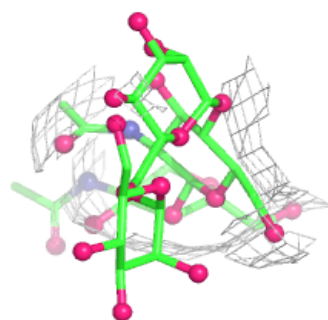
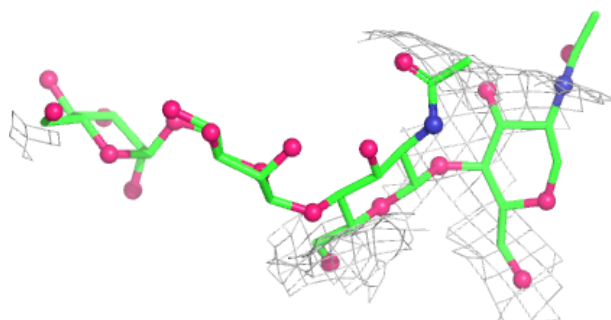
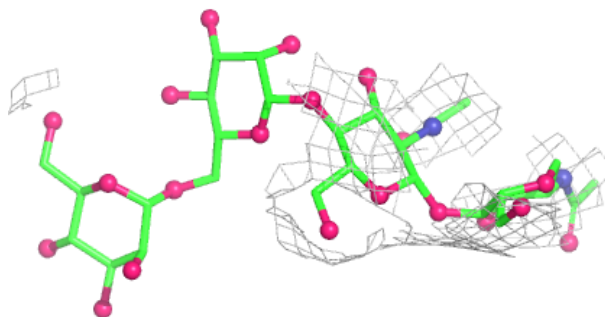
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	MAN	O	4	11/12	0.41	0.08	300,300,300,300	0
2	NAG	J	2	14/15	0.42	0.09	300,300,300,300	0
2	NAG	G	2	14/15	0.54	0.09	291,292,293,294	0
3	NAG	M	1	14/15	0.56	0.15	300,300,300,300	0
3	BMA	F	3	11/12	0.62	0.10	289,290,291,291	0
4	NAG	U	2	14/15	0.64	0.08	300,300,300,300	0
4	NAG	H	2	14/15	0.65	0.10	296,299,300,300	0
4	NAG	L	1	14/15	0.65	0.11	300,300,300,300	0
4	NAG	H	1	14/15	0.68	0.12	295,297,299,299	0
4	NAG	T	1	14/15	0.69	0.10	290,291,292,293	0
4	NAG	P	1	14/15	0.69	0.11	300,300,300,300	0
4	NAG	S	1	14/15	0.70	0.10	300,300,300,300	0
2	MAN	V	4	11/12	0.71	0.10	293,294,295,296	0
2	NAG	E	2	14/15	0.71	0.10	295,296,297,297	0
4	NAG	N	2	14/15	0.72	0.09	300,300,300,300	0
4	NAG	T	2	14/15	0.72	0.08	290,291,292,292	0
4	NAG	S	2	14/15	0.72	0.10	300,300,300,300	0
3	BMA	I	3	11/12	0.73	0.08	300,300,300,300	0
3	NAG	F	1	14/15	0.73	0.10	284,285,287,287	0
4	NAG	K	2	14/15	0.74	0.08	300,300,300,300	0
3	NAG	R	2	14/15	0.75	0.13	289,300,300,300	0
3	NAG	F	2	14/15	0.75	0.08	288,289,290,290	0
4	NAG	K	1	14/15	0.76	0.09	296,300,300,300	0
2	NAG	G	1	14/15	0.79	0.09	291,291,292,292	0
2	NAG	V	1	14/15	0.79	0.12	286,293,298,299	0
4	NAG	U	1	14/15	0.80	0.09	296,300,300,300	0
2	NAG	O	1	14/15	0.80	0.14	268,287,296,297	0
2	NAG	O	2	14/15	0.82	0.10	297,299,300,300	0
3	NAG	I	2	14/15	0.82	0.08	295,300,300,300	0
2	NAG	V	2	14/15	0.83	0.08	296,300,300,300	0
4	NAG	N	1	14/15	0.83	0.12	298,300,300,300	0
2	MAN	G	4	11/12	0.84	0.12	294,295,296,296	0
2	NAG	J	1	14/15	0.87	0.09	300,300,300,300	0
3	NAG	R	1	14/15	0.89	0.14	252,274,288,289	0
4	NAG	Q	1	14/15	0.89	0.09	290,291,292,294	0
2	NAG	E	1	14/15	0.89	0.11	295,297,298,298	0
3	NAG	I	1	14/15	0.90	0.09	259,291,300,300	0

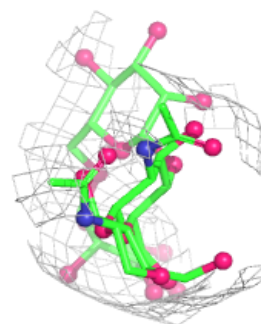
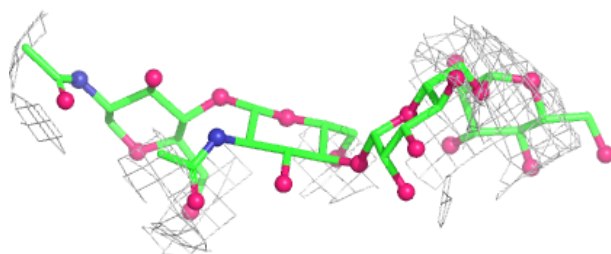
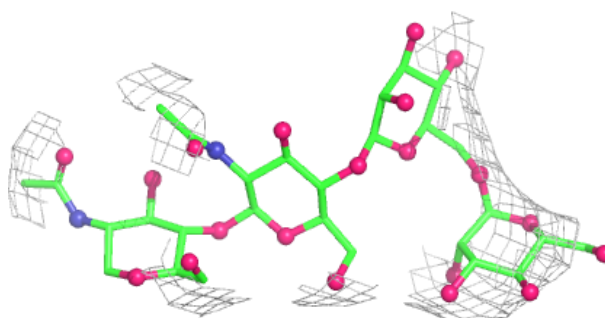
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain E:

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

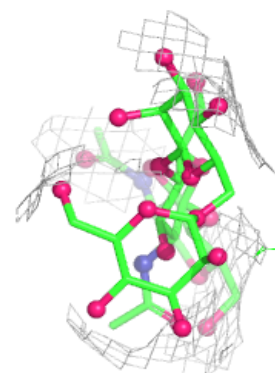
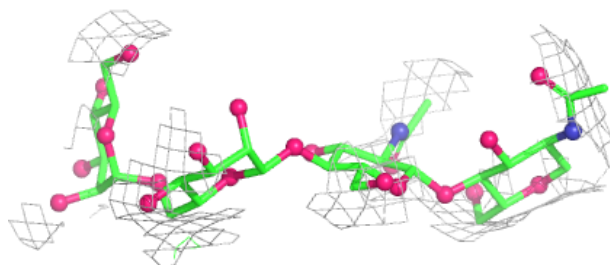
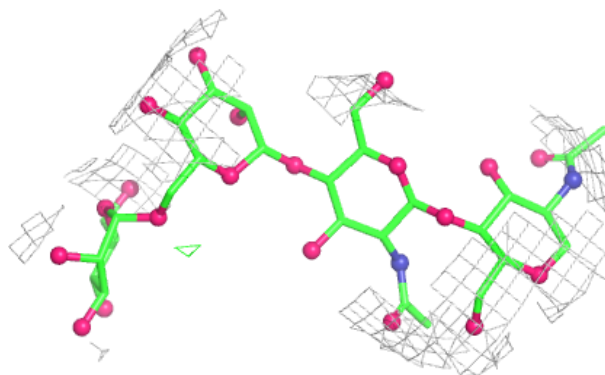
**Electron density around Chain G:**

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

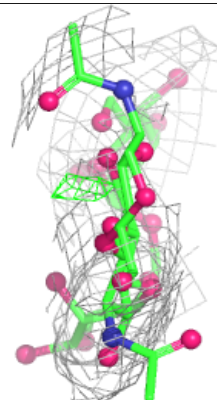
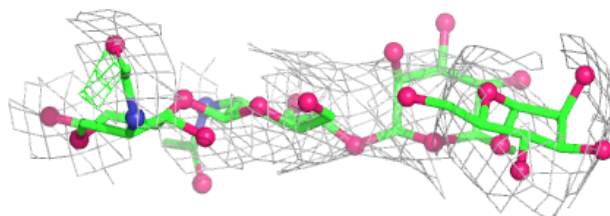
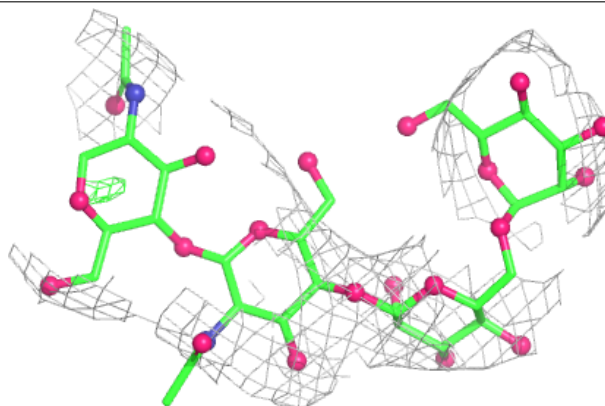


Electron density around Chain J:

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

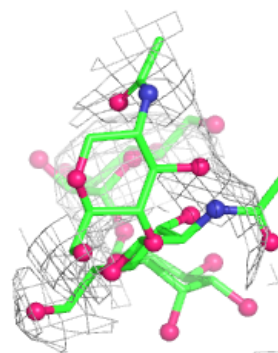
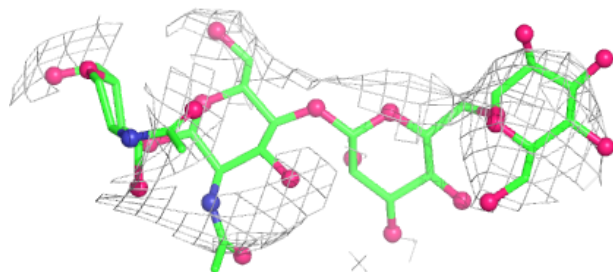
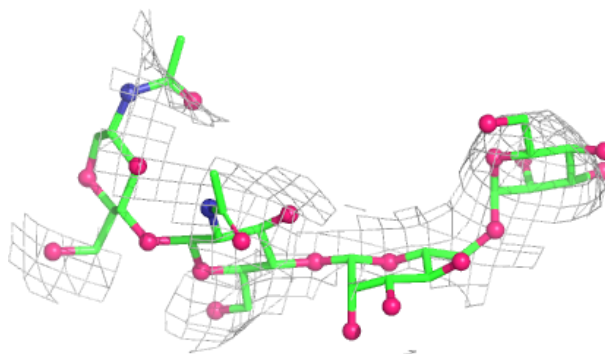
**Electron density around Chain O:**

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



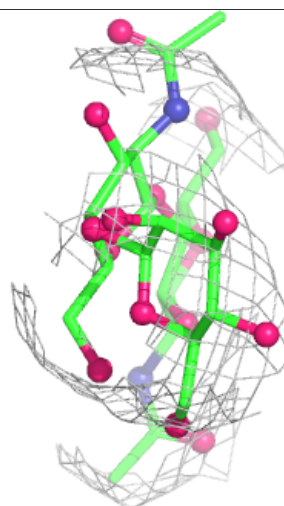
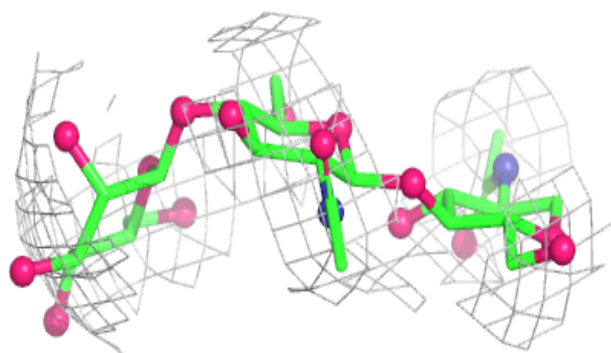
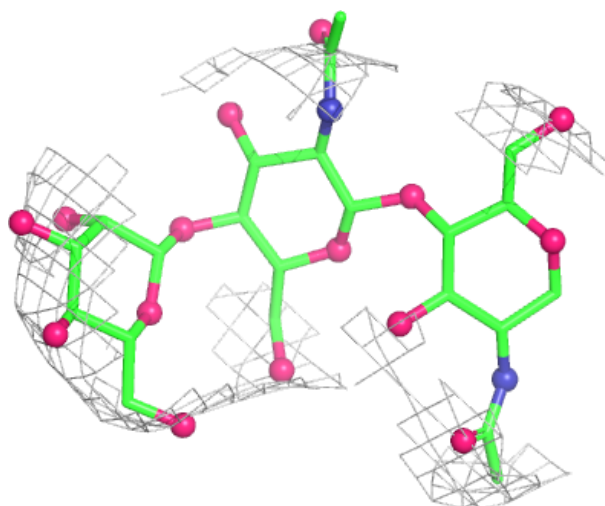
Electron density around Chain V:

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



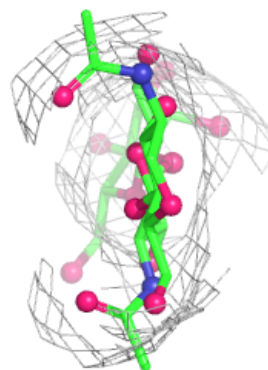
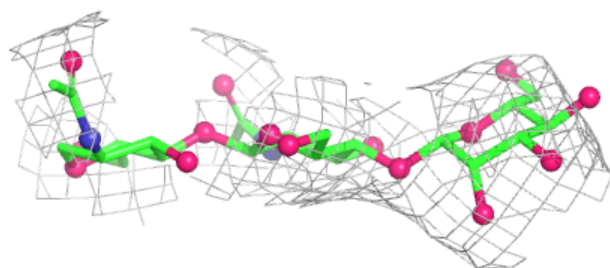
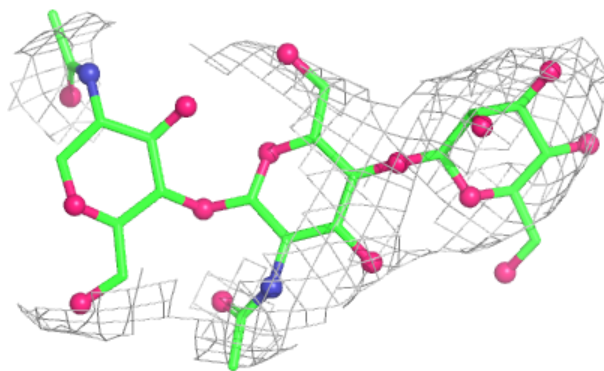
Electron density around Chain F:

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



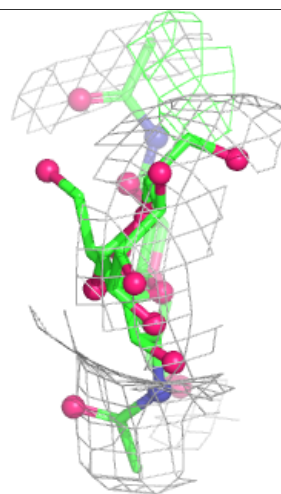
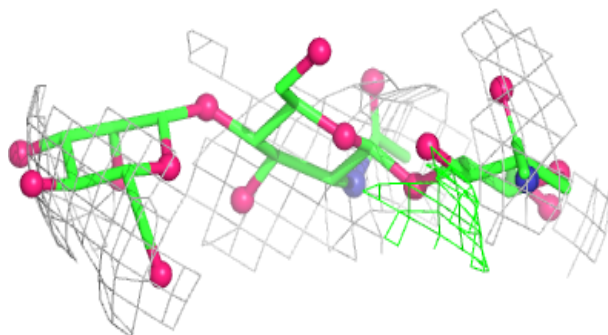
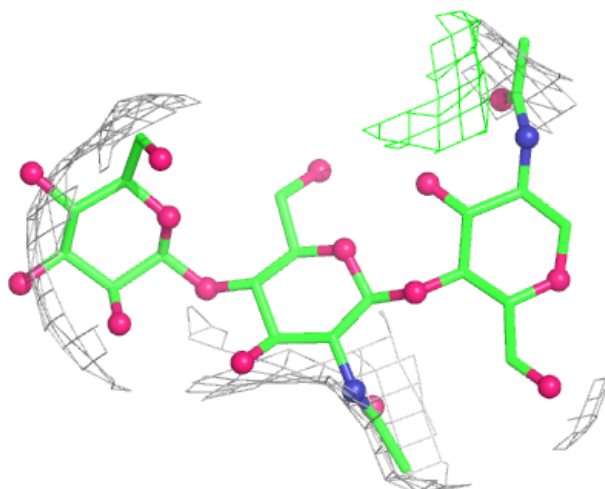
Electron density around Chain I:

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



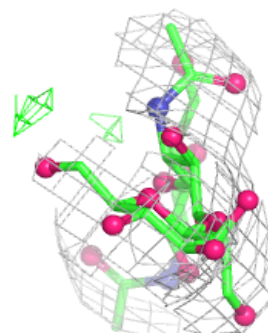
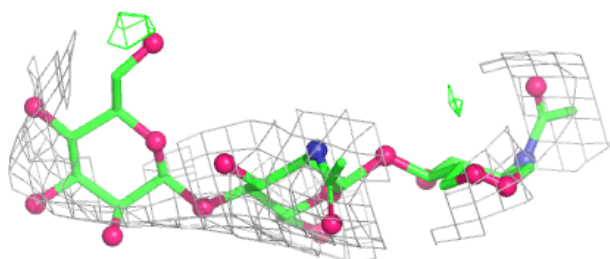
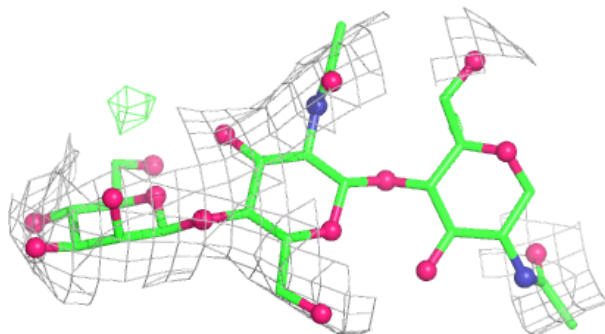
Electron density around Chain M:

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

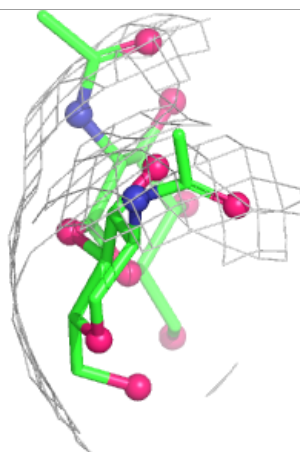
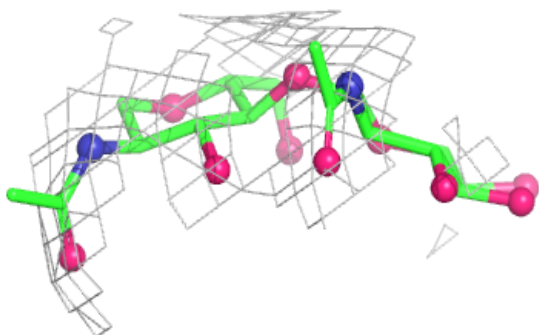
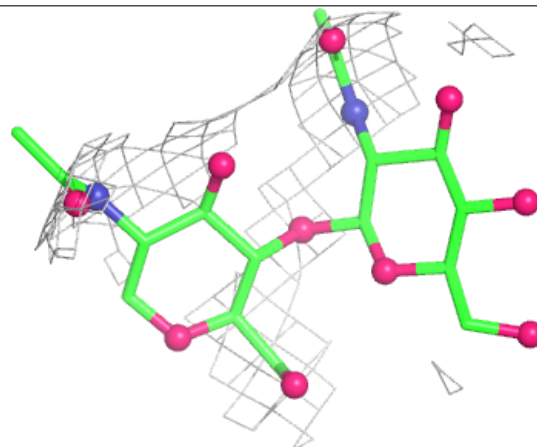


Electron density around Chain R:

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

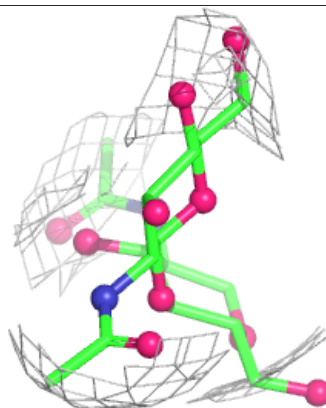
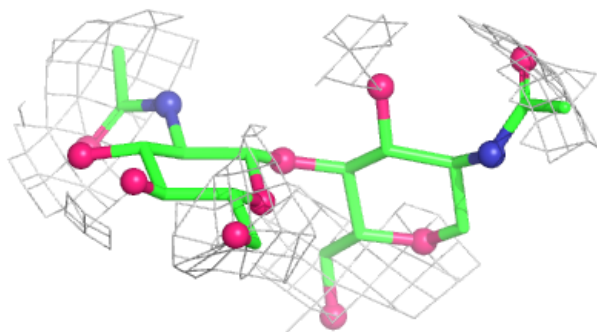
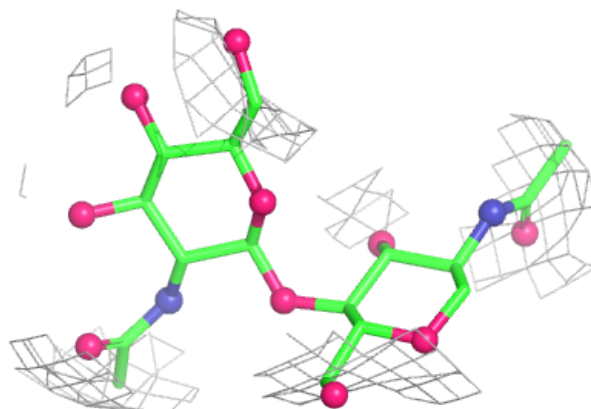
**Electron density around Chain H:**

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



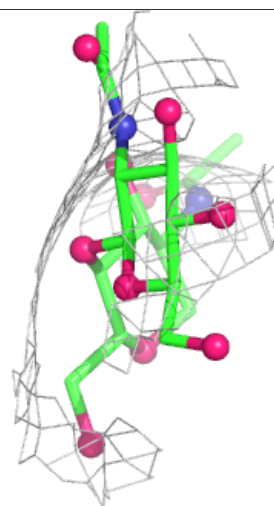
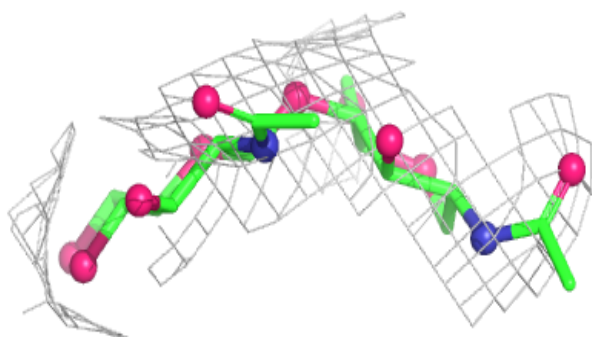
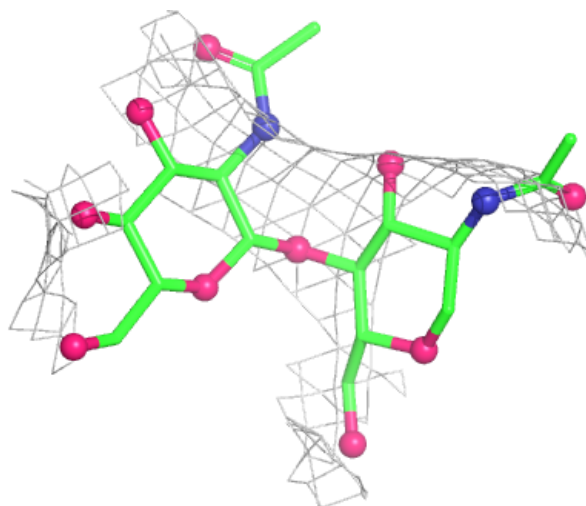
Electron density around Chain K:

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



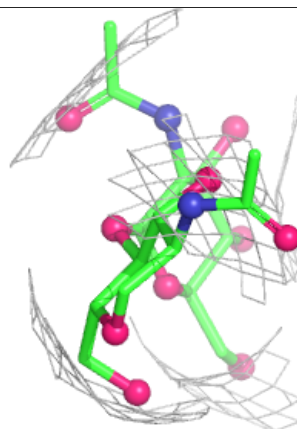
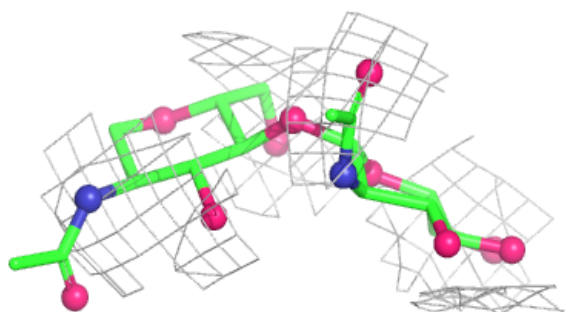
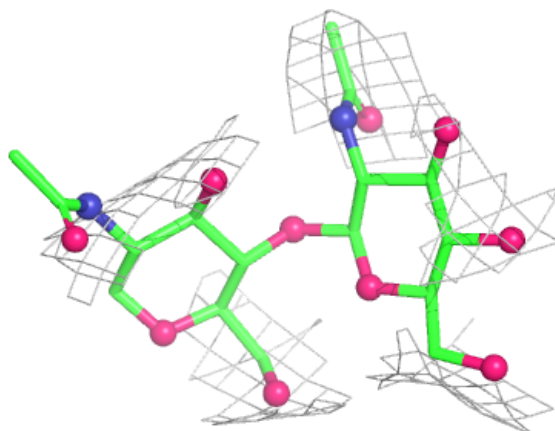
Electron density around Chain L:

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



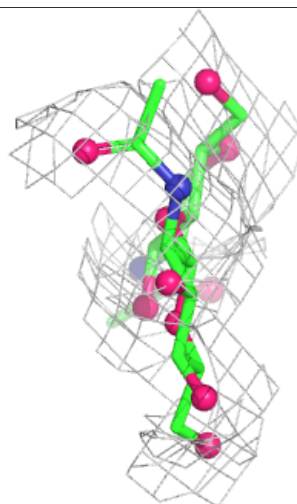
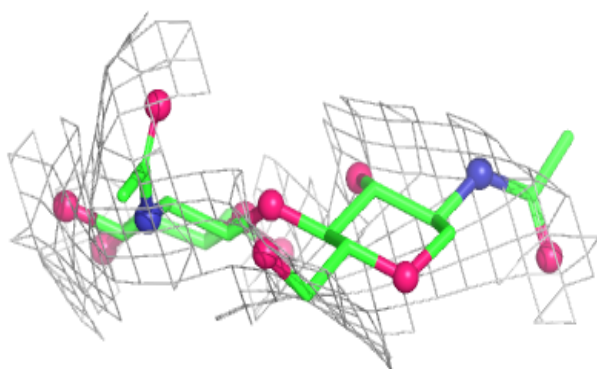
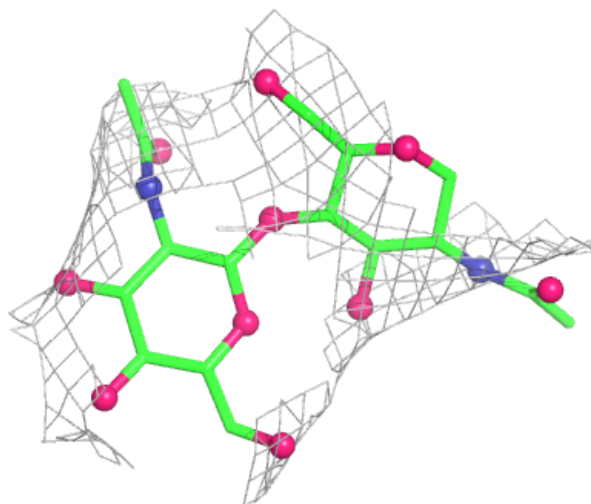
Electron density around Chain N:

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



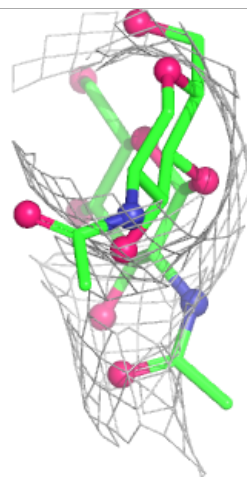
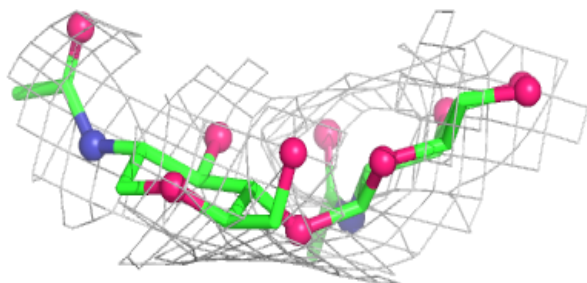
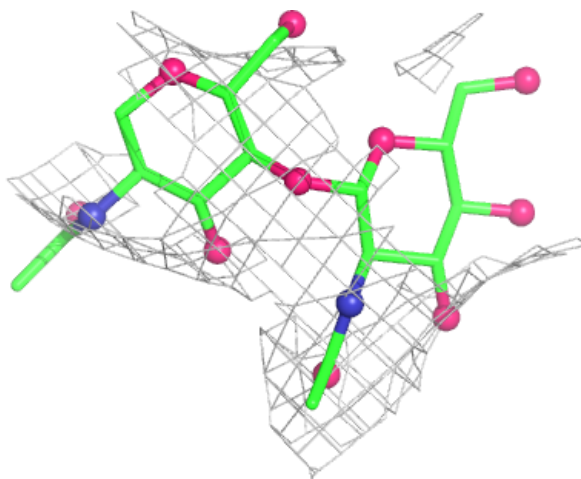
Electron density around Chain P:

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



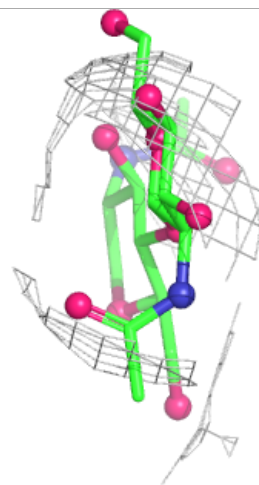
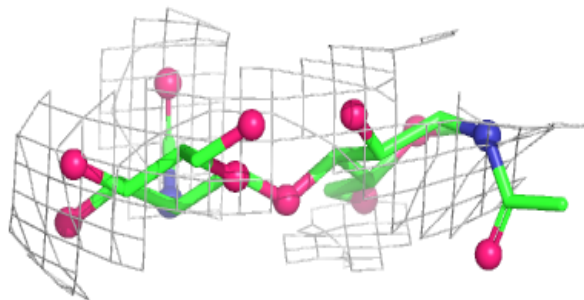
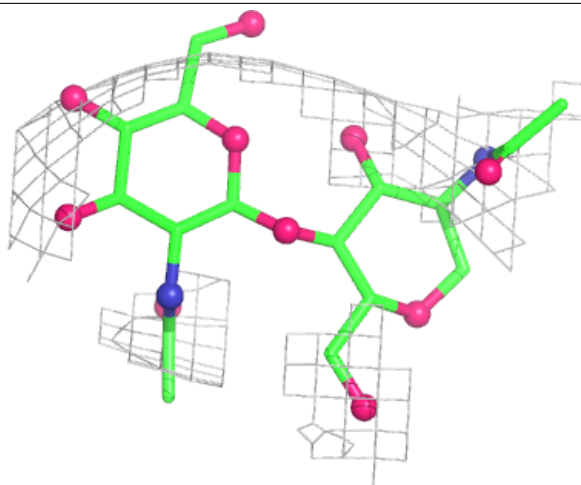
Electron density around Chain Q:

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



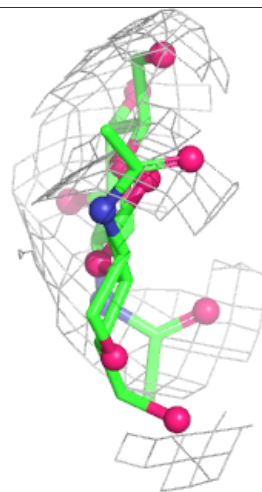
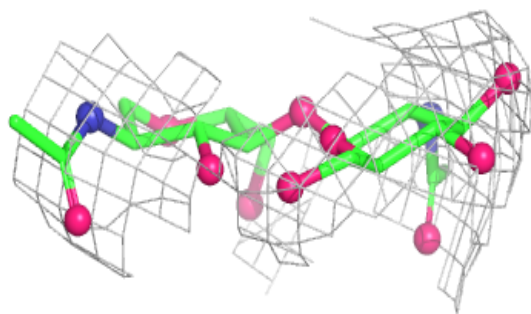
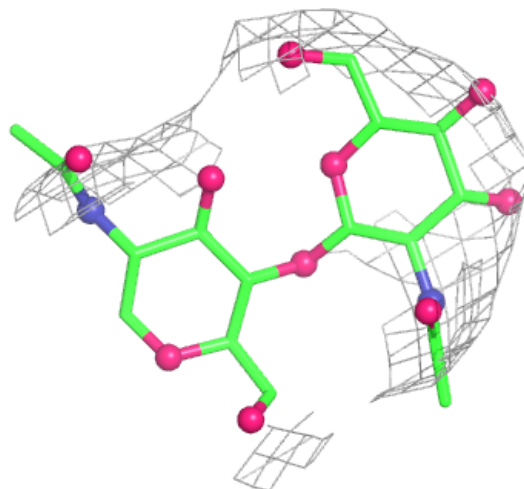
Electron density around Chain S:

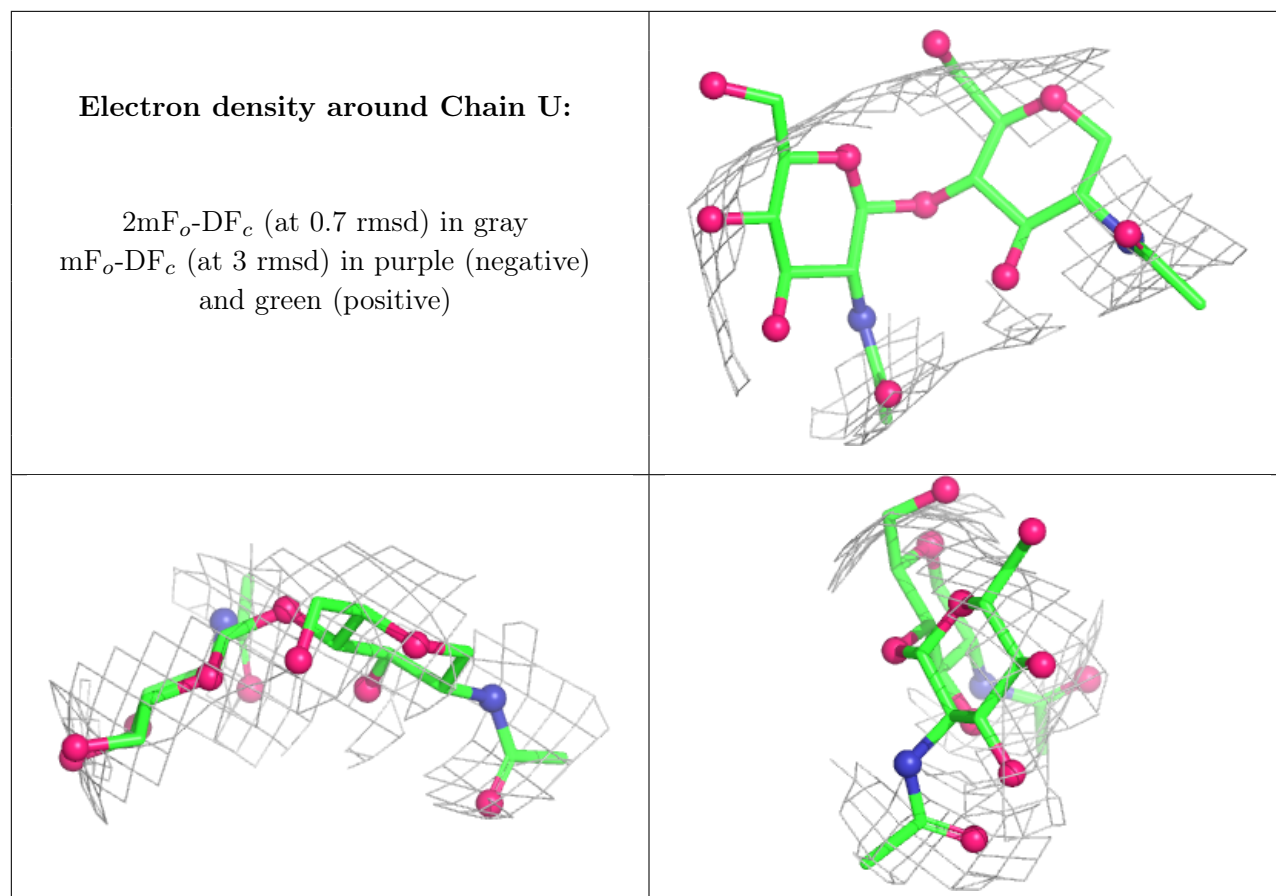
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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)





6.4 Ligands ⓘ

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
5	NAG	D	2003	14/15	-0.18	0.11	287,287,287,287	0
5	NAG	C	2003	14/15	0.46	0.13	296,297,297,297	0
5	NAG	B	2012	14/15	0.51	0.11	300,300,300,300	0
5	NAG	C	2001	14/15	0.62	0.09	297,298,298,299	0
5	NAG	D	2007	14/15	0.74	0.12	293,294,295,295	0
5	NAG	A	2019	14/15	0.76	0.09	300,300,300,300	0
5	NAG	D	2004	14/15	0.76	0.09	290,292,293,294	0
5	NAG	A	2013	14/15	0.76	0.08	292,299,300,300	0
5	NAG	C	2004	14/15	0.77	0.12	300,300,300,300	0
5	NAG	A	2008	14/15	0.80	0.06	297,299,300,300	0
5	NAG	C	2002	14/15	0.85	0.07	293,295,296,297	0

6.5 Other polymers [i](#)

There are no such residues in this entry.