



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 2, 2020 – 02:15 PM JST

PDB ID : 6LXJ
Title : Crystal structure of human Z2B3 Fab in complex with influenza virus neuraminidase from A/Anhui/1/2013 (H7N9)
Authors : Jiang, H.; Peng, W.; Qi, J.; Chai, Y.; Song, H.; Shi, Y.; Gao, G.F.; Wu, Y.
Deposited on : 2020-02-11
Resolution : 2.90 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

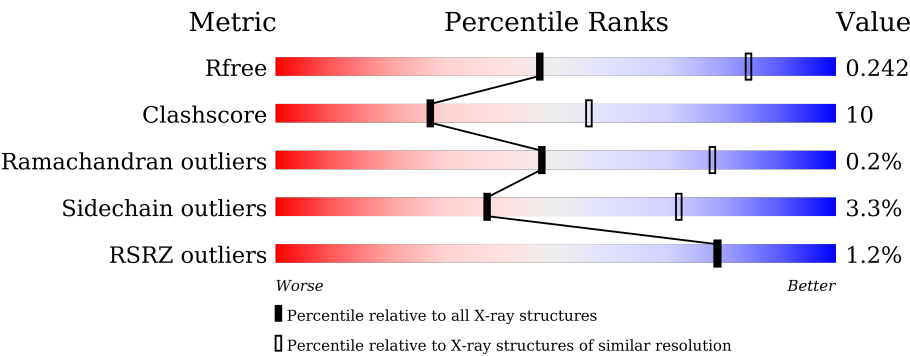
MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.14.6
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.14.6

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.90 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}	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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 on 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	388	<div><div></div><div>86%13%.</div></div>
1	B	388	<div><div></div><div>80%19%.</div></div>
1	C	388	<div><div></div><div>84%14%.</div></div>
1	D	388	<div><div></div><div>80%19%.</div></div>
2	E	237	<div><div>%</div><div>72%17%.10%</div></div>
2	H	237	<div><div>2%</div><div>74%21%5%</div></div>

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Mol	Chain	Length	Quality of chain
2	J	237	
2	M	237	
3	F	216	
3	K	216	
3	L	216	
3	N	216	
4	G	5	
5	I	9	
5	P	9	
5	R	9	
5	T	9	
6	O	4	
6	Q	4	
6	S	4	

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 25523 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Neuraminidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	388	Total	C	N	O	S	0	0	0
			3055	1902	541	589	23			
1	B	388	Total	C	N	O	S	0	0	0
			3055	1902	541	589	23			
1	C	388	Total	C	N	O	S	0	0	0
			3055	1902	541	589	23			
1	D	388	Total	C	N	O	S	0	0	0
			3055	1902	541	589	23			

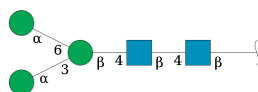
- Molecule 2 is a protein called Heavy chain of Z2B3 Fab.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	226	Total	C	N	O	S	0	0	0
			1694	1074	275	338	7			
2	E	214	Total	C	N	O	S	0	0	0
			1614	1026	262	319	7			
2	J	206	Total	C	N	O	S	0	0	0
			1561	993	253	308	7			
2	M	208	Total	C	N	O	S	0	0	0
			1563	994	255	307	7			

- Molecule 3 is a protein called Light chain of Z2B3 Fab.

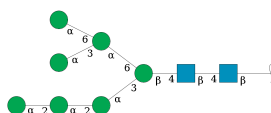
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	213	Total	C	N	O	S	0	0	0
			1579	982	262	330	5			
3	F	207	Total	C	N	O	S	0	0	0
			1540	960	256	319	5			
3	K	204	Total	C	N	O	S	0	0	0
			1517	948	251	313	5			
3	N	208	Total	C	N	O	S	0	0	0
			1544	962	257	320	5			

- Molecule 4 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[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
4	G	5	Total	C	N	O	0	0	0
			61	34	2	25			

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	I	9	Total	C	N	O	0	0	0
			105	58	2	45			
5	P	9	Total	C	N	O	0	0	0
			105	58	2	45			
5	R	9	Total	C	N	O	0	0	0
			105	58	2	45			
5	T	9	Total	C	N	O	0	0	0
			105	58	2	45			

- Molecule 6 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.



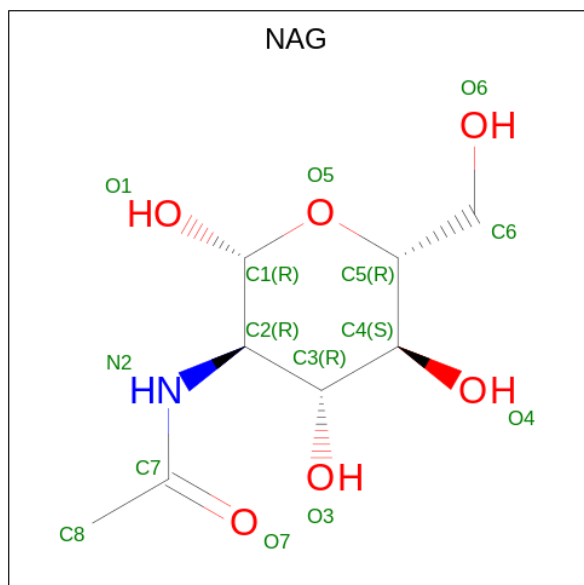
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	O	4	Total	C	N	O	0	0	0
			50	28	2	20			
6	Q	4	Total	C	N	O	0	0	0
			50	28	2	20			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	S	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$) (labeled as "Ligand of Interest" by author).



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

- Molecule 8 is CALCIUM ION (three-letter code: CA) (formula: Ca) (labeled as "Ligand of Interest" by author).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	B	1	Total	Ca	0	0
			1	1		
8	A	1	Total	Ca	0	0
			1	1		
8	D	1	Total	Ca	0	0
			1	1		

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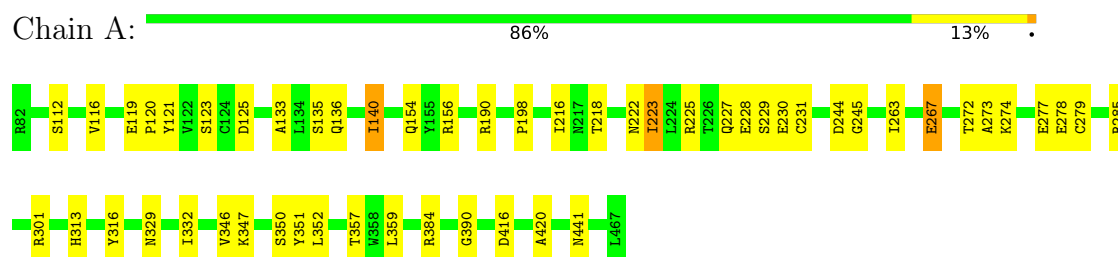
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	C	1	Total	Ca	0	0
			1	1		

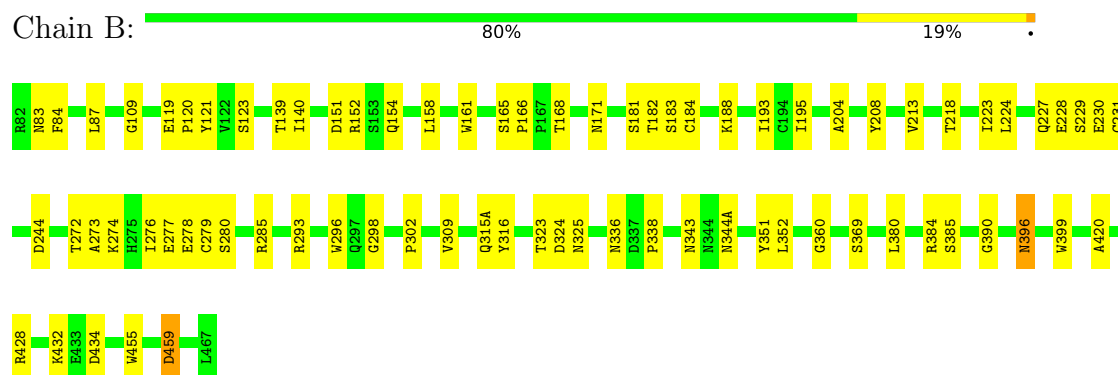
3 Residue-property plots

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.

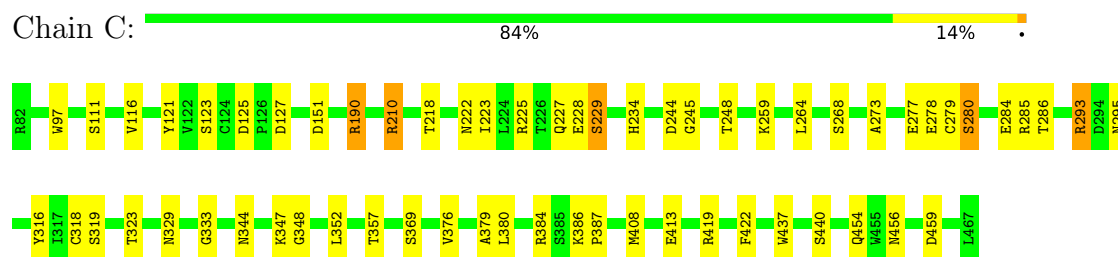
• Molecule 1: Neuraminidase



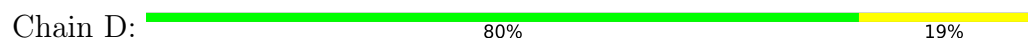
• Molecule 1: Neuraminidase

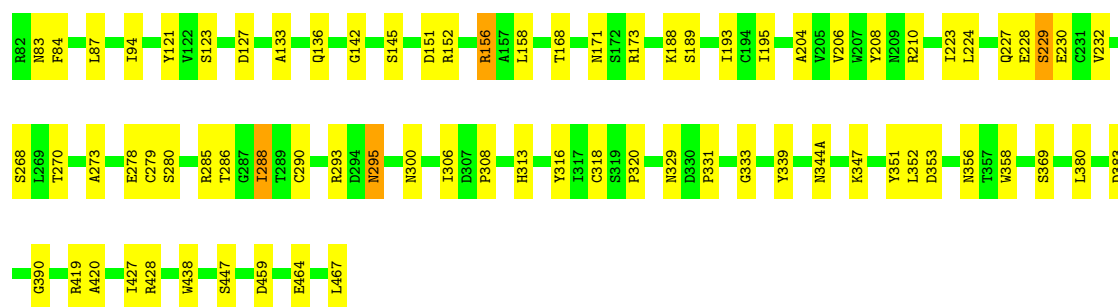


• Molecule 1: Neuraminidase

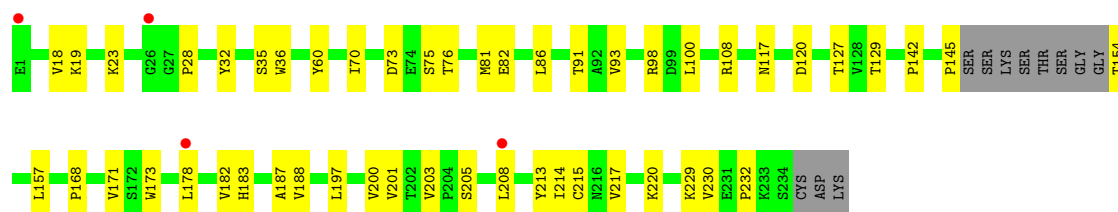
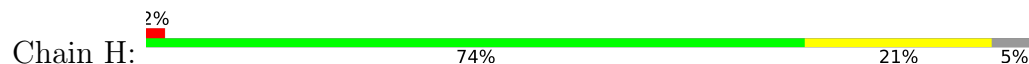


• Molecule 1: Neuraminidase

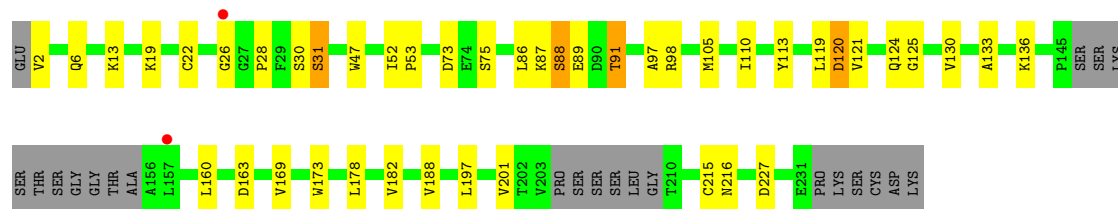




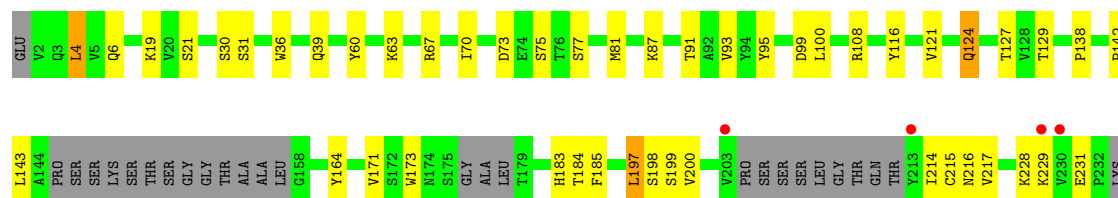
• Molecule 2: Heavy chain of Z2B3 Fab



• Molecule 2: Heavy chain of Z2B3 Fab



• Molecule 2: Heavy chain of Z2B3 Fab



• Molecule 2: Heavy chain of Z2B3 Fab







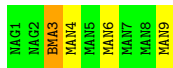
- Molecule 4: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G: 40% 40% 20%



- Molecule 5: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I: 56% 33% 11%



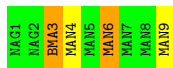
- Molecule 5: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain P: 33% 56% 11%



- Molecule 5: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain R: 56% 22% 22%



- Molecule 5: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-

(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain T:  56% 22% 22%

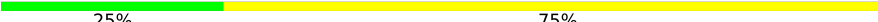


- Molecule 6: alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain O:  50% 50%



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

Chain Q:  25% 75%



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

Chain S:  75% 25%



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	201.31Å 207.51Å 207.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.91 – 2.90 48.91 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.1 (48.91-2.90) 99.1 (48.91-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.52 (at 2.91Å)	Xtriage
Refinement program	PHENIX 1.12_2829	Depositor
R, R_{free}	0.193 , 0.241 0.193 , 0.242	Depositor DCC
R_{free} test set	4742 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	52.8	Xtriage
Anisotropy	0.050	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 27.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.012 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	25523	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.31% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CA, BMA, NAG, MAN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.65	0/3137	0.65	0/4271
1	B	0.65	0/3137	0.66	0/4271
1	C	0.66	0/3137	0.69	0/4271
1	D	0.71	0/3137	0.68	0/4271
2	E	0.67	0/1652	0.62	0/2251
2	H	0.65	0/1735	0.62	0/2366
2	J	0.61	0/1598	0.67	0/2175
2	M	0.58	0/1600	0.59	0/2179
3	F	0.52	0/1575	0.61	0/2145
3	K	0.53	0/1551	0.61	0/2111
3	L	0.62	0/1616	0.62	0/2205
3	N	0.52	0/1580	0.64	0/2154
All	All	0.63	0/25455	0.65	0/34670

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3055	0	2877	40	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3055	0	2877	53	0
1	C	3055	0	2877	50	0
1	D	3055	0	2877	53	0
2	E	1614	0	1574	35	0
2	H	1694	0	1657	39	0
2	J	1561	0	1516	38	0
2	M	1563	0	1528	34	0
3	F	1540	0	1488	37	0
3	K	1517	0	1465	52	0
3	L	1579	0	1518	38	0
3	N	1544	0	1488	54	0
4	G	61	0	52	2	0
5	I	105	0	88	1	0
5	P	105	0	88	3	0
5	R	105	0	88	2	0
5	T	105	0	88	2	0
6	O	50	0	43	3	0
6	Q	50	0	43	4	0
6	S	50	0	43	0	0
7	A	14	0	13	0	0
7	B	14	0	13	1	0
7	C	14	0	13	0	0
7	D	14	0	13	0	0
8	A	1	0	0	0	0
8	B	1	0	0	0	0
8	C	1	0	0	0	0
8	D	1	0	0	0	0
All	All	25523	0	24327	496	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 10.

All (496) 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)
3:K:27:SER:HB2	3:K:95:ARG:HG3	1.46	0.97
1:C:437:TRP:CD1	6:Q:1:NAG:H82	2.00	0.97
2:J:228:LYS:NZ	3:K:127:GLU:OE1	1.99	0.94
1:C:123:SER:OG	1:C:190:ARG:NH2	2.01	0.93
1:D:121:TYR:CD1	1:D:228:GLU:O	2.23	0.92
1:C:125:ASP:OD1	1:C:190:ARG:NH1	2.03	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:121:TYR:CD1	1:C:228:GLU:O	2.25	0.90
1:C:210:ARG:HG3	1:C:210:ARG:HH11	1.35	0.89
3:L:87:ASP:OD1	3:L:106:LYS:NZ	2.08	0.87
3:N:187:GLU:OE1	3:N:187:GLU:N	2.06	0.87
1:B:121:TYR:CD1	1:B:228:GLU:O	2.29	0.86
2:E:188:VAL:HG22	3:F:166:THR:HG22	1.59	0.85
3:N:185:THR:HG22	3:N:187:GLU:OE1	1.77	0.85
2:M:169:VAL:CG2	2:M:197:LEU:HD21	2.06	0.85
2:M:35:SER:HG	2:M:47:TRP:HE1	1.25	0.84
1:C:227:GLN:HB3	1:C:279:CYS:O	1.77	0.84
1:A:301:ARG:NH2	1:A:346:VAL:O	2.11	0.84
2:E:73:ASP:OD2	6:O:3:BMA:H5	1.82	0.80
1:C:413:GLU:O	1:C:419:ARG:NH2	2.14	0.80
2:H:145:PRO:HD2	2:H:232:PRO:HA	1.63	0.78
2:H:182:VAL:HG12	2:H:201:VAL:HG22	1.66	0.78
2:J:214:ILE:HD13	2:J:229:LYS:CG	2.14	0.77
1:B:123:SER:HB2	1:B:230:GLU:HG3	1.67	0.77
1:A:121:TYR:CD1	1:A:228:GLU:O	2.37	0.77
1:D:428:ARG:NH1	1:D:459:ASP:OD2	2.18	0.77
3:K:81:GLN:NE2	3:K:83:GLU:OE2	2.18	0.76
2:E:178:LEU:HD21	2:E:201:VAL:HG11	1.68	0.76
1:C:284:GLU:OE1	1:C:285:ARG:NH1	2.19	0.76
3:N:185:THR:HB	3:N:188:GLN:HB2	1.67	0.75
1:C:210:ARG:NH1	1:C:210:ARG:HG3	2.01	0.74
2:H:145:PRO:HG3	2:H:157:LEU:HB3	1.69	0.74
3:K:27:SER:HB2	3:K:95:ARG:CG	2.18	0.74
3:F:15:GLY:HA2	3:F:79:GLY:HA2	1.70	0.74
2:M:28:PRO:HB2	2:M:32:TYR:CE1	2.23	0.73
3:L:63:ARG:NH2	3:L:84:ASP:OD2	2.22	0.72
1:D:227:GLN:HA	1:D:278:GLU:HA	1.71	0.72
1:C:376:VAL:HG23	1:C:379:ALA:HB2	1.71	0.71
3:N:125:SER:O	3:N:129:LEU:HD12	1.89	0.71
2:M:169:VAL:CG2	2:M:197:LEU:CD2	2.68	0.71
1:D:227:GLN:HB3	1:D:279:CYS:O	1.91	0.71
2:H:93:VAL:HG22	2:H:127:THR:HG22	1.71	0.71
2:J:214:ILE:HD13	2:J:229:LYS:HG2	1.73	0.71
3:N:166:THR:HB	3:N:179:SER:H	1.55	0.70
3:K:185:THR:N	3:K:188:GLN:OE1	2.25	0.69
3:N:190:LYS:O	3:N:190:LYS:HE3	1.90	0.69
3:F:39:GLN:HB2	3:F:88:TYR:CE1	2.27	0.69
2:H:214:ILE:HG12	2:H:229:LYS:HB2	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:142:ASP:OD1	3:N:171:GLN:NE2	2.23	0.69
2:E:19:LYS:NZ	6:O:4:MAN:O2	2.26	0.69
1:A:227:GLN:HA	1:A:278:GLU:HA	1.75	0.68
1:B:344(A):ASN:ND2	2:E:105:MET:O	2.27	0.68
3:F:37:TRP:HD1	3:F:50:ILE:HD11	1.59	0.67
3:F:50:ILE:HD13	3:F:54:SER:H	1.59	0.67
3:L:17:SER:HB2	3:L:78:SER:HA	1.76	0.67
2:M:197:LEU:HD12	2:M:197:LEU:C	2.15	0.67
3:F:7:PRO:O	3:F:105:THR:HG22	1.95	0.67
1:B:434:ASP:OD2	2:E:31:SER:OG	2.11	0.66
3:N:198:GLN:NE2	3:N:207:GLU:OE2	2.24	0.66
3:L:171:GLN:OE1	3:L:171:GLN:N	2.25	0.65
2:J:91:THR:HG23	2:J:129:THR:HA	1.79	0.65
3:K:187:GLU:OE1	3:K:187:GLU:N	2.28	0.65
3:F:148:VAL:HG12	3:F:201:HIS:HB2	1.77	0.65
2:H:28:PRO:HD2	2:H:98:ARG:HH12	1.62	0.65
1:D:195:ILE:HG12	1:D:204:ALA:HB2	1.80	0.64
3:F:67:SER:OG	3:F:68:LYS:N	2.30	0.64
2:E:182:VAL:HG22	2:E:201:VAL:HG22	1.80	0.63
2:H:201:VAL:HG12	2:H:203:VAL:HG13	1.79	0.63
1:A:227:GLN:HB3	1:A:279:CYS:O	1.98	0.63
2:J:93:VAL:HG22	2:J:127:THR:HG22	1.80	0.63
3:L:19:THR:HG23	3:L:76:THR:HG22	1.81	0.63
1:D:173:ARG:HH11	1:D:210:ARG:HH12	1.45	0.62
2:J:185:PHE:O	2:J:197:LEU:HD12	1.98	0.62
3:F:63:ARG:HD2	3:F:78:SER:O	1.99	0.62
3:N:155:ASP:HB2	3:N:193:ARG:HB3	1.80	0.62
1:D:127:ASP:N	1:D:127:ASP:OD1	2.31	0.62
1:B:278:GLU:OE1	1:B:293:ARG:NH1	2.32	0.62
1:C:227:GLN:O	1:C:228:GLU:CB	2.48	0.61
1:D:227:GLN:O	1:D:228:GLU:CB	2.48	0.61
3:L:26:SER:HA	3:L:30:GLY:HA3	1.83	0.61
2:J:63:LYS:HD2	2:J:63:LYS:O	2.00	0.61
1:A:119:GLU:N	1:A:120:PRO:HD3	2.16	0.61
1:A:125:ASP:OD1	1:A:190:ARG:NH2	2.28	0.61
2:H:120:ASP:HB3	3:L:48:LEU:HD23	1.83	0.61
3:L:11:SER:HB3	3:L:108:THR:HB	1.83	0.61
3:N:153:LYS:HE3	3:N:156:SER:HA	1.83	0.61
1:D:273:ALA:HA	1:D:316:TYR:CE1	2.36	0.61
3:N:80:LEU:HD21	3:N:109:VAL:HG22	1.82	0.61
2:J:4:LEU:HD11	2:J:121:VAL:HG12	1.81	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:227:GLN:O	1:A:228:GLU:CB	2.48	0.60
1:D:145:SER:HB2	1:D:438:TRP:HB3	1.84	0.60
2:H:18:VAL:HG12	2:H:86:LEU:HD11	1.82	0.60
2:M:28:PRO:HB2	2:M:32:TYR:HE1	1.66	0.60
2:J:30:SER:O	2:J:31:SER:OG	2.19	0.60
3:N:148:VAL:HG12	3:N:201:HIS:HB2	1.84	0.60
2:J:4:LEU:CD1	2:J:121:VAL:HG12	2.32	0.60
3:N:154:ALA:HA	3:N:195:TYR:HA	1.82	0.60
1:B:227:GLN:O	1:B:228:GLU:CB	2.48	0.59
2:E:87:LYS:O	2:E:130:VAL:HG21	2.01	0.59
4:G:3:BMA:H3	4:G:4:MAN:H5	1.85	0.59
2:H:73:ASP:OD1	2:H:75:SER:OG	2.19	0.59
1:D:195:ILE:HD13	1:D:224:LEU:HG	1.85	0.59
3:K:33:ASN:CA	3:K:53:VAL:HG21	2.32	0.59
1:C:437:TRP:NE1	6:Q:1:NAG:H82	2.16	0.59
2:H:154:THR:N	2:H:205:SER:HG	2.01	0.59
2:H:203:VAL:HG11	2:H:213:TYR:CE1	2.38	0.59
1:B:272:THR:OG1	1:B:315(A):GLN:HA	2.02	0.58
2:E:91:THR:HG22	2:E:130:VAL:H	1.67	0.58
3:N:6:GLN:NE2	3:N:105:THR:HG23	2.18	0.58
3:N:153:LYS:HD3	3:N:198:GLN:NE2	2.18	0.58
1:C:227:GLN:C	1:C:228:GLU:HG2	2.24	0.58
3:F:171:GLN:HG2	3:F:175:LYS:O	2.04	0.58
2:H:157:LEU:HD12	2:H:230:VAL:CG2	2.33	0.58
1:B:227:GLN:C	1:B:228:GLU:HG2	2.24	0.58
3:N:187:GLU:C	3:N:189:TRP:N	2.55	0.58
3:L:32:TYR:N	3:L:32:TYR:CD1	2.71	0.58
1:A:227:GLN:C	1:A:228:GLU:HG2	2.24	0.58
1:D:136:GLN:HG2	1:D:156:ARG:HE	1.69	0.58
1:D:227:GLN:C	1:D:228:GLU:HG2	2.24	0.58
2:M:169:VAL:HG21	2:M:197:LEU:HD21	1.82	0.57
1:D:173:ARG:NH1	1:D:210:ARG:HH12	2.03	0.57
2:M:218:ASN:HD22	2:M:225:LYS:HG3	1.68	0.57
1:A:223:ILE:O	1:A:223:ILE:HG22	2.03	0.57
2:J:116:TYR:HH	3:K:38:TYR:HH	1.51	0.57
3:N:7:PRO:O	3:N:105:THR:HG22	2.05	0.57
2:J:73:ASP:OD1	2:J:75:SER:OG	2.21	0.57
2:H:19:LYS:HZ2	4:G:5:MAN:H4	1.69	0.56
2:M:169:VAL:HG22	2:M:197:LEU:CD2	2.35	0.56
1:B:87:LEU:O	1:B:285:ARG:HA	2.05	0.56
3:K:27:SER:CB	3:K:95:ARG:HG3	2.30	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:125:SER:O	3:F:129:LEU:HD12	2.05	0.56
3:N:65:SER:OG	3:N:76:THR:O	2.22	0.56
1:D:227:GLN:O	1:D:228:GLU:HG2	2.06	0.56
2:E:73:ASP:OD1	2:E:75:SER:OG	2.20	0.56
1:A:227:GLN:O	1:A:228:GLU:HG2	2.06	0.56
1:B:83:ASN:HB2	7:B:501:NAG:H83	1.87	0.56
1:C:227:GLN:HA	1:C:278:GLU:HA	1.86	0.56
1:B:227:GLN:O	1:B:228:GLU:HG2	2.06	0.56
2:E:136:LYS:NZ	2:E:163:ASP:O	2.37	0.56
1:B:227:GLN:HA	1:B:278:GLU:HA	1.87	0.55
2:E:73:ASP:OD2	6:O:3:BMA:C5	2.53	0.55
2:H:208:LEU:HD12	2:H:208:LEU:H	1.71	0.55
3:K:33:ASN:HA	3:K:53:VAL:HG21	1.87	0.55
2:M:116:TYR:HB3	3:N:93:TYR:HB2	1.86	0.55
2:M:145:PRO:HG3	2:M:157:LEU:HB3	1.88	0.55
1:C:121:TYR:CE1	1:C:228:GLU:O	2.60	0.55
1:C:227:GLN:O	1:C:228:GLU:HB2	2.07	0.55
1:C:227:GLN:O	1:C:228:GLU:HG2	2.06	0.55
1:C:437:TRP:NE1	6:Q:1:NAG:C8	2.70	0.55
3:N:136:LEU:HD11	3:N:184:LEU:HD11	1.87	0.55
1:D:94:ILE:HG23	1:D:447:SER:HB2	1.88	0.55
3:F:173:ASN:HD22	3:F:175:LYS:HG3	1.71	0.55
3:K:142:ASP:HA	3:K:175:LYS:HB2	1.88	0.55
1:A:272:THR:O	1:A:274:LYS:NZ	2.39	0.55
1:B:182:THR:OG1	1:B:229:SER:O	2.14	0.55
2:M:218:ASN:HB2	2:M:225:LYS:HG2	1.87	0.55
1:B:168:THR:OG1	1:B:171:ASN:OD1	2.18	0.55
2:E:188:VAL:HG22	3:F:166:THR:CG2	2.35	0.55
2:E:89:GLU:N	2:E:89:GLU:OE1	2.39	0.55
3:N:171:GLN:HE21	3:N:173:ASN:HB3	1.70	0.55
1:A:119:GLU:N	1:A:120:PRO:CD	2.70	0.55
1:A:227:GLN:O	1:A:347:LYS:HE2	2.07	0.55
1:B:227:GLN:HB3	1:B:279:CYS:O	2.07	0.55
2:M:36:TRP:CE2	2:M:81:MET:HB2	2.42	0.54
1:A:227:GLN:O	1:A:228:GLU:HB2	2.07	0.54
3:F:50:ILE:CD1	3:F:54:SER:H	2.20	0.54
2:J:19:LYS:NZ	6:Q:4:MAN:O2	2.41	0.54
1:D:353:ASP:HB3	1:D:356:ASN:HB3	1.90	0.54
2:M:190:GLN:HG2	3:N:164:GLU:OE1	2.07	0.54
1:D:193:ILE:HG12	1:D:206:VAL:HG13	1.90	0.54
2:J:60:TYR:HE1	2:J:70:ILE:HG13	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:227:GLN:O	1:D:228:GLU:HB2	2.07	0.54
1:C:218:THR:OG1	1:C:244:ASP:OD2	2.18	0.54
3:N:152:TRP:O	3:N:159:VAL:HG22	2.07	0.54
1:B:396:ASN:ND2	1:B:396:ASN:O	2.31	0.54
2:H:173:TRP:HB3	2:H:178:LEU:HD23	1.89	0.54
1:C:127:ASP:N	1:C:127:ASP:OD1	2.39	0.54
3:F:37:TRP:CD1	3:F:50:ILE:HD11	2.42	0.54
2:J:185:PHE:CZ	3:K:139:LEU:HB3	2.43	0.54
3:L:132:ASN:ND2	3:L:132:ASN:O	2.41	0.53
1:B:227:GLN:O	1:B:228:GLU:HB2	2.07	0.53
1:B:208:TYR:HB3	1:B:213:VAL:HG21	1.90	0.53
3:K:7:PRO:O	3:K:105:THR:OG1	2.16	0.53
2:E:91:THR:HG22	2:E:130:VAL:CG2	2.38	0.53
2:H:208:LEU:HB3	2:H:232:PRO:HG2	1.90	0.53
3:L:196:SER:OG	3:L:209:THR:HG22	2.08	0.53
3:L:63:ARG:HB3	3:L:78:SER:O	2.09	0.53
1:A:416:ASP:OD1	1:A:416:ASP:N	2.39	0.53
3:K:41:HIS:CD2	3:K:86:ALA:HB2	2.43	0.53
3:N:47:LYS:HG2	3:N:49:MET:HE3	1.89	0.53
1:D:464:GLU:HA	1:D:467:LEU:HG	1.91	0.53
3:F:124:PRO:HB2	3:F:129:LEU:HD11	1.90	0.53
2:J:36:TRP:HD1	2:J:70:ILE:HD13	1.74	0.53
2:H:117:ASN:O	3:L:51:TYR:HB2	2.09	0.53
1:B:351:TYR:CE2	1:B:420:ALA:HB1	2.44	0.52
1:D:123:SER:HB2	1:D:230:GLU:HB3	1.91	0.52
3:K:124:PRO:HD3	3:K:136:LEU:HD23	1.91	0.52
2:M:169:VAL:HG12	2:M:219:HIS:CD2	2.45	0.52
3:N:11:SER:HB3	3:N:108:THR:OG1	2.09	0.52
1:A:222:ASN:HB3	1:A:245:GLY:HA2	1.91	0.52
1:C:278:GLU:OE1	1:C:293:ARG:NH1	2.42	0.52
2:J:197:LEU:HG	2:J:198:SER:N	2.24	0.52
1:B:272:THR:HG21	1:B:336:ASN:OD1	2.09	0.52
1:B:123:SER:CB	1:B:230:GLU:HG3	2.37	0.52
1:C:273:ALA:HA	1:C:316:TYR:CE1	2.45	0.52
1:C:376:VAL:CG2	1:C:379:ALA:HB2	2.39	0.52
3:L:185:THR:OG1	3:L:187:GLU:OE1	2.25	0.52
2:J:99:ASP:OD1	2:J:100:LEU:N	2.43	0.51
2:J:143:LEU:HB3	3:K:122:PHE:CD2	2.46	0.51
3:K:125:SER:O	3:K:129:LEU:HD12	2.10	0.51
3:L:39:GLN:HB2	3:L:88:TYR:CE1	2.46	0.51
2:M:184:THR:HG22	2:M:199:SER:OG	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:149:THR:HG23	3:F:200:THR:OG1	2.10	0.51
3:F:57:PRO:HD2	3:F:60:VAL:HG21	1.92	0.51
1:B:276:ILE:O	1:B:277:GLU:HG2	2.10	0.51
3:N:154:ALA:HB2	3:N:195:TYR:CE2	2.46	0.51
3:L:38:TYR:O	3:L:88:TYR:HA	2.10	0.51
1:D:121:TYR:HD1	1:D:228:GLU:O	1.88	0.51
2:J:200:VAL:HG21	3:K:139:LEU:HD13	1.92	0.51
2:E:124:GLN:HG2	2:E:125:GLY:N	2.25	0.51
2:E:169:VAL:HG22	2:E:197:LEU:HD21	1.93	0.50
2:H:168:PRO:O	2:H:220:LYS:NZ	2.43	0.50
3:K:12:GLY:O	3:K:109:VAL:HA	2.11	0.50
3:F:185:THR:HG22	3:F:188:GLN:HG2	1.93	0.50
1:D:168:THR:OG1	1:D:171:ASN:OD1	2.12	0.50
3:F:53:VAL:O	3:F:54:SER:OG	2.23	0.50
1:B:273:ALA:HA	1:B:316:TYR:CE1	2.47	0.50
1:C:329:ASN:HA	5:P:6:MAN:O3	2.11	0.50
2:E:28:PRO:HD2	2:E:98:ARG:NH2	2.26	0.50
3:K:125:SER:O	3:K:128:GLU:N	2.45	0.50
2:J:116:TYR:HB3	3:K:93:TYR:HB2	1.94	0.50
3:K:186:PRO:O	3:K:189:TRP:HB3	2.11	0.50
3:L:154:ALA:HB2	3:L:195:TYR:CE1	2.47	0.50
1:D:133:ALA:O	1:D:158:LEU:HD12	2.11	0.49
3:K:187:GLU:O	3:K:191:SER:HB2	2.12	0.49
3:N:187:GLU:C	3:N:189:TRP:H	2.14	0.49
3:K:49:MET:O	3:K:50:ILE:HD13	2.13	0.49
1:A:329:ASN:HA	5:T:6:MAN:O3	2.11	0.49
2:E:120:ASP:OD1	2:E:121:VAL:HG23	2.12	0.49
1:A:332:ILE:HG12	1:A:384:ARG:HD3	1.94	0.49
3:N:155:ASP:CB	3:N:193:ARG:HB3	2.42	0.49
3:K:33:ASN:CB	3:K:53:VAL:HG21	2.43	0.49
1:A:120:PRO:HG3	1:A:441:ASN:ND2	2.28	0.49
2:J:173:TRP:CZ3	2:J:215:CYS:HB3	2.48	0.49
3:N:14:PRO:HD3	3:N:111:GLY:H	1.77	0.49
2:J:138:PRO:HB3	2:J:164:TYR:HB3	1.95	0.49
1:C:227:GLN:O	1:C:228:GLU:CG	2.61	0.49
1:A:227:GLN:O	1:A:228:GLU:CG	2.61	0.48
3:F:47:LYS:HG2	3:F:49:MET:HE2	1.95	0.48
1:D:227:GLN:O	1:D:228:GLU:CG	2.61	0.48
1:B:218:THR:OG1	1:B:244:ASP:OD2	2.25	0.48
2:H:28:PRO:HG2	2:H:32:TYR:CE1	2.48	0.48
2:J:184:THR:HG22	2:J:199:SER:OG	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:184:LEU:HD22	3:F:188:GLN:HG3	1.94	0.48
1:D:320:PRO:HD3	1:D:383:ASP:O	2.13	0.48
1:C:277:GLU:HB2	1:C:293:ARG:HD2	1.94	0.48
3:L:37:TRP:CZ3	3:L:90:CYS:HB3	2.49	0.48
1:A:116:VAL:HG12	1:A:136:GLN:HG3	1.96	0.48
1:C:210:ARG:CG	1:C:210:ARG:HH11	2.15	0.48
1:C:376:VAL:HG12	1:C:387:PRO:HA	1.96	0.48
3:F:9:SER:OG	3:F:106:LYS:HB2	2.14	0.48
1:B:227:GLN:O	1:B:228:GLU:CG	2.61	0.48
1:D:270:THR:HG22	1:D:313:HIS:NE2	2.29	0.48
2:H:60:TYR:HE1	2:H:70:ILE:HG13	1.79	0.48
1:B:166:PRO:O	1:B:168:THR:HG23	2.14	0.47
2:E:2:VAL:HG22	2:E:26:GLY:O	2.13	0.47
2:E:13:LYS:NZ	2:E:133:ALA:O	2.46	0.47
3:K:186:PRO:O	3:K:190:LYS:HG3	2.14	0.47
3:N:173:ASN:OD1	3:N:173:ASN:O	2.32	0.47
1:B:352:LEU:HD13	1:B:380:LEU:HD13	1.96	0.47
2:M:158:GLY:HA2	2:M:173:TRP:CH2	2.49	0.47
3:N:50:ILE:HD11	3:N:56:ARG:HG2	1.97	0.47
1:D:121:TYR:CG	1:D:229:SER:HA	2.50	0.47
1:D:351:TYR:CE2	1:D:420:ALA:HB1	2.50	0.47
3:L:153:LYS:HD2	3:L:198:GLN:NE2	2.29	0.47
1:A:218:THR:OG1	1:A:244:ASP:OD2	2.26	0.47
2:E:88:SER:O	2:E:91:THR:HG23	2.14	0.47
3:K:22:CYS:HB2	3:K:37:TRP:CH2	2.49	0.47
1:A:352:LEU:HA	1:A:357:THR:HG23	1.97	0.47
1:A:350:SER:HB2	1:A:359:LEU:HD23	1.96	0.47
3:K:198:GLN:NE2	3:K:207:GLU:OE1	2.44	0.47
3:L:18:ILE:HD11	3:L:77:ILE:HD12	1.97	0.47
1:C:116:VAL:HG13	1:C:440:SER:HB2	1.97	0.47
3:K:39:GLN:HB2	3:K:88:TYR:CE1	2.49	0.47
1:C:386:LYS:HD2	5:P:5:MAN:H61	1.97	0.47
2:J:142:PRO:O	3:K:125:SER:HB2	2.15	0.47
3:K:152:TRP:HB2	3:K:159:VAL:HG13	1.96	0.47
2:M:101:GLN:O	2:M:115:TYR:OH	2.25	0.47
1:D:189:SER:HB2	1:D:208:TYR:CZ	2.50	0.47
3:K:53:VAL:HG12	3:K:53:VAL:O	2.15	0.46
1:B:161:TRP:NE1	1:B:165:SER:O	2.48	0.46
2:H:36:TRP:CE2	2:H:81:MET:HB2	2.50	0.46
3:N:6:GLN:HE21	3:N:105:THR:HG23	1.80	0.46
1:D:84:PHE:CE1	1:D:188:LYS:HD3	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:36:TRP:CE2	2:J:81:MET:HB2	2.50	0.46
1:B:296:TRP:C	1:B:296:TRP:CD1	2.86	0.46
2:J:185:PHE:CD1	3:K:139:LEU:HD22	2.51	0.46
3:K:142:ASP:HB3	3:K:175:LYS:NZ	2.30	0.46
3:K:63:ARG:O	3:K:77:ILE:HA	2.15	0.46
2:E:30:SER:HA	2:E:53:PRO:HB2	1.97	0.46
2:H:23:LYS:NZ	2:H:76:THR:O	2.49	0.46
3:L:32:TYR:O	3:L:68:LYS:NZ	2.48	0.46
3:N:154:ALA:HA	3:N:194:SER:O	2.15	0.46
1:A:216:ILE:HG12	1:A:263:ILE:HD11	1.98	0.46
1:C:151:ASP:OD2	2:J:108:ARG:HA	2.16	0.46
1:C:229:SER:HB3	1:C:347:LYS:HE2	1.96	0.46
3:N:196:SER:OG	3:N:209:THR:HG23	2.15	0.46
1:B:195:ILE:HG12	1:B:204:ALA:HB2	1.96	0.46
2:H:19:LYS:HG3	2:H:82:GLU:HB2	1.97	0.46
2:M:91:THR:HG23	2:M:129:THR:HA	1.98	0.46
1:C:352:LEU:HD13	1:C:380:LEU:HD13	1.98	0.46
3:F:12:GLY:O	3:F:109:VAL:HA	2.15	0.46
1:D:329:ASN:HA	5:R:6:MAN:O3	2.16	0.46
1:A:121:TYR:CE1	1:A:228:GLU:O	2.69	0.46
1:B:296:TRP:O	1:B:343:ASN:HA	2.14	0.46
1:D:295:ASN:OD1	1:D:344(A):ASN:C	2.55	0.46
2:E:91:THR:HG22	2:E:130:VAL:HG22	1.98	0.46
1:B:390:GLY:HA3	5:I:3:BMA:O2	2.14	0.46
3:K:68:LYS:HA	3:K:73:ALA:HA	1.98	0.46
1:A:120:PRO:HB3	1:A:133:ALA:HB2	1.96	0.46
1:D:300:ASN:ND2	1:D:316:TYR:CD2	2.84	0.46
2:E:28:PRO:HD2	2:E:98:ARG:HH21	1.80	0.46
3:F:18:ILE:HD13	3:F:80:LEU:HD11	1.96	0.46
2:H:220:LYS:HD3	2:H:220:LYS:H	1.81	0.46
1:D:229:SER:HB3	1:D:347:LYS:HE2	1.98	0.45
3:N:10:VAL:HG23	3:N:107:LEU:HD13	1.97	0.45
3:N:27:SER:OG	3:N:28:ASP:OD1	2.23	0.45
3:N:47:LYS:HE3	3:N:49:MET:CE	2.46	0.45
1:A:225:ARG:HE	1:A:277:GLU:CD	2.20	0.45
1:B:351:TYR:CZ	1:B:420:ALA:HB1	2.51	0.45
2:E:216:ASN:ND2	2:E:227:ASP:OD1	2.45	0.45
2:E:52:ILE:HD12	2:E:113:TYR:CE1	2.51	0.45
2:J:87:LYS:HE3	2:J:87:LYS:HB2	1.53	0.45
3:L:190:LYS:HE2	3:L:190:LYS:HB3	1.77	0.45
3:N:49:MET:O	3:N:50:ILE:HD12	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:84:PHE:CE1	1:B:188:LYS:HD2	2.51	0.45
3:F:85:GLU:OE2	3:F:109:VAL:HG22	2.15	0.45
1:C:97:TRP:CE3	1:C:422:PHE:HE1	2.35	0.45
1:D:390:GLY:HA3	5:R:3:BMA:O2	2.17	0.45
1:D:352:LEU:HD13	1:D:380:LEU:HB2	1.97	0.45
3:F:68:LYS:HA	3:F:73:ALA:HA	1.98	0.45
2:H:201:VAL:CG1	2:H:203:VAL:HG13	2.44	0.45
2:H:208:LEU:HB3	2:H:232:PRO:CG	2.46	0.45
2:J:185:PHE:O	2:J:197:LEU:CD1	2.65	0.45
3:K:84:ASP:N	3:K:84:ASP:OD1	2.49	0.45
3:L:26:SER:O	3:L:32:TYR:HE1	1.99	0.45
1:D:121:TYR:CE1	1:D:228:GLU:O	2.67	0.45
1:C:357:THR:HG21	1:C:379:ALA:HB3	1.99	0.45
2:M:116:TYR:HE1	2:M:119:LEU:HD22	1.81	0.45
1:C:259:LYS:HB2	1:C:264:LEU:HD11	1.99	0.45
2:J:184:THR:HA	2:J:199:SER:HA	1.98	0.45
3:F:173:ASN:ND2	3:F:175:LYS:HG3	2.32	0.44
2:H:200:VAL:HG11	3:L:139:LEU:HD13	1.98	0.44
2:H:142:PRO:HB3	2:H:230:VAL:HG12	1.98	0.44
3:K:82:ALA:HA	3:K:109:VAL:HG21	1.98	0.44
3:K:146:GLY:HA3	3:K:176:TYR:CD2	2.51	0.44
1:A:123:SER:HB2	1:A:230:GLU:HB2	1.99	0.44
1:C:408:MET:HG2	1:C:419:ARG:O	2.17	0.44
1:B:154:GLN:HG2	1:C:456:ASN:O	2.18	0.44
1:A:228:GLU:OE2	2:H:108:ARG:NH2	2.50	0.44
1:B:139:THR:OG1	1:C:111:SER:HB3	2.16	0.44
1:C:248:THR:O	1:C:248:THR:OG1	2.28	0.44
1:A:351:TYR:CZ	1:A:420:ALA:HB1	2.52	0.44
1:C:234:HIS:CE1	1:C:286:THR:HG23	2.52	0.44
1:B:181:SER:HA	1:B:193:ILE:O	2.18	0.44
2:E:173:TRP:CZ3	2:E:215:CYS:HB3	2.53	0.44
3:F:84:ASP:OD1	3:F:84:ASP:N	2.50	0.44
3:K:124:PRO:HD3	3:K:136:LEU:CD2	2.47	0.44
2:M:218:ASN:ND2	2:M:225:LYS:HG3	2.31	0.44
3:N:149:THR:HB	3:N:200:THR:HB	2.00	0.44
1:A:230:GLU:HG2	1:A:231:CYS:O	2.18	0.44
1:B:121:TYR:CG	1:B:229:SER:HA	2.51	0.44
1:D:87:LEU:HB2	1:D:285:ARG:O	2.17	0.44
3:K:126:SER:HA	3:K:129:LEU:HD13	2.00	0.44
3:L:112:GLN:H	3:L:112:GLN:HG2	1.70	0.44
2:M:197:LEU:HD12	2:M:198:SER:N	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:171:VAL:HG22	2:H:217:VAL:HG22	2.00	0.44
2:J:171:VAL:HG22	2:J:217:VAL:HG22	2.00	0.44
2:M:97:ALA:HB3	2:M:119:LEU:HG	1.98	0.44
2:M:164:TYR:OH	2:M:197:LEU:HD23	2.17	0.44
1:D:270:THR:HG22	1:D:313:HIS:CE1	2.53	0.43
1:D:288:ILE:HB	1:D:306:ILE:HB	1.99	0.43
2:E:91:THR:HG22	2:E:130:VAL:HG23	2.00	0.43
2:J:214:ILE:HD13	2:J:229:LYS:CA	2.48	0.43
3:K:37:TRP:CZ3	3:K:90:CYS:HB3	2.52	0.43
3:L:106:LYS:HE2	3:L:106:LYS:HB2	1.75	0.43
3:N:61:SER:OG	3:N:63:ARG:HG3	2.17	0.43
1:A:390:GLY:HA3	5:T:3:BMA:O2	2.17	0.43
1:B:151:ASP:OD2	1:B:152:ARG:HG3	2.18	0.43
3:F:165:THR:HG22	3:F:180:SER:CB	2.48	0.43
2:M:31:SER:O	2:M:103:THR:HG22	2.17	0.43
1:D:427:ILE:O	1:D:428:ARG:HD2	2.18	0.43
2:E:86:LEU:HB3	2:E:130:VAL:HG11	1.99	0.43
3:F:25:ALA:O	3:F:28:ASP:OD1	2.36	0.43
2:H:157:LEU:HD23	2:H:201:VAL:O	2.18	0.43
3:L:124:PRO:HD3	3:L:136:LEU:CD2	2.49	0.43
3:L:56:ARG:HD2	3:L:64:PHE:O	2.18	0.43
2:M:169:VAL:HG21	2:M:197:LEU:CD2	2.44	0.43
3:N:85:GLU:HG2	3:N:108:THR:HA	2.01	0.43
1:A:273:ALA:HA	1:A:316:TYR:CE1	2.52	0.43
1:B:298:GLY:CA	1:B:338:PRO:HB3	2.49	0.43
2:J:185:PHE:CE1	3:K:139:LEU:HD22	2.52	0.43
2:M:57:THR:OG1	2:M:111:GLY:O	2.33	0.43
1:B:109:GLY:HA3	1:B:140:ILE:HD12	2.01	0.43
3:K:50:ILE:HD12	3:K:56:ARG:HG2	2.00	0.43
2:M:116:TYR:CE1	2:M:118:GLY:HA2	2.54	0.43
3:F:39:GLN:HB2	3:F:88:TYR:HE1	1.81	0.43
3:K:185:THR:HG22	3:K:188:GLN:OE1	2.19	0.43
2:H:173:TRP:CB	2:H:178:LEU:HD23	2.48	0.43
3:N:187:GLU:O	3:N:189:TRP:N	2.52	0.43
1:C:151:ASP:OD1	1:C:151:ASP:N	2.44	0.43
3:L:187:GLU:CD	3:L:187:GLU:H	2.21	0.43
2:M:52:ILE:HD11	2:M:115:TYR:HD1	1.84	0.43
3:N:26:SER:O	3:N:32:TYR:HE2	2.02	0.43
1:D:286:THR:O	1:D:308:PRO:HD2	2.19	0.42
2:E:97:ALA:HB1	2:E:119:LEU:HB3	2.00	0.42
2:H:220:LYS:N	2:H:220:LYS:HD3	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:52:ILE:CD1	2:E:113:TYR:CE1	3.02	0.42
3:F:37:TRP:HB2	3:F:50:ILE:HG13	2.01	0.42
3:L:18:ILE:HG12	3:L:107:LEU:HD11	2.00	0.42
3:L:84:ASP:O	3:L:107:LEU:HD23	2.18	0.42
2:M:34:PHE:CZ	2:M:98:ARG:HG3	2.54	0.42
3:N:137:VAL:HG22	3:N:181:TYR:CD2	2.54	0.42
2:E:160:LEU:HD13	3:F:137:VAL:HG21	2.02	0.42
3:L:207:GLU:O	3:L:208:LYS:HG2	2.19	0.42
3:N:171:GLN:OE1	3:N:177:ALA:HB2	2.19	0.42
1:D:142:GLY:O	1:D:145:SER:OG	2.36	0.42
1:D:279:CYS:HB3	1:D:290:CYS:HB3	2.01	0.42
2:M:73:ASP:OD1	2:M:76:THR:OG1	2.28	0.42
2:J:36:TRP:CD1	2:J:70:ILE:HD13	2.54	0.42
3:N:163:VAL:HG12	3:N:182:LEU:HD13	2.01	0.42
3:N:173:ASN:OD1	3:N:175:LYS:HG3	2.20	0.42
3:N:81:GLN:HB2	3:N:83:GLU:HG2	2.00	0.42
1:B:323:THR:HB	1:B:360:GLY:O	2.19	0.42
1:A:154:GLN:N	1:A:154:GLN:OE1	2.50	0.42
1:D:94:ILE:HB	1:D:358:TRP:NE1	2.34	0.42
1:A:135:SER:O	1:A:156:ARG:HA	2.20	0.42
1:C:295:ASN:O	1:C:344:ASN:HA	2.20	0.42
2:E:169:VAL:CG2	2:E:197:LEU:HD21	2.50	0.42
2:J:6:GLN:O	2:J:124:GLN:OE1	2.37	0.42
3:L:29:VAL:HG13	3:L:35:VAL:HG21	2.01	0.42
2:M:142:PRO:O	3:N:125:SER:HB3	2.19	0.42
3:N:20:ILE:CG2	3:N:105:THR:HG21	2.50	0.42
1:B:324:ASP:OD1	1:B:325:ASN:N	2.41	0.42
1:D:232:VAL:HB	1:D:288:ILE:CD1	2.50	0.42
2:H:188:VAL:HB	3:L:166:THR:HG22	2.02	0.42
1:A:140:ILE:HG21	1:A:140:ILE:HD13	1.77	0.41
1:D:318:CYS:O	1:D:333:GLY:HA3	2.20	0.41
1:D:331:PRO:HG3	1:D:339:TYR:CZ	2.55	0.41
2:H:230:VAL:O	2:H:230:VAL:HG23	2.20	0.41
3:N:81:GLN:O	3:N:109:VAL:HG21	2.20	0.41
3:L:37:TRP:CH2	3:L:90:CYS:HB3	2.55	0.41
3:N:131:ALA:O	3:N:132:ASN:HB3	2.20	0.41
1:B:158:LEU:HD22	1:B:181:SER:HB2	2.02	0.41
1:B:428:ARG:NH1	1:B:459:ASP:OD2	2.53	0.41
1:C:222:ASN:HB3	1:C:245:GLY:HA2	2.02	0.41
2:E:47:TRP:HB2	3:F:101:PHE:HE1	1.86	0.41
3:F:165:THR:HG22	3:F:180:SER:HB2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:222:SER:OG	2:M:224:THR:HG23	2.20	0.41
3:N:170:LYS:NZ	3:N:176:TYR:OH	2.53	0.41
1:C:318:CYS:O	1:C:333:GLY:HA3	2.20	0.41
1:B:276:ILE:HD11	1:B:302:PRO:HB2	2.02	0.41
1:B:396:ASN:HD22	1:B:396:ASN:C	2.20	0.41
1:D:229:SER:HB3	1:D:347:LYS:CE	2.50	0.41
1:D:152:ARG:HH11	1:D:152:ARG:HG3	1.85	0.41
3:K:163:VAL:HG23	3:K:182:LEU:HD13	2.01	0.41
2:J:39:GLN:NE2	3:K:40:GLN:OE1	2.45	0.41
3:N:47:LYS:HG2	3:N:49:MET:CE	2.49	0.41
1:C:223:ILE:O	1:C:225:ARG:NH1	2.49	0.41
1:D:223:ILE:O	1:D:223:ILE:HG22	2.20	0.41
3:L:57:PRO:HD2	3:L:60:VAL:HG21	2.02	0.41
2:M:214:ILE:HA	2:M:228:LYS:O	2.20	0.41
1:B:352:LEU:HD13	1:B:380:LEU:HB2	2.03	0.41
3:L:140:ILE:HG12	3:L:199:VAL:HG21	2.02	0.41
3:L:51:TYR:O	3:L:55:ASN:HB2	2.20	0.41
1:A:267:GLU:OE1	1:A:313:HIS:ND1	2.35	0.41
1:B:119:GLU:N	1:B:120:PRO:HD3	2.36	0.41
2:H:220:LYS:HB2	2:H:220:LYS:HE2	1.89	0.41
2:J:6:GLN:OE1	2:J:95:TYR:HA	2.21	0.41
1:C:280:SER:OG	1:C:348:GLY:O	2.39	0.41
1:A:198:PRO:HD3	1:B:455:TRP:CD1	2.55	0.40
1:B:184:CYS:HB3	1:B:231:CYS:O	2.22	0.40
3:F:136:LEU:HD12	3:F:182:LEU:HD23	2.02	0.40
2:H:91:THR:HG23	2:H:129:THR:HA	2.03	0.40
3:K:33:ASN:HB3	3:K:53:VAL:HG21	2.03	0.40
1:A:121:TYR:CG	1:A:229:SER:HA	2.57	0.40
1:B:399:TRP:CZ3	1:B:432:LYS:HD3	2.56	0.40
2:H:187:ALA:HB2	2:H:197:LEU:HD23	2.03	0.40
3:K:75:LEU:HD22	3:K:76:THR:H	1.86	0.40
1:C:121:TYR:CG	1:C:229:SER:HA	2.57	0.40
1:D:151:ASP:O	1:D:156:ARG:HD3	2.21	0.40
3:K:184:LEU:HB3	3:K:188:GLN:OE1	2.20	0.40
3:K:155:ASP:HB3	3:K:193:ARG:NH1	2.36	0.40
1:C:454:GLN:HG2	5:P:1:NAG:O6	2.21	0.40
1:B:224:LEU:HD13	1:B:244:ASP:HB2	2.02	0.40
1:C:376:VAL:HG23	1:C:376:VAL:O	2.21	0.40
3:K:143:PHE:CE2	3:K:146:GLY:HA2	2.56	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	386/388 (100%)	366 (95%)	19 (5%)	1 (0%)	41	71
1	B	386/388 (100%)	369 (96%)	16 (4%)	1 (0%)	41	71
1	C	386/388 (100%)	365 (95%)	21 (5%)	0	100	100
1	D	386/388 (100%)	366 (95%)	20 (5%)	0	100	100
2	E	208/237 (88%)	197 (95%)	11 (5%)	0	100	100
2	H	222/237 (94%)	217 (98%)	5 (2%)	0	100	100
2	J	198/237 (84%)	192 (97%)	6 (3%)	0	100	100
2	M	202/237 (85%)	194 (96%)	8 (4%)	0	100	100
3	F	201/216 (93%)	180 (90%)	20 (10%)	1 (0%)	29	61
3	K	196/216 (91%)	186 (95%)	9 (5%)	1 (0%)	29	61
3	L	211/216 (98%)	203 (96%)	8 (4%)	0	100	100
3	N	204/216 (94%)	190 (93%)	13 (6%)	1 (0%)	29	61
All	All	3186/3364 (95%)	3025 (95%)	156 (5%)	5 (0%)	47	78

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	K	53	VAL
1	A	223	ILE
3	N	53	VAL
1	B	223	ILE
3	F	53	VAL

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	339/339 (100%)	335 (99%)	4 (1%)	71	91
1	B	339/339 (100%)	330 (97%)	9 (3%)	44	77
1	C	339/339 (100%)	328 (97%)	11 (3%)	39	73
1	D	339/339 (100%)	329 (97%)	10 (3%)	42	76
2	E	181/200 (90%)	174 (96%)	7 (4%)	32	66
2	H	191/200 (96%)	187 (98%)	4 (2%)	53	81
2	J	176/200 (88%)	167 (95%)	9 (5%)	24	56
2	M	175/200 (88%)	166 (95%)	9 (5%)	24	56
3	F	176/183 (96%)	170 (97%)	6 (3%)	37	71
3	K	173/183 (94%)	167 (96%)	6 (4%)	36	70
3	L	180/183 (98%)	172 (96%)	8 (4%)	28	61
3	N	176/183 (96%)	168 (96%)	8 (4%)	27	61
All	All	2784/2888 (96%)	2693 (97%)	91 (3%)	38	72

All (91) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	112	SER
1	A	140	ILE
1	A	267	GLU
1	A	285	ARG
1	B	183	SER
1	B	274	LYS
1	B	280	SER
1	B	309	VAL
1	B	369	SER
1	B	384	ARG
1	B	385	SER
1	B	396	ASN
1	B	459	ASP
1	C	190	ARG
1	C	210	ARG
1	C	229	SER
1	C	268	SER
1	C	280	SER
1	C	293	ARG

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Mol	Chain	Res	Type
1	C	319	SER
1	C	323	THR
1	C	369	SER
1	C	384	ARG
1	C	459	ASP
1	D	83	ASN
1	D	156	ARG
1	D	229	SER
1	D	268	SER
1	D	280	SER
1	D	288	ILE
1	D	293	ARG
1	D	295	ASN
1	D	369	SER
1	D	419	ARG
2	H	35	SER
2	H	100	LEU
2	H	183	HIS
2	H	215	CYS
3	L	17	SER
3	L	27	SER
3	L	28	ASP
3	L	32	TYR
3	L	83	GLU
3	L	85	GLU
3	L	87	ASP
3	L	141	SER
2	E	6	GLN
2	E	22	CYS
2	E	31	SER
2	E	88	SER
2	E	91	THR
2	E	110	ILE
2	E	120	ASP
3	F	26	SER
3	F	65	SER
3	F	68	LYS
3	F	84	ASP
3	F	191	SER
3	F	193	ARG
2	J	4	LEU
2	J	21	SER

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Mol	Chain	Res	Type
2	J	67	ARG
2	J	77	SER
2	J	124	GLN
2	J	183	HIS
2	J	197	LEU
2	J	216	ASN
2	J	231	GLU
3	K	19	THR
3	K	28	ASP
3	K	62	ASN
3	K	67	SER
3	K	84	ASP
3	K	174	ASN
2	M	6	GLN
2	M	22	CYS
2	M	35	SER
2	M	67	ARG
2	M	119	LEU
2	M	131	SER
2	M	197	LEU
2	M	216	ASN
2	M	227	ASP
3	N	9	SER
3	N	55	ASN
3	N	62	ASN
3	N	153	LYS
3	N	183	SER
3	N	190	LYS
3	N	192	HIS
3	N	193	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
3	K	171	GLN
3	K	174	ASN
2	M	117	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 ⓘ

53 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	$\# Z > 2$
4	NAG	G	1	1,4	14,14,15	0.29	0	17,19,21	0.71	0
4	NAG	G	2	4	14,14,15	0.29	0	17,19,21	0.64	0
4	BMA	G	3	4	11,11,12	0.73	0	15,15,17	1.93	3 (20%)
4	MAN	G	4	4	11,11,12	0.26	0	15,15,17	0.64	0
4	MAN	G	5	4	11,11,12	0.26	0	15,15,17	0.65	0
5	NAG	I	1	1,5	14,14,15	0.56	0	17,19,21	0.69	0
5	NAG	I	2	5	14,14,15	0.57	0	17,19,21	0.68	0
5	BMA	I	3	5	11,11,12	0.27	0	15,15,17	0.97	1 (6%)
5	MAN	I	4	5	11,11,12	0.48	0	15,15,17	1.39	2 (13%)
5	MAN	I	5	5	11,11,12	0.51	0	15,15,17	0.79	0
5	MAN	I	6	5	11,11,12	0.43	0	15,15,17	0.97	1 (6%)
5	MAN	I	7	5	11,11,12	0.57	0	15,15,17	0.75	0
5	MAN	I	8	5	11,11,12	0.55	0	15,15,17	0.78	0
5	MAN	I	9	5	11,11,12	0.57	0	15,15,17	1.05	2 (13%)
6	NAG	O	1	1,6	14,14,15	0.29	0	17,19,21	0.74	0
6	NAG	O	2	6	14,14,15	0.30	0	17,19,21	0.64	0
6	BMA	O	3	6	11,11,12	0.33	0	15,15,17	0.69	0
6	MAN	O	4	6	11,11,12	0.26	0	15,15,17	0.64	0
5	NAG	P	1	1,5	14,14,15	0.56	0	17,19,21	0.68	0
5	NAG	P	2	5	14,14,15	0.57	0	17,19,21	0.68	0
5	BMA	P	3	5	11,11,12	0.26	0	15,15,17	0.97	1 (6%)
5	MAN	P	4	5	11,11,12	0.47	0	15,15,17	1.38	2 (13%)
5	MAN	P	5	5	11,11,12	0.50	0	15,15,17	0.78	0
5	MAN	P	6	5	11,11,12	0.43	0	15,15,17	0.98	1 (6%)
5	MAN	P	7	5	11,11,12	0.58	0	15,15,17	0.76	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	MAN	P	8	5	11,11,12	0.55	0	15,15,17	0.78	0
5	MAN	P	9	5	11,11,12	0.57	0	15,15,17	1.06	2 (13%)
6	NAG	Q	1	1,6	14,14,15	0.31	0	17,19,21	0.78	0
6	NAG	Q	2	6	14,14,15	0.29	0	17,19,21	0.76	0
6	BMA	Q	3	6	11,11,12	0.36	0	15,15,17	0.94	1 (6%)
6	MAN	Q	4	6	11,11,12	0.27	0	15,15,17	0.63	0
5	NAG	R	1	1,5	14,14,15	0.55	0	17,19,21	0.69	0
5	NAG	R	2	5	14,14,15	0.57	0	17,19,21	0.68	0
5	BMA	R	3	5	11,11,12	0.26	0	15,15,17	0.97	1 (6%)
5	MAN	R	4	5	11,11,12	0.48	0	15,15,17	1.39	2 (13%)
5	MAN	R	5	5	11,11,12	0.52	0	15,15,17	0.79	0
5	MAN	R	6	5	11,11,12	0.44	0	15,15,17	0.98	1 (6%)
5	MAN	R	7	5	11,11,12	0.57	0	15,15,17	0.75	0
5	MAN	R	8	5	11,11,12	0.54	0	15,15,17	0.78	0
5	MAN	R	9	5	11,11,12	0.57	0	15,15,17	1.06	2 (13%)
6	NAG	S	1	1,6	14,14,15	0.28	0	17,19,21	0.77	0
6	NAG	S	2	6	14,14,15	0.29	0	17,19,21	0.64	0
6	BMA	S	3	6	11,11,12	0.43	0	15,15,17	1.26	2 (13%)
6	MAN	S	4	6	11,11,12	0.23	0	15,15,17	0.76	0
5	NAG	T	1	1,5	14,14,15	0.56	0	17,19,21	0.68	0
5	NAG	T	2	5	14,14,15	0.57	0	17,19,21	0.68	0
5	BMA	T	3	5	11,11,12	0.27	0	15,15,17	0.97	1 (6%)
5	MAN	T	4	5	11,11,12	0.46	0	15,15,17	1.38	2 (13%)
5	MAN	T	5	5	11,11,12	0.50	0	15,15,17	0.79	0
5	MAN	T	6	5	11,11,12	0.43	0	15,15,17	0.97	1 (6%)
5	MAN	T	7	5	11,11,12	0.56	0	15,15,17	0.75	0
5	MAN	T	8	5	11,11,12	0.54	0	15,15,17	0.77	0
5	MAN	T	9	5	11,11,12	0.58	0	15,15,17	1.05	2 (13%)

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

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	I	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	I	2	5	-	0/6/23/26	0/1/1/1
5	BMA	I	3	5	-	0/2/19/22	0/1/1/1
5	MAN	I	4	5	-	0/2/19/22	0/1/1/1
5	MAN	I	5	5	-	0/2/19/22	0/1/1/1
5	MAN	I	6	5	-	0/2/19/22	0/1/1/1
5	MAN	I	7	5	-	0/2/19/22	0/1/1/1
5	MAN	I	8	5	-	0/2/19/22	0/1/1/1
5	MAN	I	9	5	-	1/2/19/22	0/1/1/1
6	NAG	O	1	1,6	-	2/6/23/26	0/1/1/1
6	NAG	O	2	6	-	1/6/23/26	0/1/1/1
6	BMA	O	3	6	-	1/2/19/22	0/1/1/1
6	MAN	O	4	6	-	2/2/19/22	0/1/1/1
5	NAG	P	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	P	2	5	-	0/6/23/26	0/1/1/1
5	BMA	P	3	5	-	0/2/19/22	0/1/1/1
5	MAN	P	4	5	-	0/2/19/22	0/1/1/1
5	MAN	P	5	5	-	0/2/19/22	0/1/1/1
5	MAN	P	6	5	-	0/2/19/22	0/1/1/1
5	MAN	P	7	5	-	0/2/19/22	0/1/1/1
5	MAN	P	8	5	-	0/2/19/22	0/1/1/1
5	MAN	P	9	5	-	1/2/19/22	0/1/1/1
6	NAG	Q	1	1,6	-	2/6/23/26	0/1/1/1
6	NAG	Q	2	6	-	2/6/23/26	0/1/1/1
6	BMA	Q	3	6	-	0/2/19/22	0/1/1/1
6	MAN	Q	4	6	-	2/2/19/22	0/1/1/1
5	NAG	R	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	R	2	5	-	0/6/23/26	0/1/1/1
5	BMA	R	3	5	-	0/2/19/22	0/1/1/1
5	MAN	R	4	5	-	0/2/19/22	0/1/1/1
5	MAN	R	5	5	-	0/2/19/22	0/1/1/1
5	MAN	R	6	5	-	0/2/19/22	0/1/1/1
5	MAN	R	7	5	-	0/2/19/22	0/1/1/1
5	MAN	R	8	5	-	0/2/19/22	0/1/1/1
5	MAN	R	9	5	-	1/2/19/22	0/1/1/1
6	NAG	S	1	1,6	-	2/6/23/26	0/1/1/1
6	NAG	S	2	6	-	0/6/23/26	0/1/1/1
6	BMA	S	3	6	-	0/2/19/22	0/1/1/1
6	MAN	S	4	6	-	2/2/19/22	0/1/1/1
5	NAG	T	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	T	2	5	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	BMA	T	3	5	-	0/2/19/22	0/1/1/1
5	MAN	T	4	5	-	0/2/19/22	0/1/1/1
5	MAN	T	5	5	-	0/2/19/22	0/1/1/1
5	MAN	T	6	5	-	0/2/19/22	0/1/1/1
5	MAN	T	7	5	-	0/2/19/22	0/1/1/1
5	MAN	T	8	5	-	0/2/19/22	0/1/1/1
5	MAN	T	9	5	-	1/2/19/22	0/1/1/1

There are no bond length outliers.

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	3	BMA	C1-C2-C3	5.18	116.04	109.67
4	G	3	BMA	C2-C3-C4	3.67	117.24	110.89
5	P	4	MAN	O2-C2-C1	-2.75	103.53	109.15
5	I	4	MAN	O2-C2-C1	-2.74	103.56	109.15
5	T	4	MAN	O2-C2-C1	-2.73	103.56	109.15
5	R	4	MAN	O2-C2-C1	-2.72	103.58	109.15
6	S	3	BMA	O5-C1-C2	2.68	114.91	110.77
6	S	3	BMA	C1-O5-C5	2.61	115.73	112.19
5	R	3	BMA	C1-C2-C3	2.43	112.65	109.67
5	P	3	BMA	C1-C2-C3	2.41	112.63	109.67
5	I	3	BMA	C1-C2-C3	2.41	112.62	109.67
5	T	3	BMA	C1-C2-C3	2.40	112.62	109.67
4	G	3	BMA	C3-C4-C5	2.39	114.50	110.24
6	Q	3	BMA	C1-O5-C5	2.34	115.37	112.19
5	P	4	MAN	O2-C2-C3	2.32	114.78	110.14
5	I	4	MAN	O2-C2-C3	2.32	114.78	110.14
5	T	4	MAN	O2-C2-C3	2.32	114.78	110.14
5	R	4	MAN	O2-C2-C3	2.31	114.76	110.14
5	I	9	MAN	O5-C5-C6	2.16	110.59	107.20
5	P	9	MAN	O5-C5-C6	2.15	110.57	107.20
5	R	9	MAN	O5-C5-C6	2.14	110.57	107.20
5	T	9	MAN	O5-C5-C6	2.14	110.56	107.20
5	P	9	MAN	O5-C1-C2	-2.10	107.53	110.77
5	R	9	MAN	O5-C1-C2	-2.09	107.54	110.77
5	I	9	MAN	O5-C1-C2	-2.08	107.56	110.77
5	T	9	MAN	O5-C1-C2	-2.07	107.58	110.77
5	P	6	MAN	C1-O5-C5	2.03	114.94	112.19
5	R	6	MAN	C1-O5-C5	2.02	114.93	112.19
5	T	6	MAN	C1-O5-C5	2.02	114.92	112.19
5	I	6	MAN	C1-O5-C5	2.01	114.92	112.19

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	S	4	MAN	O5-C5-C6-O6
6	Q	1	NAG	C4-C5-C6-O6
6	S	1	NAG	C4-C5-C6-O6
6	S	4	MAN	C4-C5-C6-O6
6	O	1	NAG	C4-C5-C6-O6
6	Q	1	NAG	O5-C5-C6-O6
6	S	1	NAG	O5-C5-C6-O6
6	O	1	NAG	O5-C5-C6-O6
5	P	9	MAN	O5-C5-C6-O6
5	I	9	MAN	O5-C5-C6-O6
5	T	9	MAN	O5-C5-C6-O6
5	R	9	MAN	O5-C5-C6-O6
4	G	2	NAG	C4-C5-C6-O6
6	Q	4	MAN	C4-C5-C6-O6
4	G	2	NAG	O5-C5-C6-O6
6	O	4	MAN	C4-C5-C6-O6
6	Q	4	MAN	O5-C5-C6-O6
4	G	1	NAG	C4-C5-C6-O6
6	O	4	MAN	O5-C5-C6-O6
6	Q	2	NAG	C4-C5-C6-O6
6	Q	2	NAG	O5-C5-C6-O6
6	O	3	BMA	C4-C5-C6-O6
4	G	5	MAN	C4-C5-C6-O6
6	O	2	NAG	C4-C5-C6-O6

There are no ring outliers.

15 monomers are involved in 17 short contacts:

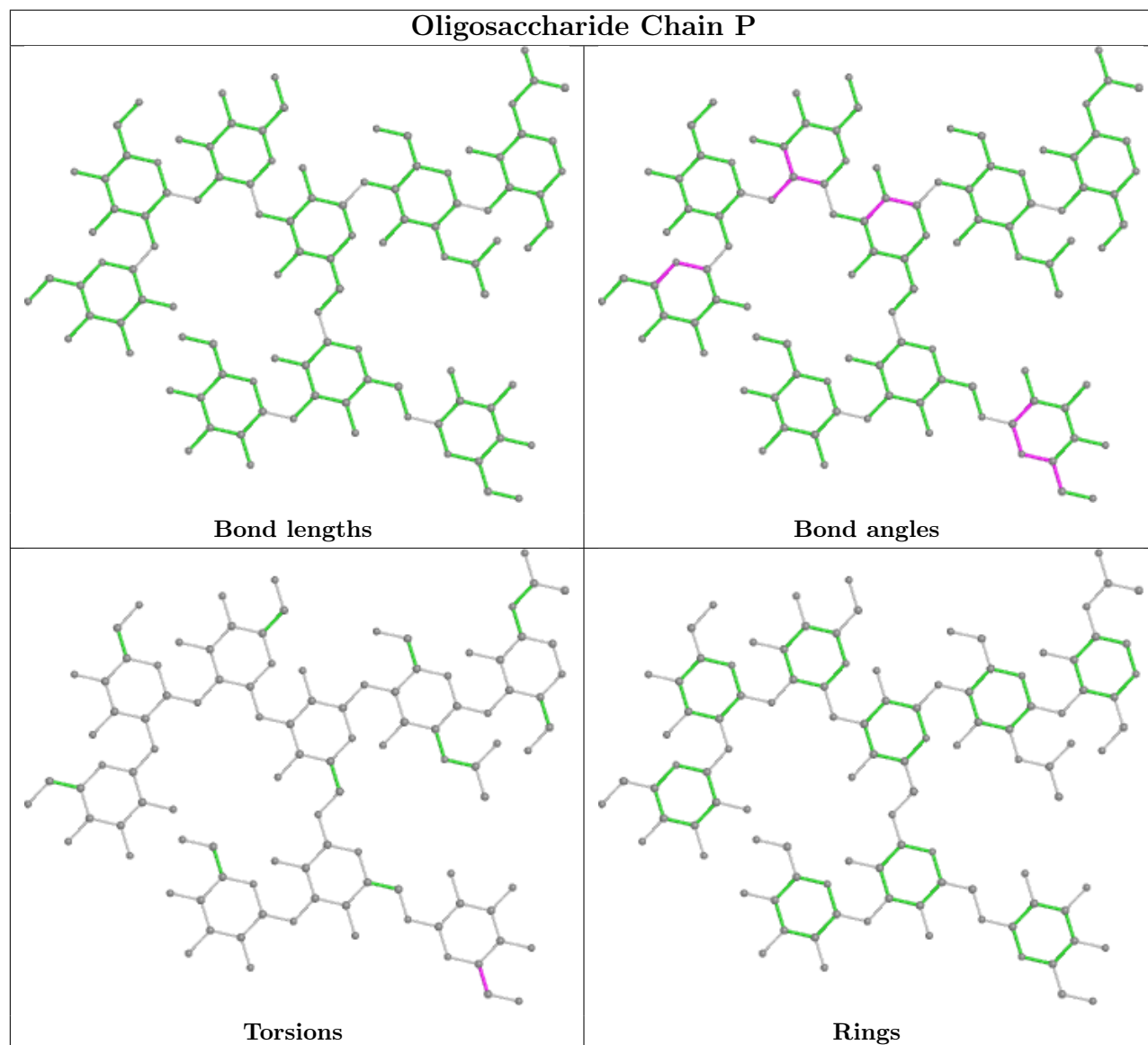
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	O	3	BMA	2	0
5	R	3	BMA	1	0
4	G	5	MAN	1	0
5	I	3	BMA	1	0
5	T	6	MAN	1	0
5	T	3	BMA	1	0
6	Q	4	MAN	1	0
5	P	1	NAG	1	0
6	Q	1	NAG	3	0
5	P	6	MAN	1	0
5	P	5	MAN	1	0

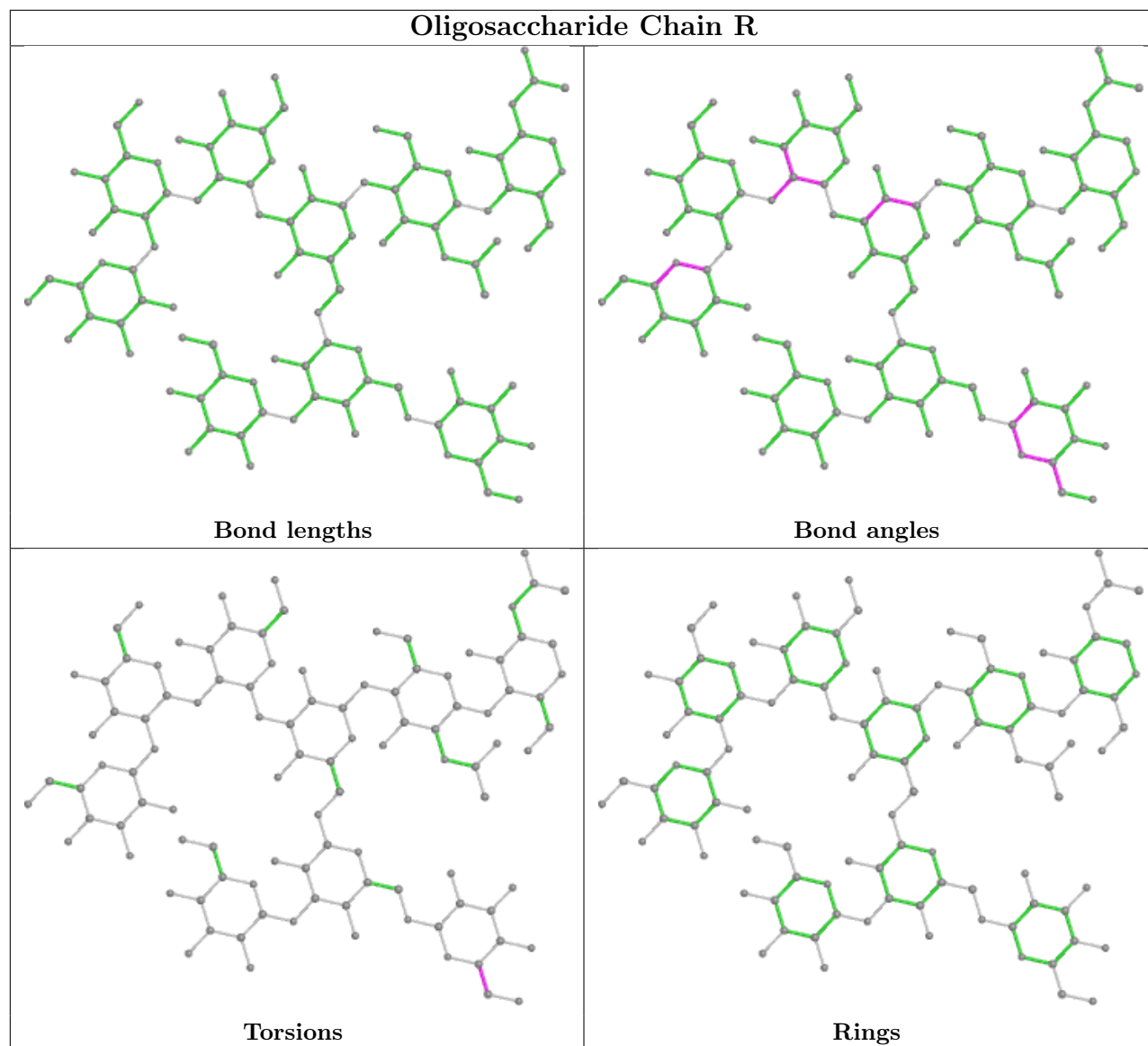
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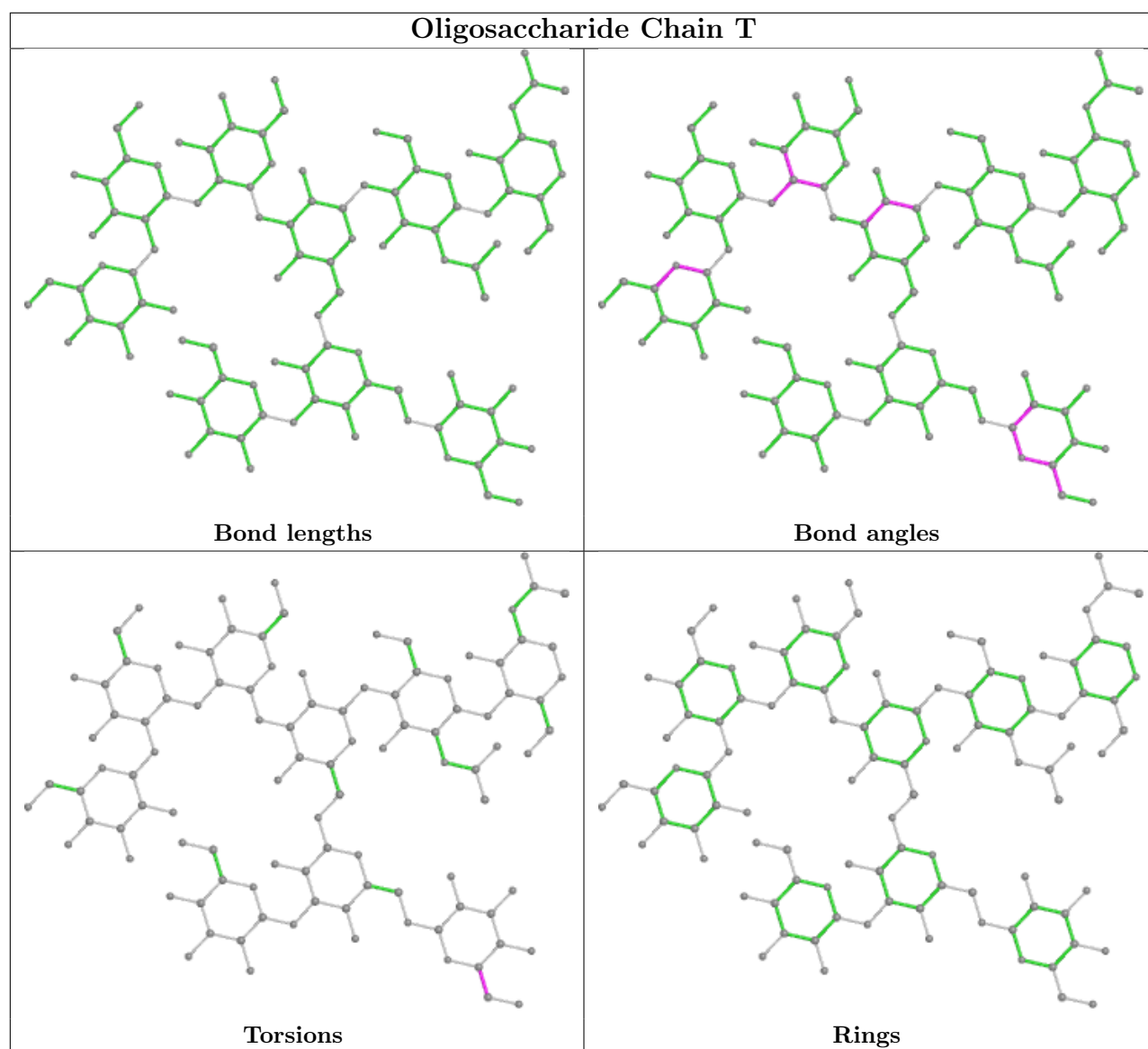
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	O	4	MAN	1	0
5	R	6	MAN	1	0
4	G	4	MAN	1	0
4	G	3	BMA	1	0

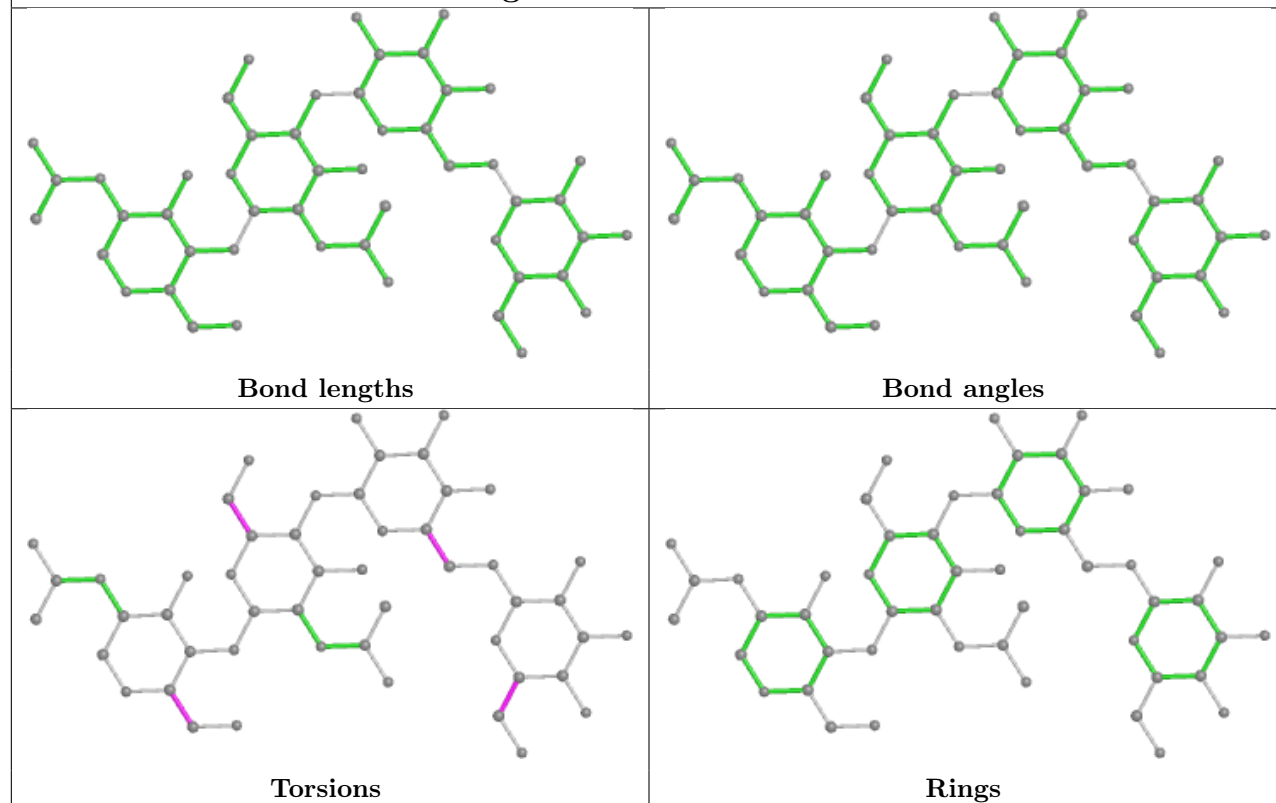
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



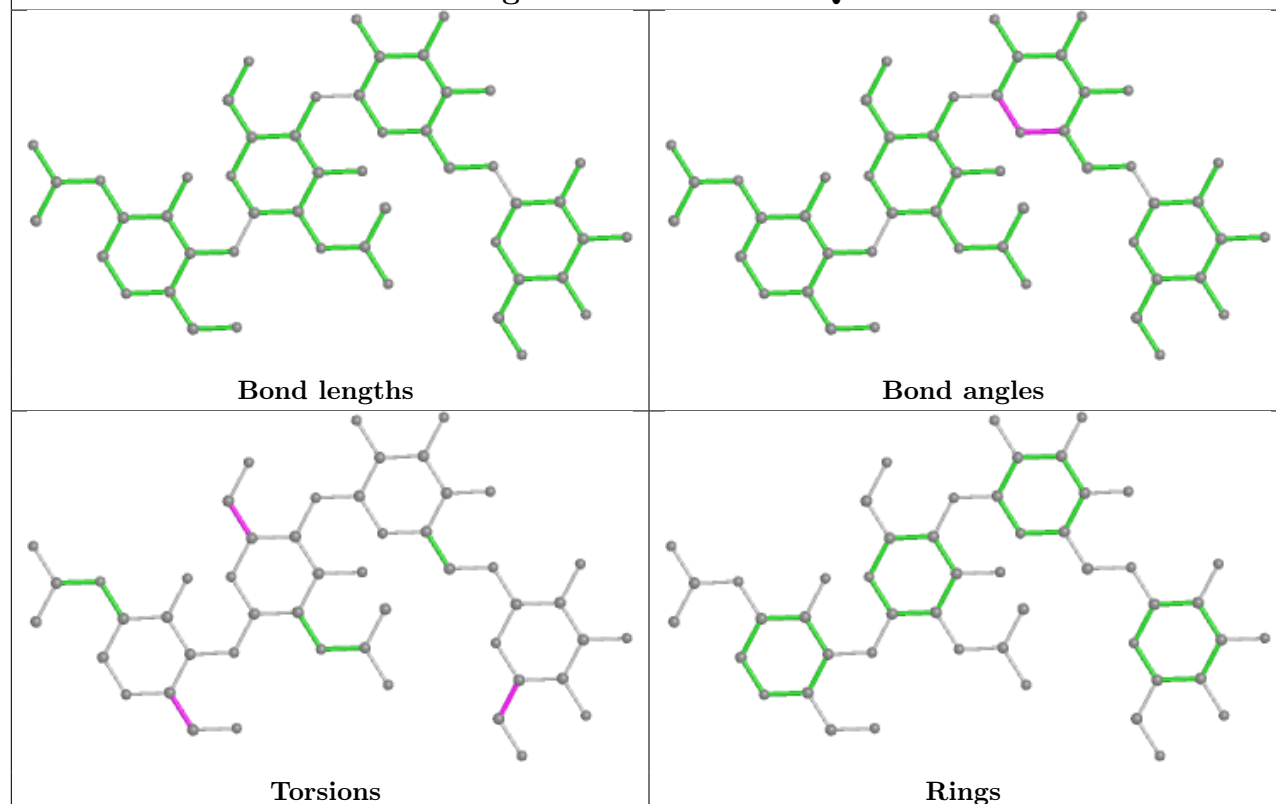


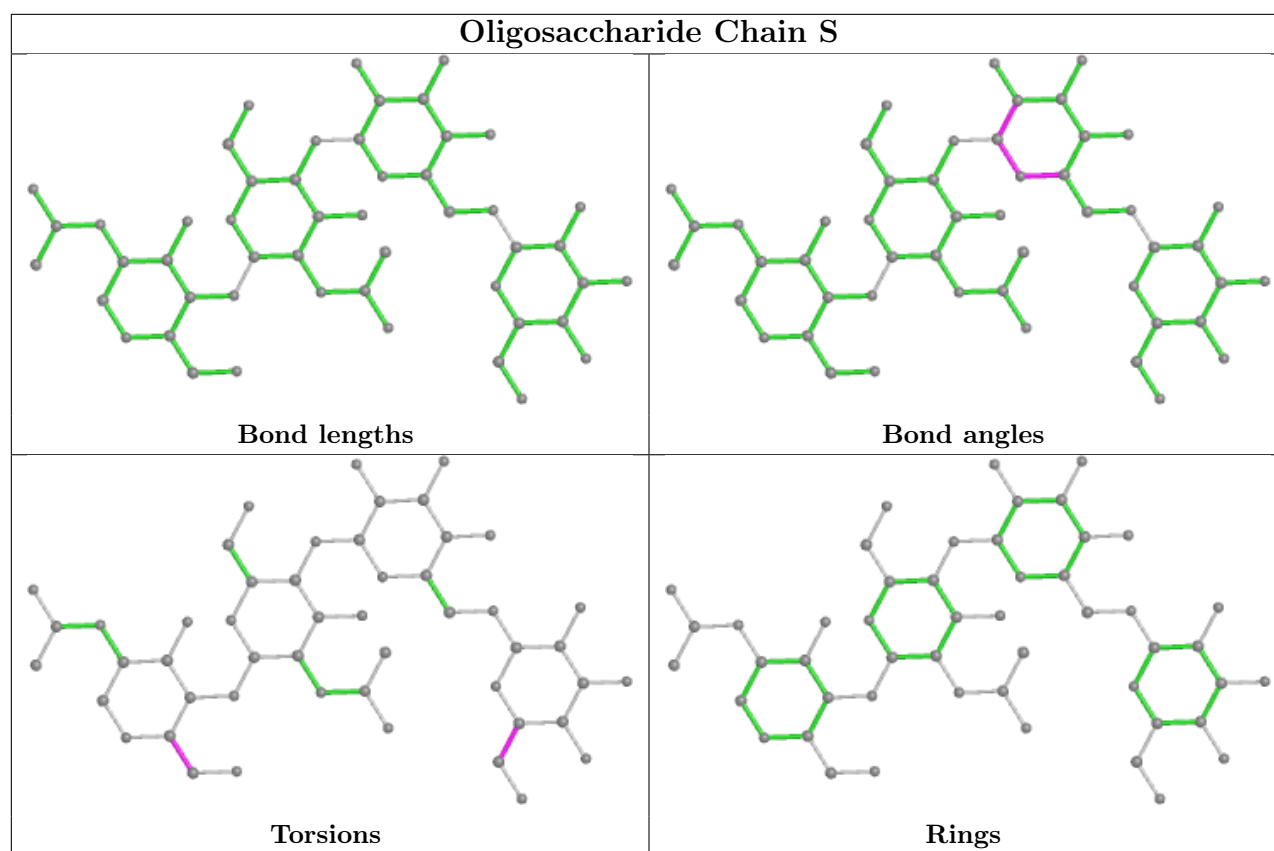


Oligosaccharide Chain O



Oligosaccharide Chain Q





5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
7	NAG	A	501	1	14,14,15	0.44	0	17,19,21	0.86	1 (5%)
7	NAG	B	501	1	14,14,15	0.44	0	17,19,21	0.86	1 (5%)
7	NAG	C	501	1	14,14,15	0.44	0	17,19,21	0.86	1 (5%)
7	NAG	D	501	1	14,14,15	0.44	0	17,19,21	0.86	1 (5%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	A	501	1	-	0/6/23/26	0/1/1/1
7	NAG	B	501	1	-	0/6/23/26	0/1/1/1
7	NAG	C	501	1	-	0/6/23/26	0/1/1/1
7	NAG	D	501	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	C	501	NAG	O5-C5-C6	2.53	111.17	107.20
7	D	501	NAG	O5-C5-C6	2.52	111.15	107.20
7	B	501	NAG	O5-C5-C6	2.51	111.14	107.20
7	A	501	NAG	O5-C5-C6	2.51	111.14	107.20

There are no chirality outliers.

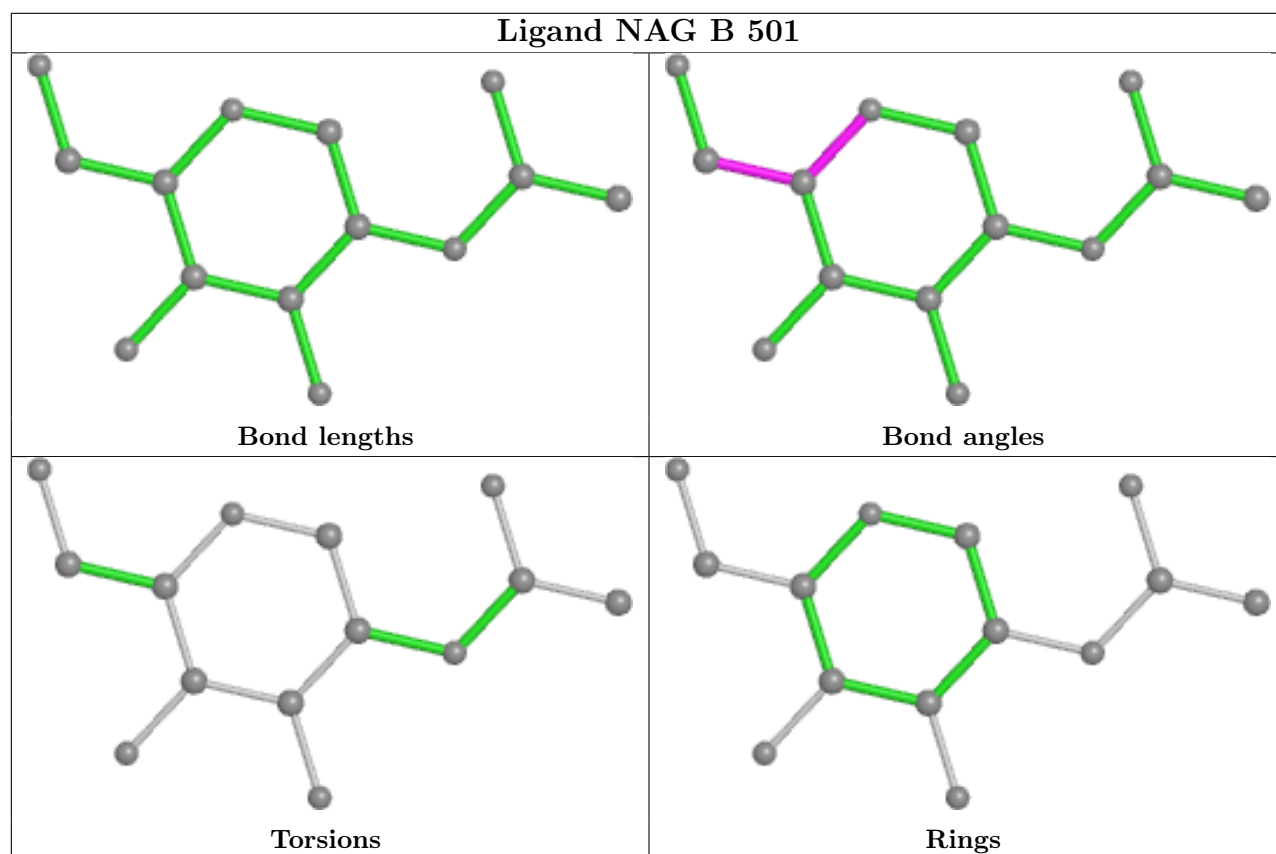
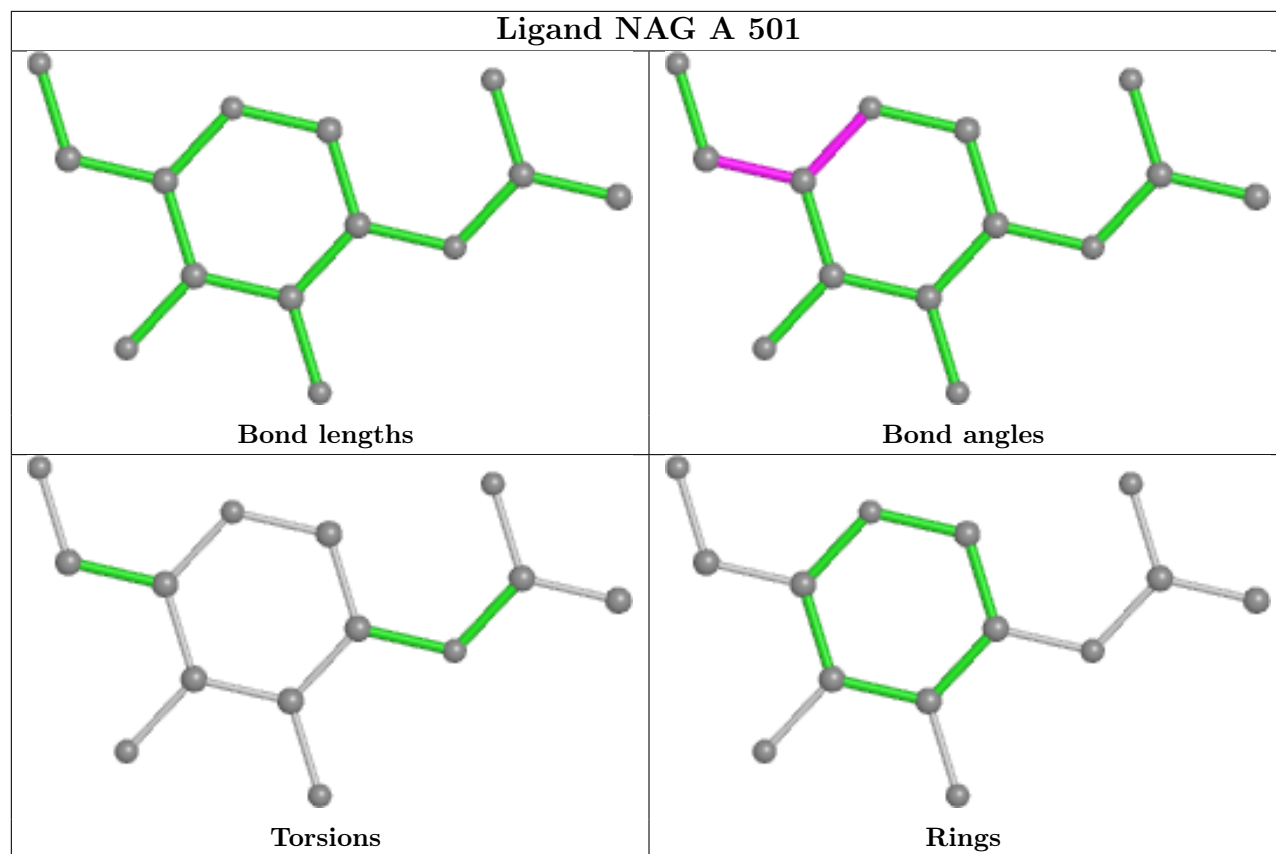
There are no torsion outliers.

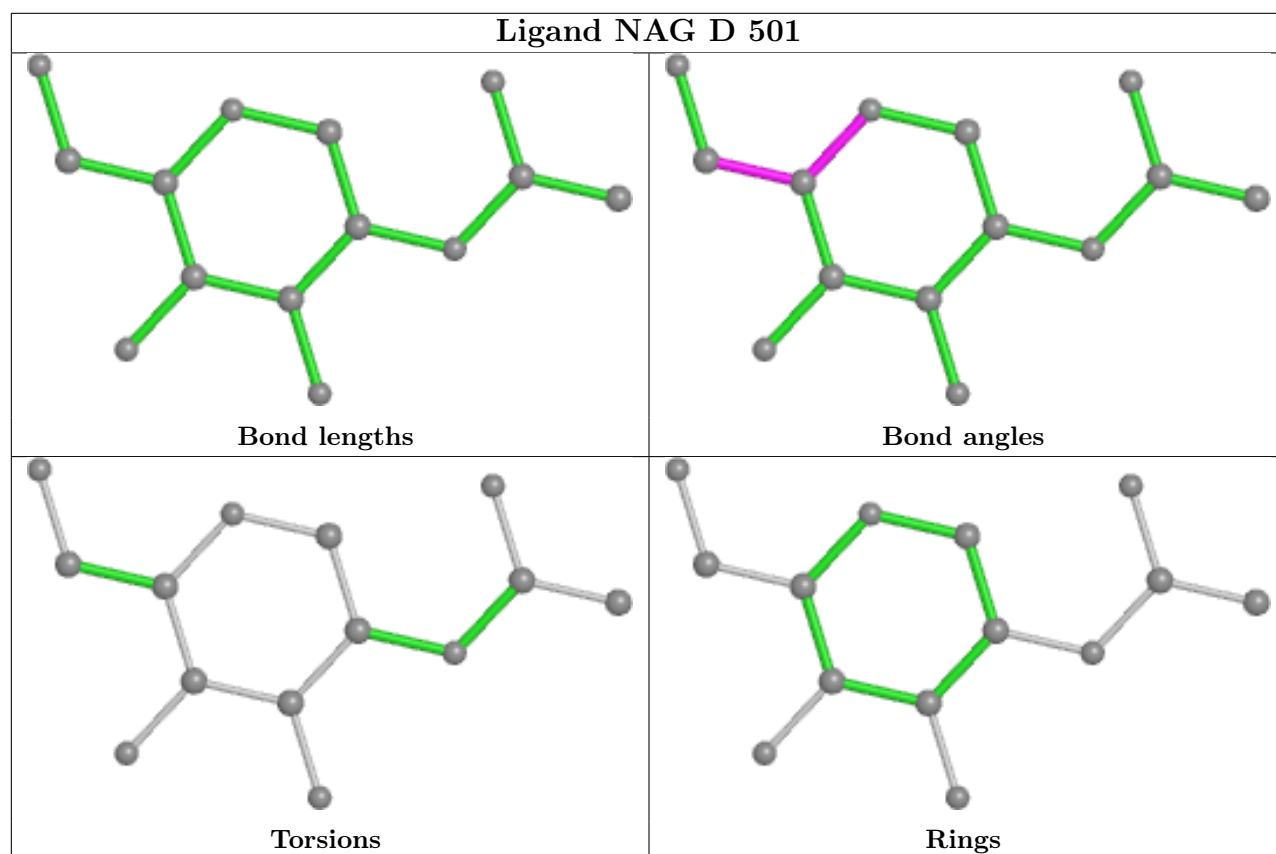
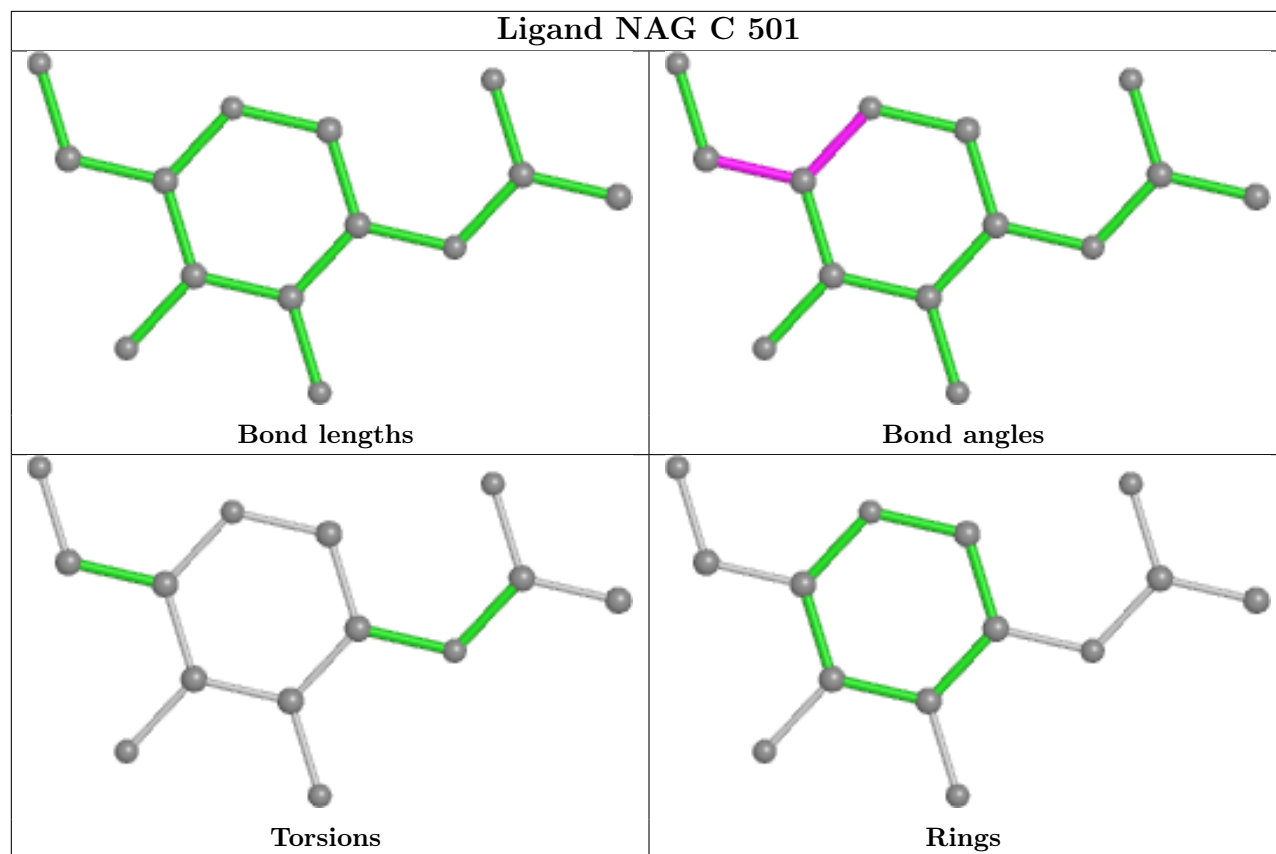
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	501	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 all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	388/388 (100%)	-0.30	0 100 100	17, 27, 41, 62	0
1	B	388/388 (100%)	-0.28	0 100 100	19, 31, 53, 62	0
1	C	388/388 (100%)	-0.29	0 100 100	17, 29, 46, 62	0
1	D	388/388 (100%)	-0.31	0 100 100	16, 27, 43, 55	0
2	E	214/237 (90%)	-0.06	2 (0%) 84 84	27, 39, 64, 78	0
2	H	226/237 (95%)	-0.17	4 (1%) 68 67	22, 33, 62, 84	0
2	J	206/237 (86%)	-0.13	4 (1%) 66 65	26, 39, 75, 96	0
2	M	208/237 (87%)	-0.08	4 (1%) 66 65	24, 37, 70, 97	0
3	F	207/216 (95%)	0.18	8 (3%) 39 35	35, 57, 96, 114	0
3	K	204/216 (94%)	0.20	6 (2%) 51 47	35, 61, 90, 113	0
3	L	213/216 (98%)	-0.15	1 (0%) 91 91	23, 43, 66, 77	0
3	N	208/216 (96%)	0.27	9 (4%) 35 31	31, 59, 92, 120	0
All	All	3238/3364 (96%)	-0.14	38 (1%) 79 79	16, 35, 77, 120	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	J	213	TYR	5.6
3	F	82	ALA	4.0
2	M	178	LEU	3.5
2	H	26	GLY	3.4
2	M	230	VAL	3.2
3	N	111	GLY	3.1
3	N	126	SER	3.1
2	E	26	GLY	3.0
2	J	229	LYS	3.0
3	N	28	ASP	3.0
3	K	2	SER	2.9

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Mol	Chain	Res	Type	RSRZ
3	F	11	SER	2.8
3	K	32	TYR	2.8
2	J	230	VAL	2.7
3	N	155	ASP	2.7
3	K	59	GLY	2.6
3	K	18	ILE	2.5
3	F	32	TYR	2.5
3	N	32	TYR	2.5
2	M	27	GLY	2.4
2	M	26	GLY	2.4
3	N	190	LYS	2.4
3	F	28	ASP	2.3
2	E	157	LEU	2.3
3	N	26	SER	2.2
2	H	178	LEU	2.2
3	N	160	LYS	2.2
3	L	111	GLY	2.2
2	H	208	LEU	2.2
3	K	159	VAL	2.2
2	J	203	VAL	2.1
3	F	64	PHE	2.1
3	F	118	SER	2.1
2	H	1	GLU	2.1
3	K	82	ALA	2.1
3	F	2	SER	2.0
3	F	61	SER	2.0
3	N	193	ARG	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(\AA^2)	Q<0.9
5	MAN	R	9	11/12	0.71	0.27	70,78,90,98	0

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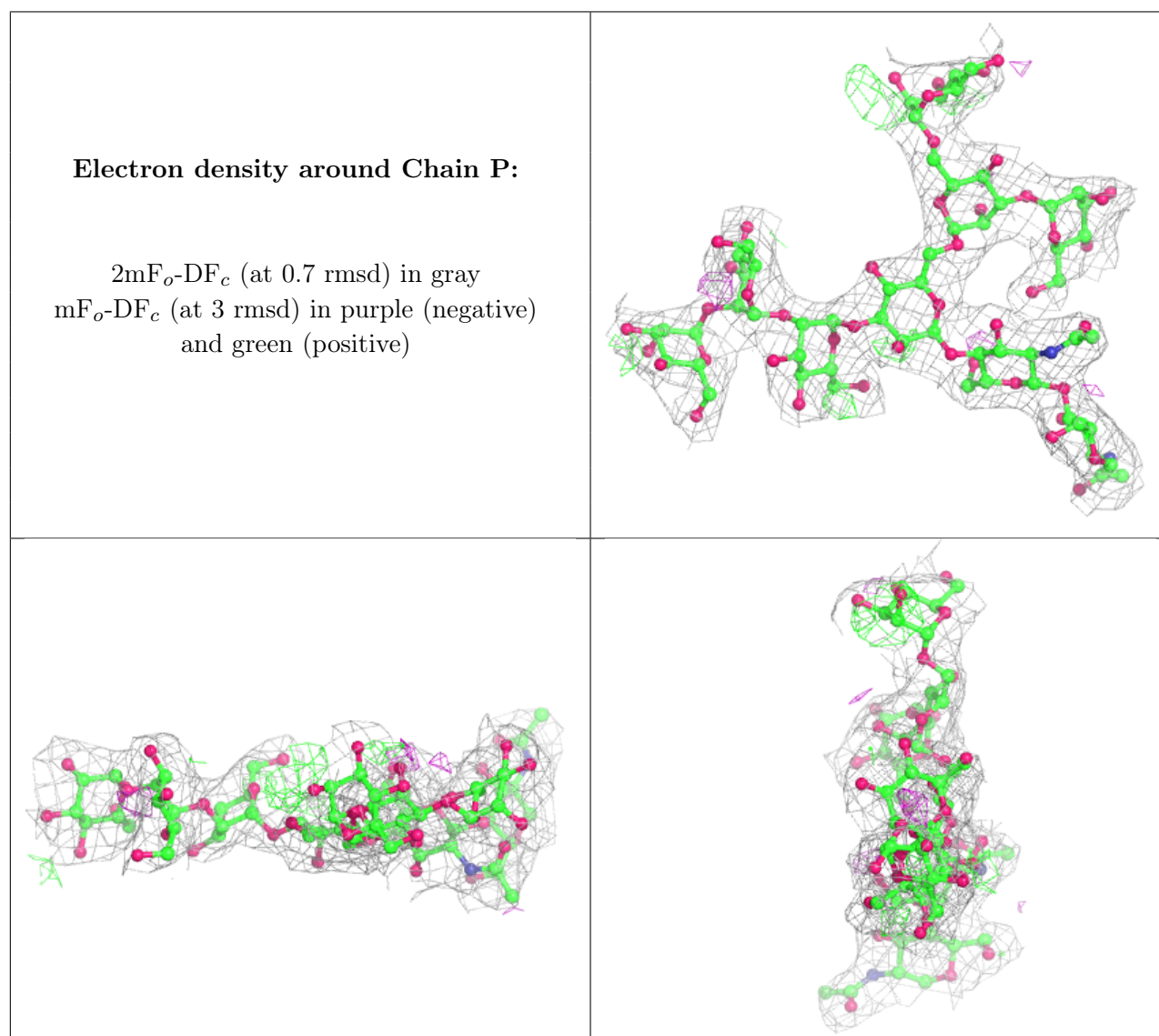
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	MAN	P	9	11/12	0.72	0.25	56,63,72,73	0
4	MAN	G	5	11/12	0.75	0.28	71,89,101,103	0
4	MAN	G	4	11/12	0.80	0.27	80,92,97,99	0
6	MAN	Q	4	11/12	0.84	0.19	51,69,73,74	0
5	MAN	I	9	11/12	0.84	0.22	54,56,61,67	0
5	MAN	T	9	11/12	0.85	0.21	45,54,61,65	0
5	MAN	T	8	11/12	0.85	0.17	37,47,56,56	0
6	BMA	S	3	11/12	0.85	0.12	54,58,63,66	0
6	BMA	Q	3	11/12	0.86	0.11	50,57,62,62	0
6	BMA	O	3	11/12	0.87	0.10	54,64,66,67	0
4	BMA	G	3	11/12	0.87	0.16	67,77,86,88	0
6	MAN	O	4	11/12	0.88	0.14	64,70,76,77	0
5	MAN	P	8	11/12	0.88	0.24	42,52,56,57	0
6	MAN	S	4	11/12	0.88	0.17	61,66,75,78	0
5	MAN	I	8	11/12	0.88	0.19	46,52,57,62	0
6	NAG	Q	1	14/15	0.90	0.16	25,32,35,37	0
4	NAG	G	2	14/15	0.90	0.14	46,56,64,70	0
5	BMA	R	3	11/12	0.90	0.18	29,38,45,47	0
5	MAN	P	5	11/12	0.90	0.25	36,42,47,48	0
5	BMA	P	3	11/12	0.91	0.15	35,39,44,45	0
5	MAN	R	7	11/12	0.91	0.14	38,44,54,66	0
6	NAG	S	2	14/15	0.91	0.15	35,42,52,61	0
5	MAN	P	4	11/12	0.92	0.18	28,31,38,38	0
5	MAN	R	4	11/12	0.92	0.19	26,32,39,41	0
5	MAN	P	6	11/12	0.92	0.18	37,41,45,48	0
6	NAG	O	2	14/15	0.92	0.14	39,56,62,66	0
5	MAN	R	5	11/12	0.92	0.30	37,40,46,47	0
5	MAN	I	5	11/12	0.93	0.15	42,44,50,52	0
5	MAN	I	7	11/12	0.93	0.15	39,49,52,59	0
5	MAN	R	8	11/12	0.93	0.20	44,45,51,51	0
5	MAN	T	7	11/12	0.94	0.15	44,50,55,62	0
5	NAG	P	1	14/15	0.94	0.13	27,31,41,48	0
5	MAN	I	6	11/12	0.94	0.13	38,43,47,48	0
5	MAN	T	5	11/12	0.94	0.19	34,37,42,45	0
5	NAG	P	2	14/15	0.94	0.17	28,33,39,49	0
6	NAG	Q	2	14/15	0.94	0.12	33,49,52,54	0
5	MAN	R	6	11/12	0.94	0.17	32,35,37,39	0
5	MAN	P	7	11/12	0.94	0.13	42,47,55,57	0
5	NAG	T	1	14/15	0.94	0.17	23,27,35,39	0
5	MAN	T	6	11/12	0.94	0.17	29,35,40,40	0
5	MAN	I	4	11/12	0.94	0.13	27,33,41,43	0
5	NAG	I	2	14/15	0.95	0.15	29,30,44,46	0

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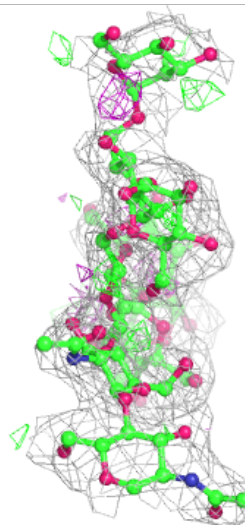
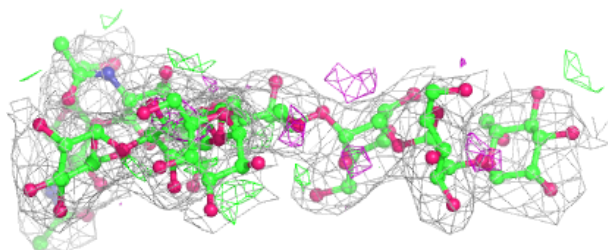
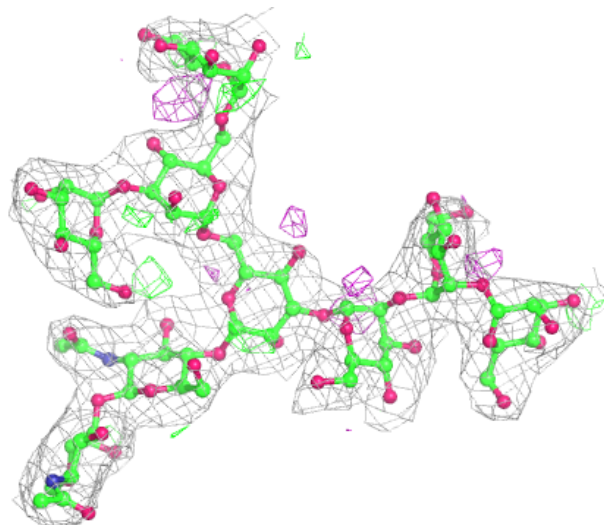
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	NAG	T	2	14/15	0.95	0.18	24,30,36,50	0
5	NAG	R	1	14/15	0.95	0.15	28,32,43,50	0
5	BMA	I	3	11/12	0.95	0.16	32,40,46,49	0
6	NAG	O	1	14/15	0.95	0.13	29,37,42,43	0
5	BMA	T	3	11/12	0.96	0.16	32,35,43,47	0
5	NAG	R	2	14/15	0.96	0.19	30,33,38,49	0
4	NAG	G	1	14/15	0.96	0.12	27,32,41,47	0
5	MAN	T	4	11/12	0.96	0.12	25,32,34,35	0
5	NAG	I	1	14/15	0.96	0.11	25,32,35,38	0
6	NAG	S	1	14/15	0.97	0.12	23,26,34,37	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.



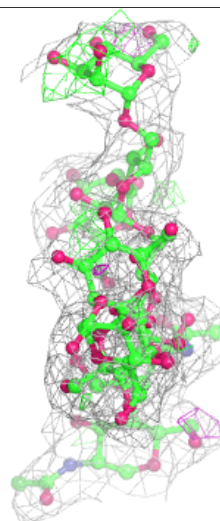
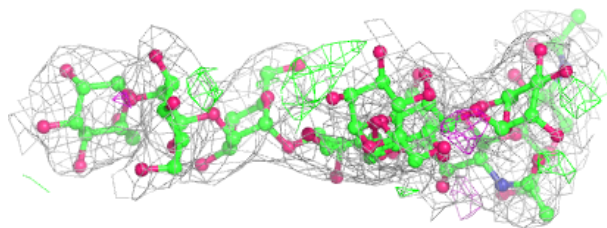
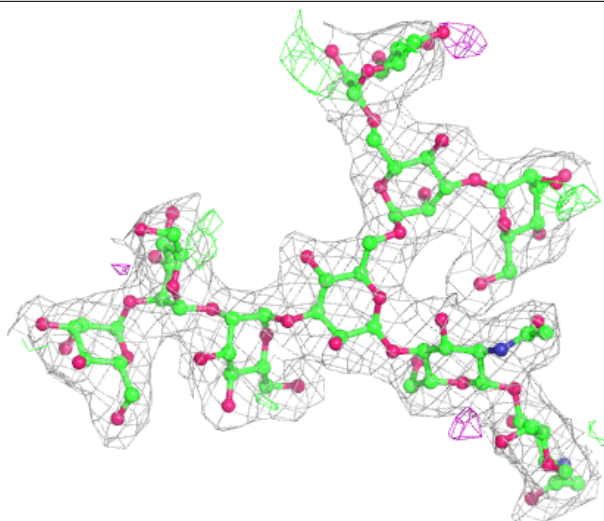
Electron density around Chain R:

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



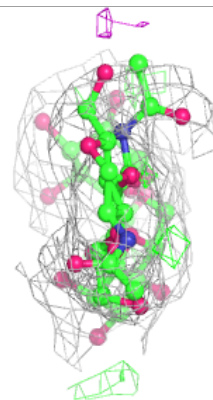
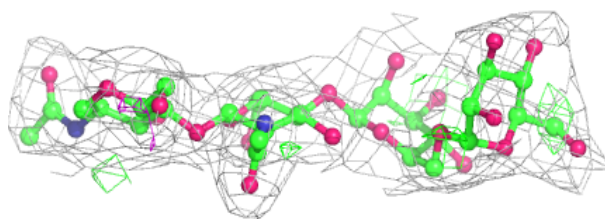
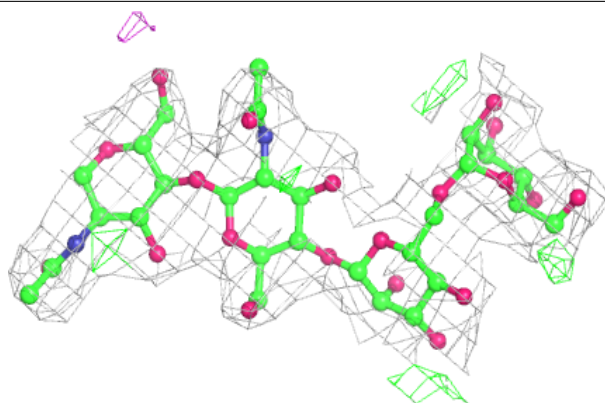
Electron density around Chain T:

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

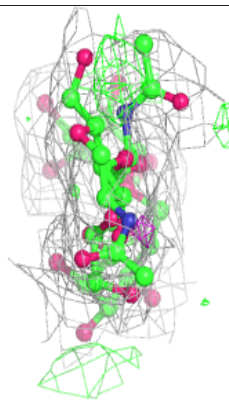
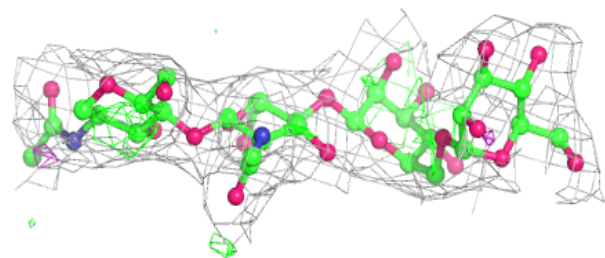
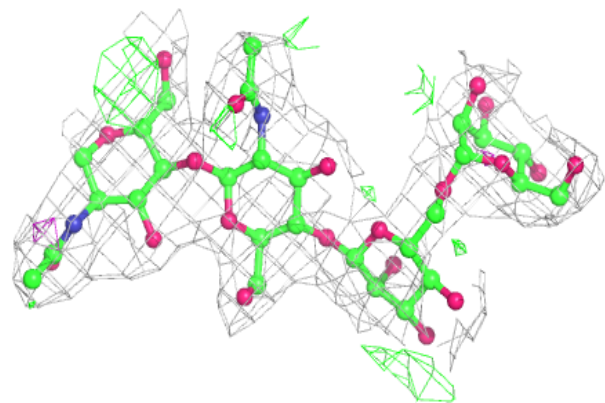


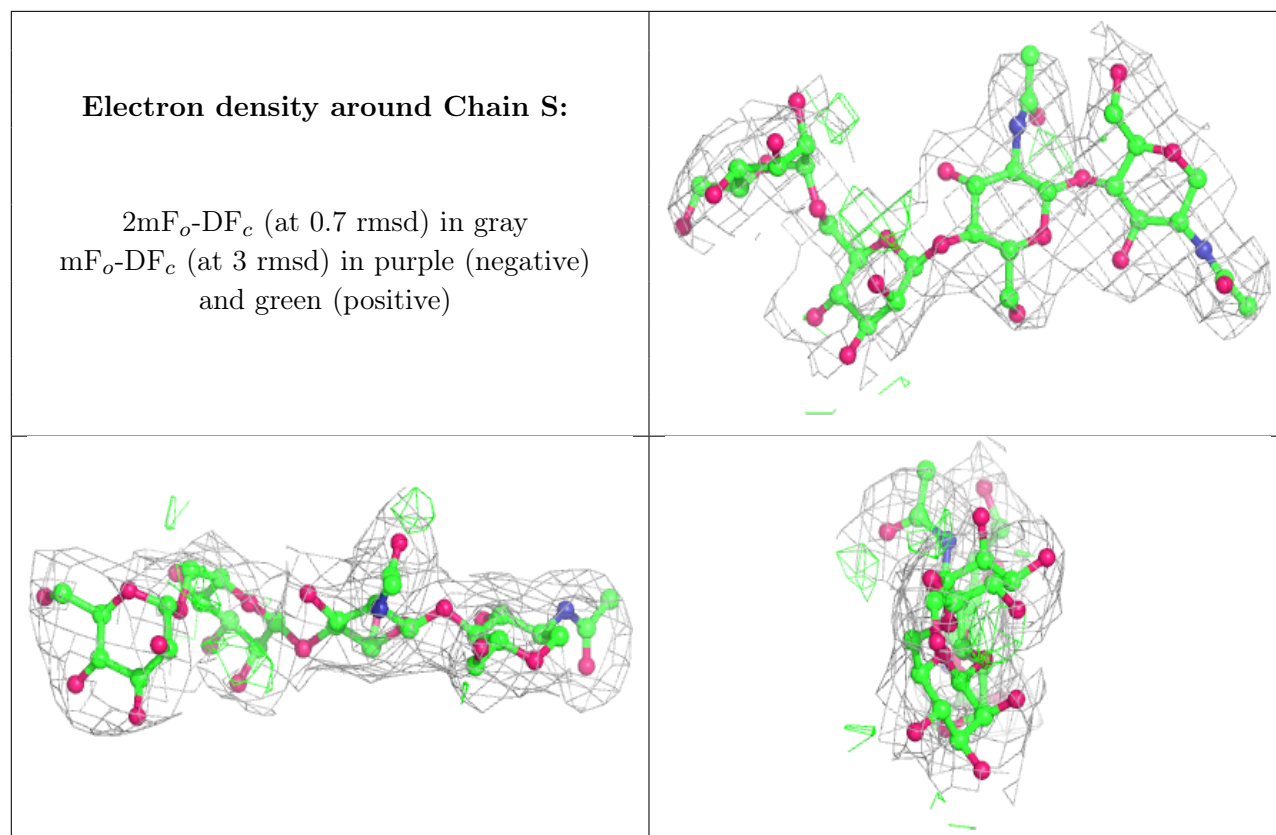
Electron density around Chain O:

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

**Electron density around Chain Q:**

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





6.4 Ligands [i](#)

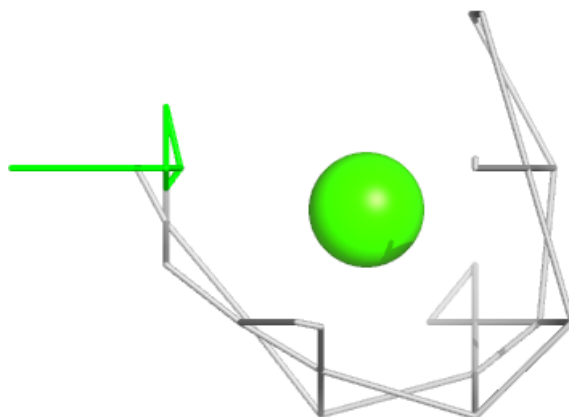
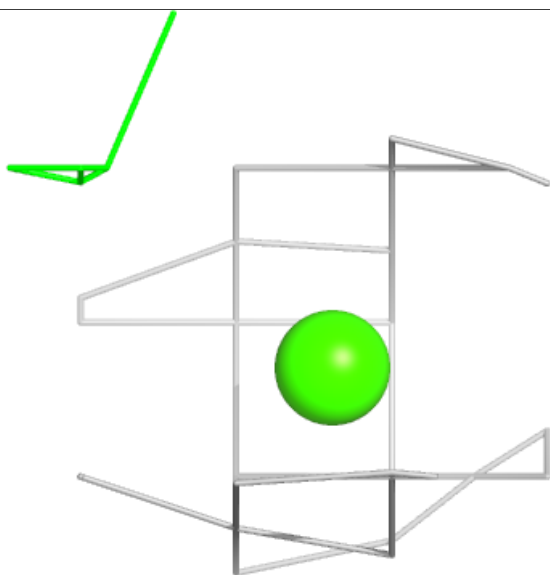
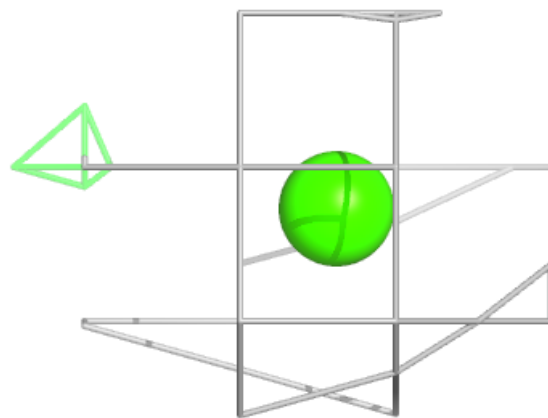
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
8	CA	D	502	1/1	0.60	0.19	90,90,90,90	0
8	CA	B	502	1/1	0.71	0.17	79,79,79,79	0
8	CA	C	502	1/1	0.79	0.11	72,72,72,72	0
7	NAG	B	501	14/15	0.80	0.32	47,58,62,65	0
7	NAG	C	501	14/15	0.81	0.42	56,68,75,76	0
7	NAG	D	501	14/15	0.84	0.28	46,58,65,66	0
7	NAG	A	501	14/15	0.86	0.30	49,58,63,64	0
8	CA	A	502	1/1	0.91	0.10	65,65,65,65	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

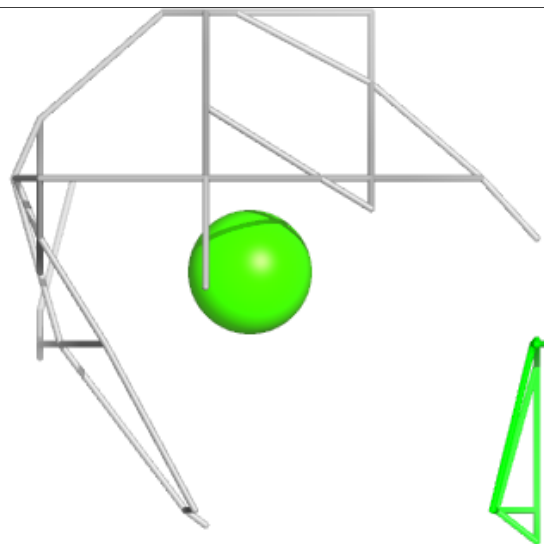
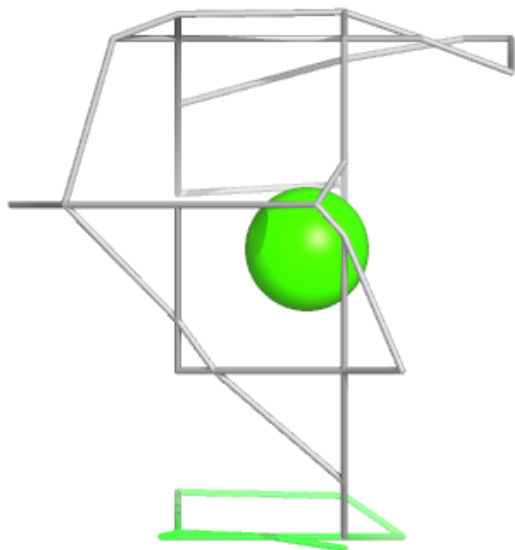
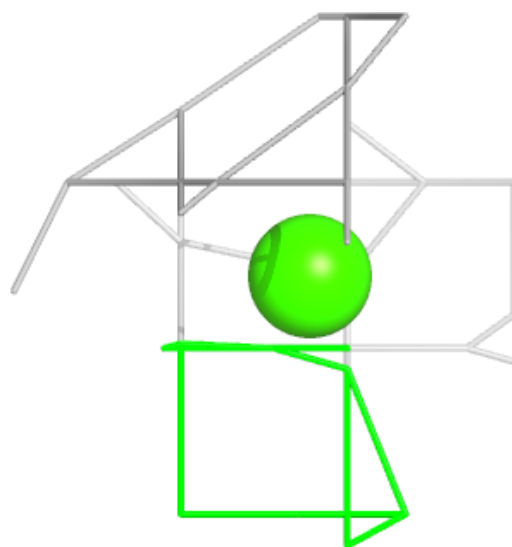
Electron density around CA D 502:

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



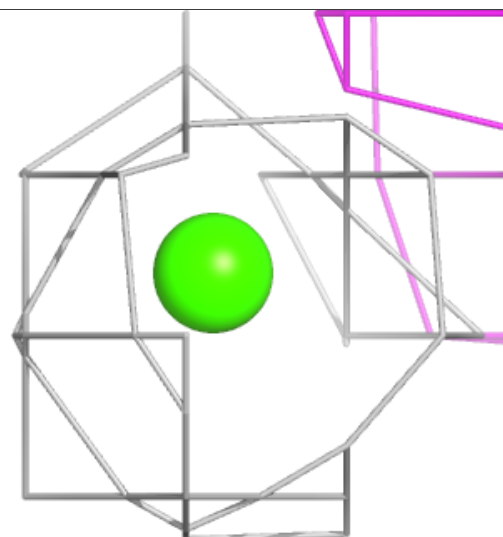
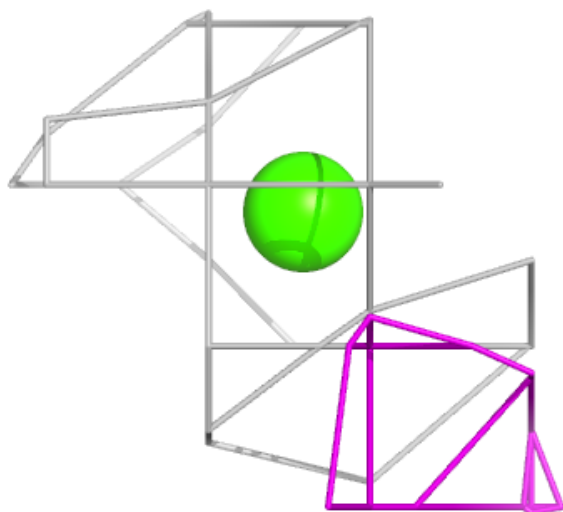
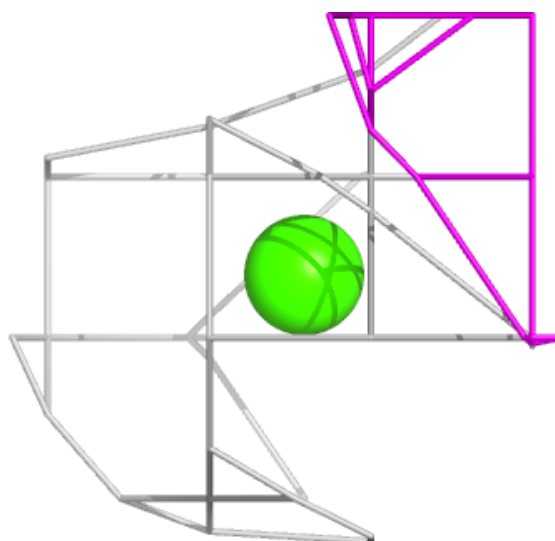
Electron density around CA B 502:

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



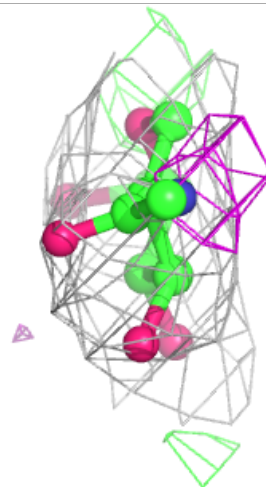
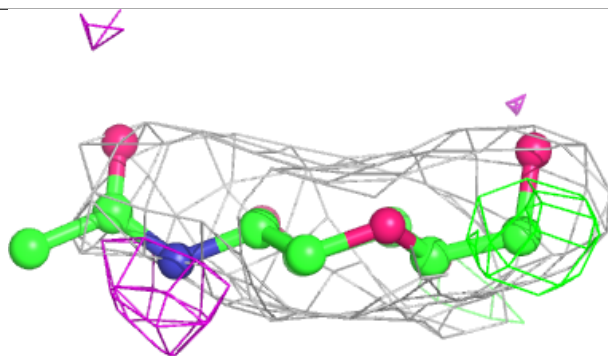
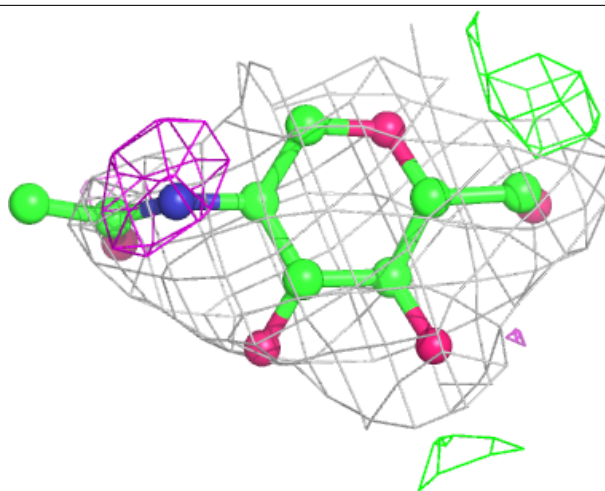
Electron density around CA C 502:

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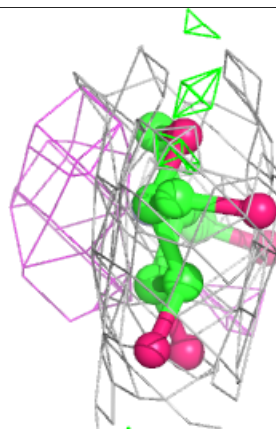
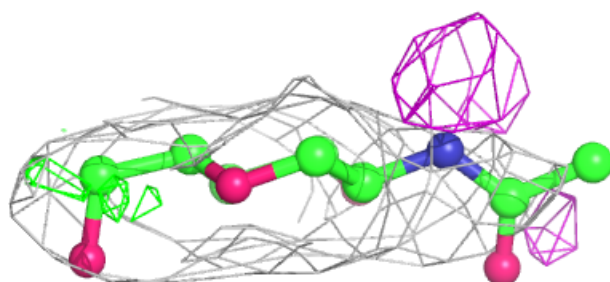
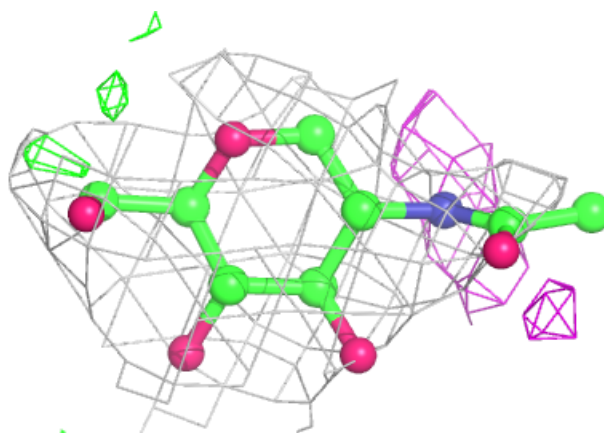
Electron density around NAG B 501:

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and green (positive)



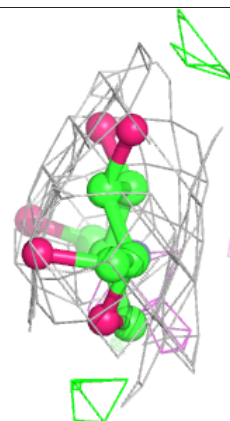
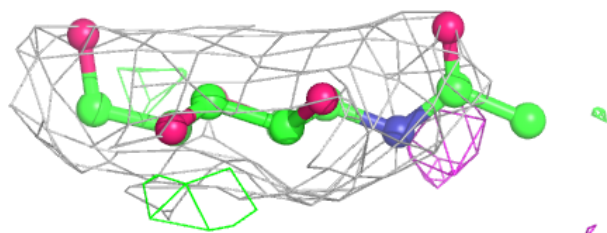
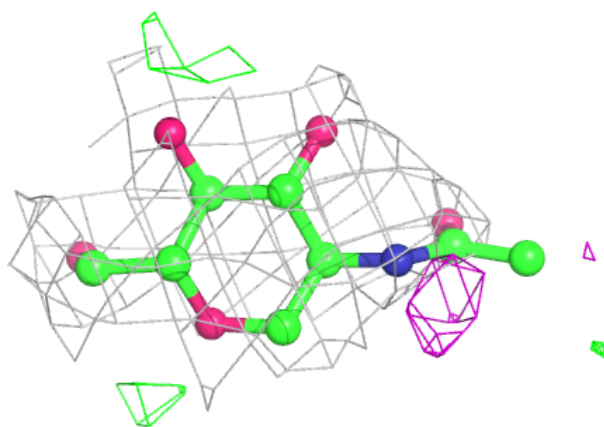
Electron density around NAG C 501:

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



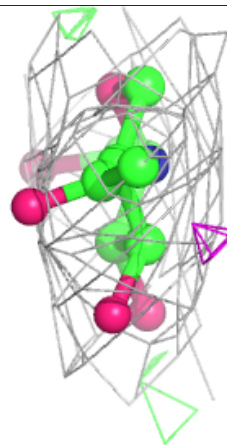
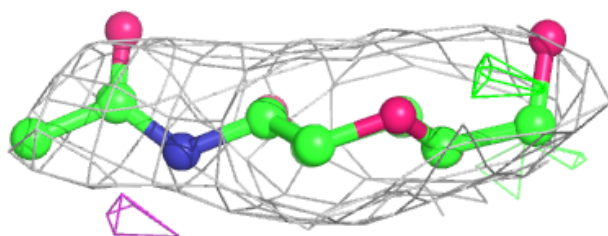
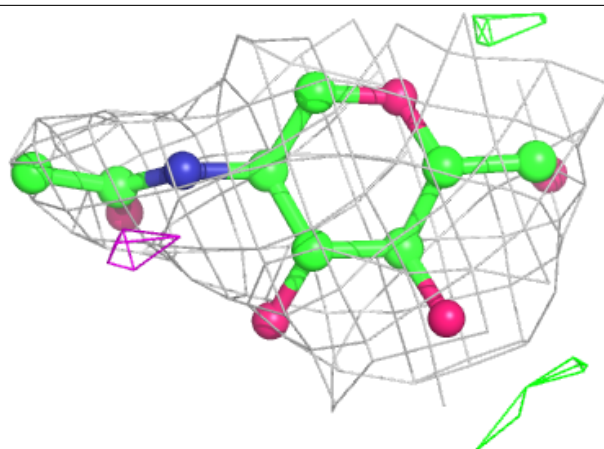
Electron density around NAG D 501:

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



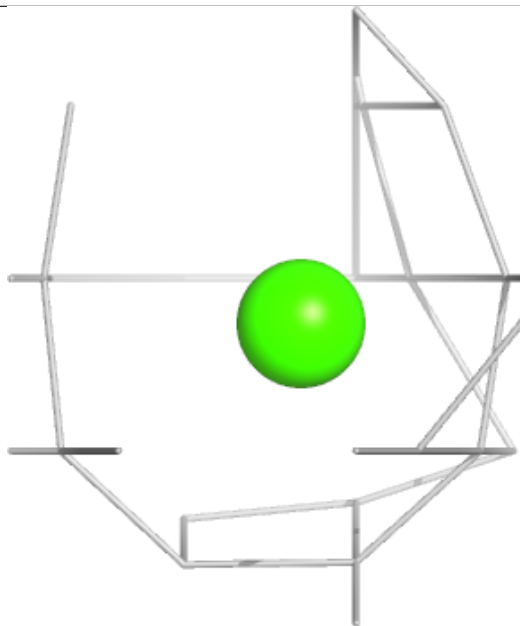
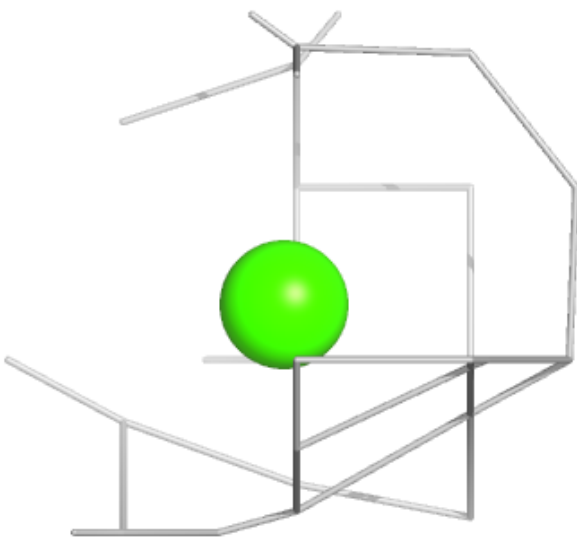
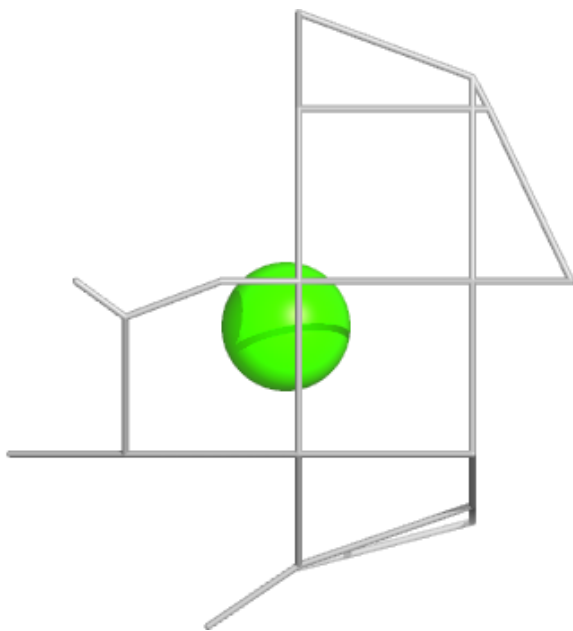
Electron density around NAG A 501:

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



Electron density around CA A 502:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.