



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 09:53 PM UTC

PDB ID : 4WSR / pdb_00004wsr
Title : The crystal structure of hemagglutinin form A/chicken/New York/14677-13/1998
Authors : Yang, H.; Carney, P.J.; Chang, J.C.; Villanueva, J.M.; Stevens, J.
Deposited on : 2014-10-28
Resolution : 2.50 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

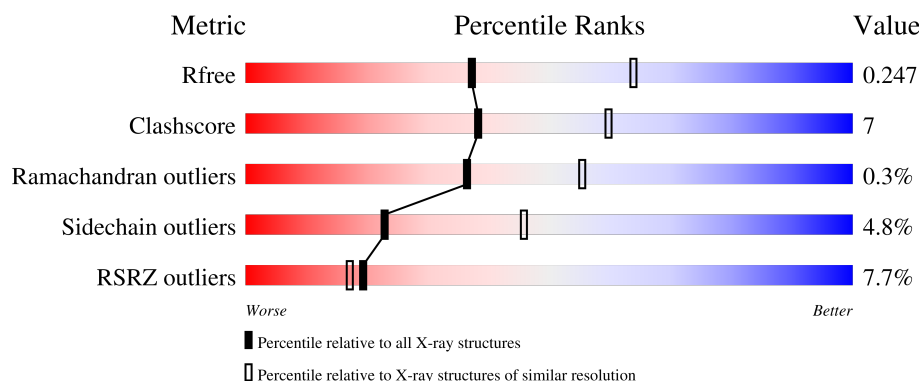
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	514	5% 81% 12% • 6%
1	B	514	6% 79% 12% • 6%
1	C	514	3% 83% 9% • 6%
1	D	514	7% 79% 16% • •
1	E	514	11% 79% 14% • 5%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	514	 11% 78% 13% 6%
2	G	2	 100%
2	H	2	 100%
2	I	2	 100%
2	J	2	 100%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NAG	A	601	X	-	-	-
3	NAG	B	601	X	-	-	-
3	NAG	C	605	X	-	-	-
3	NAG	D	601	X	-	-	-
3	NAG	D	602	X	-	-	-
3	NAG	E	601	X	-	-	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 24430 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 Hemagglutinin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	483	Total	C	N	O	S	0	0	0
			3841	2410	669	743	19			
1	B	482	Total	C	N	O	S	0	0	0
			3832	2405	667	741	19			
1	C	482	Total	C	N	O	S	0	0	0
			3832	2405	667	741	19			
1	E	489	Total	C	N	O	S	0	0	0
			3886	2441	675	751	19			
1	D	498	Total	C	N	O	S	0	0	0
			3952	2484	688	761	19			
1	F	481	Total	C	N	O	S	0	0	0
			3825	2400	666	740	19			

There are 66 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	ALA	-	expression tag	UNP Q0A3A5
A	-2	ASP	-	expression tag	UNP Q0A3A5
A	-1	PRO	-	expression tag	UNP Q0A3A5
A	0	GLY	-	expression tag	UNP Q0A3A5
A	317	THR	UNK	conflict	UNP Q0A3A5
A	504	GLY	VAL	conflict	UNP Q0A3A5
A	505	ARG	MET	conflict	UNP Q0A3A5
A	507	VAL	-	expression tag	UNP Q0A3A5
A	508	PRO	-	expression tag	UNP Q0A3A5
A	509	ARG	-	expression tag	UNP Q0A3A5
A	510	GLY	-	expression tag	UNP Q0A3A5
B	-3	ALA	-	expression tag	UNP Q0A3A5
B	-2	ASP	-	expression tag	UNP Q0A3A5
B	-1	PRO	-	expression tag	UNP Q0A3A5
B	0	GLY	-	expression tag	UNP Q0A3A5
B	317	THR	UNK	conflict	UNP Q0A3A5
B	504	GLY	VAL	conflict	UNP Q0A3A5

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	505	ARG	MET	conflict	UNP Q0A3A5
B	507	VAL	-	expression tag	UNP Q0A3A5
B	508	PRO	-	expression tag	UNP Q0A3A5
B	509	ARG	-	expression tag	UNP Q0A3A5
B	510	GLY	-	expression tag	UNP Q0A3A5
C	-3	ALA	-	expression tag	UNP Q0A3A5
C	-2	ASP	-	expression tag	UNP Q0A3A5
C	-1	PRO	-	expression tag	UNP Q0A3A5
C	0	GLY	-	expression tag	UNP Q0A3A5
C	317	THR	UNK	conflict	UNP Q0A3A5
C	504	GLY	VAL	conflict	UNP Q0A3A5
C	505	ARG	MET	conflict	UNP Q0A3A5
C	507	VAL	-	expression tag	UNP Q0A3A5
C	508	PRO	-	expression tag	UNP Q0A3A5
C	509	ARG	-	expression tag	UNP Q0A3A5
C	510	GLY	-	expression tag	UNP Q0A3A5
E	-3	ALA	-	expression tag	UNP Q0A3A5
E	-2	ASP	-	expression tag	UNP Q0A3A5
E	-1	PRO	-	expression tag	UNP Q0A3A5
E	0	GLY	-	expression tag	UNP Q0A3A5
E	317	THR	UNK	conflict	UNP Q0A3A5
E	504	GLY	VAL	conflict	UNP Q0A3A5
E	505	ARG	MET	conflict	UNP Q0A3A5
E	507	VAL	-	expression tag	UNP Q0A3A5
E	508	PRO	-	expression tag	UNP Q0A3A5
E	509	ARG	-	expression tag	UNP Q0A3A5
E	510	GLY	-	expression tag	UNP Q0A3A5
D	-3	ALA	-	expression tag	UNP Q0A3A5
D	-2	ASP	-	expression tag	UNP Q0A3A5
D	-1	PRO	-	expression tag	UNP Q0A3A5
D	0	GLY	-	expression tag	UNP Q0A3A5
D	317	THR	UNK	conflict	UNP Q0A3A5
D	504	GLY	VAL	conflict	UNP Q0A3A5
D	505	ARG	MET	conflict	UNP Q0A3A5
D	507	VAL	-	expression tag	UNP Q0A3A5
D	508	PRO	-	expression tag	UNP Q0A3A5
D	509	ARG	-	expression tag	UNP Q0A3A5
D	510	GLY	-	expression tag	UNP Q0A3A5
F	-3	ALA	-	expression tag	UNP Q0A3A5
F	-2	ASP	-	expression tag	UNP Q0A3A5
F	-1	PRO	-	expression tag	UNP Q0A3A5
F	0	GLY	-	expression tag	UNP Q0A3A5

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
F	317	THR	UNK	conflict	UNP Q0A3A5
F	504	GLY	VAL	conflict	UNP Q0A3A5
F	505	ARG	MET	conflict	UNP Q0A3A5
F	507	VAL	-	expression tag	UNP Q0A3A5
F	508	PRO	-	expression tag	UNP Q0A3A5
F	509	ARG	-	expression tag	UNP Q0A3A5
F	510	GLY	-	expression tag	UNP Q0A3A5

- Molecule 2 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
2	G	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	H	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	I	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	J	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	226	Total	O	0	0
			226	226		
4	B	219	Total	O	0	0
			219	219		
4	C	175	Total	O	0	0
			175	175		

Continued on next page...

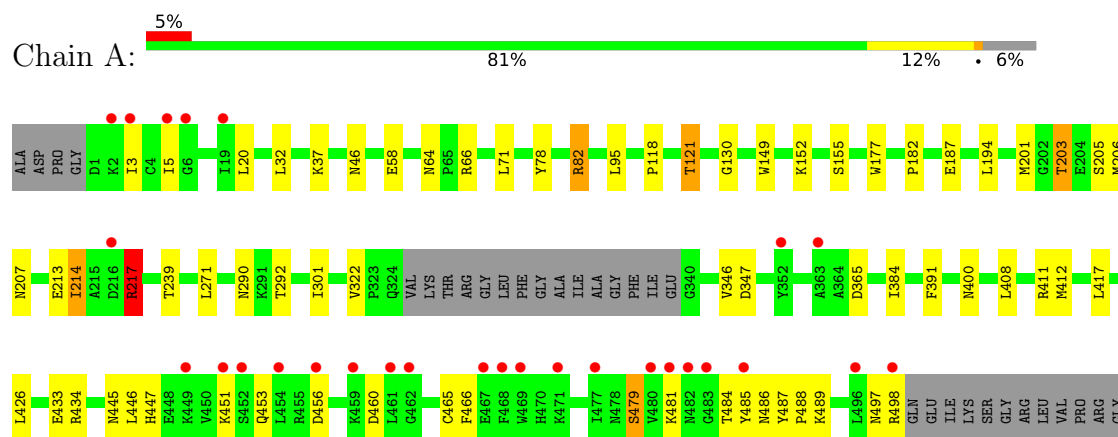
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	85	Total 85	O 85	0	0
4	D	212	Total 212	O 212	0	0
4	F	107	Total 107	O 107	0	0

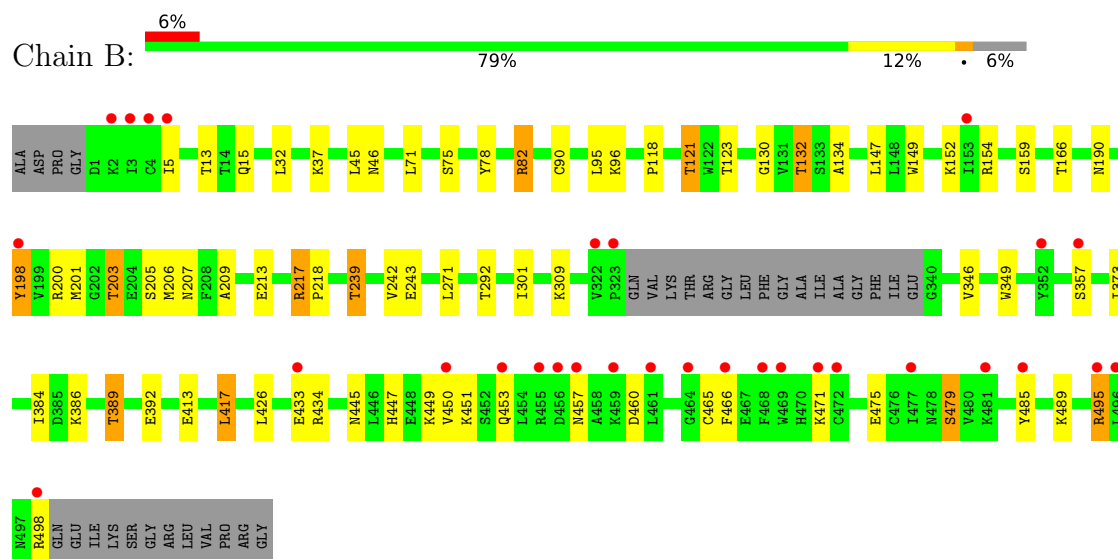
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

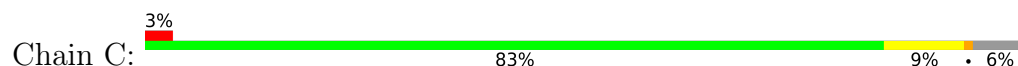
• Molecule 1: Hemagglutinin

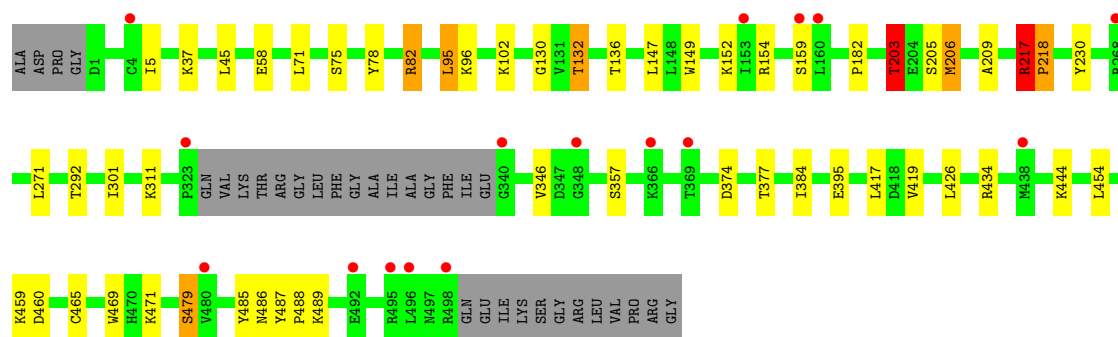


• Molecule 1: Hemagglutinin

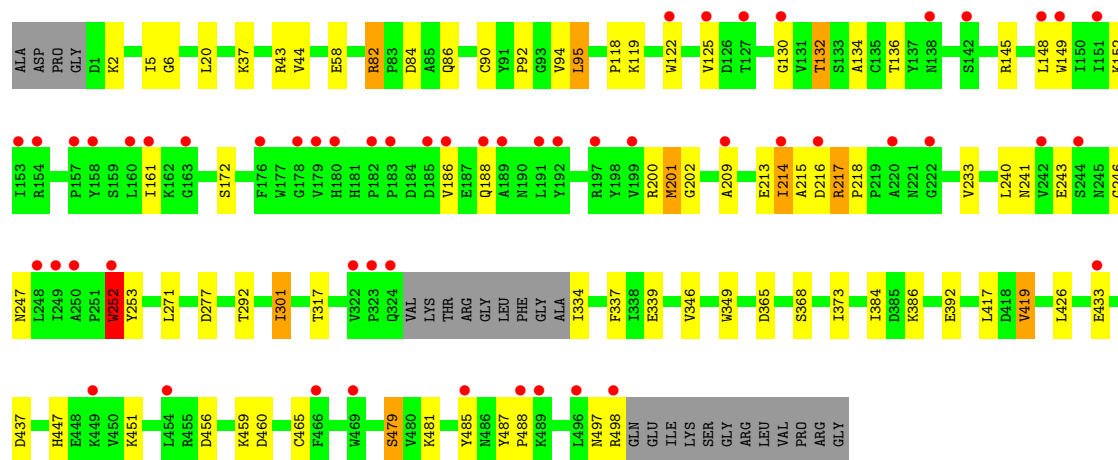
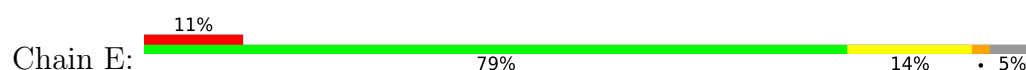


• Molecule 1: Hemagglutinin

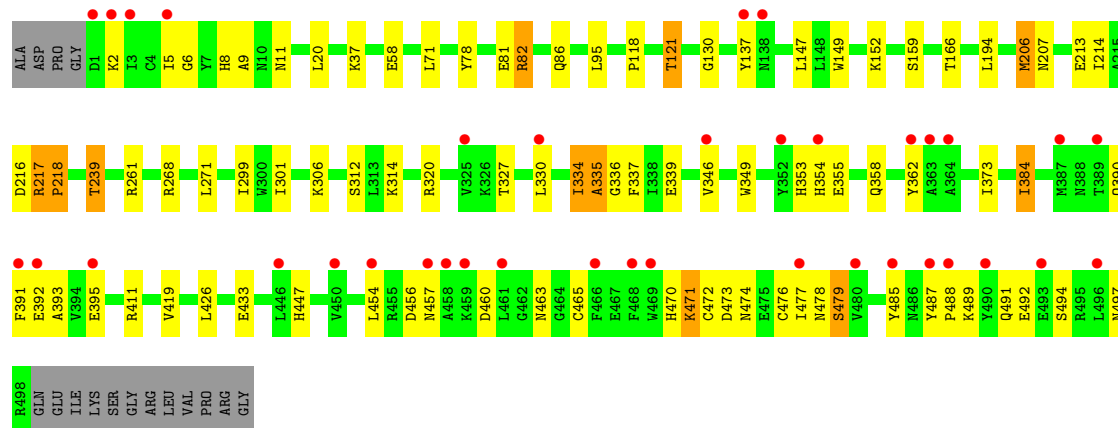
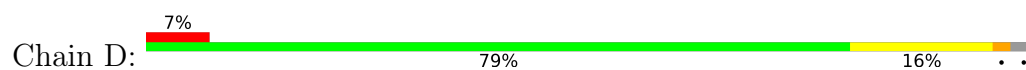




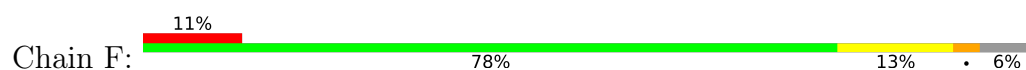
• Molecule 1: Hemagglutinin

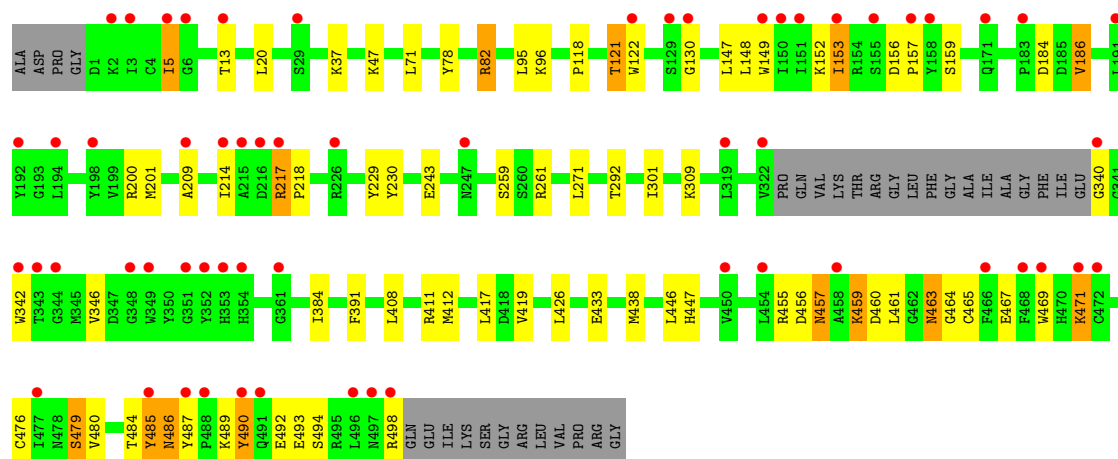


• Molecule 1: Hemagglutinin



• Molecule 1: Hemagglutinin





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

Chain G:  100%

MAG1
MAG2

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

Chain H:  100%

MAG1
MAG2

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

Chain I:  100%

MAG1
MAG2

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

Chain J:  100%

MAG1
MAG2

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	252.54Å 134.82Å 123.09Å 90.00° 113.23° 90.00°	Depositor
Resolution (Å)	48.00 – 2.50 48.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.9 (48.00-2.50) 98.9 (48.00-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.65 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.210 , 0.246 0.213 , 0.247	Depositor DCC
R_{free} test set	6504 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	49.1	Xtriage
Anisotropy	0.338	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 58.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	24430	wwPDB-VP
Average B, all atoms (Å ²)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.95% 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: NAG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.96	0/3928	0.93	3/5323 (0.1%)
1	B	0.92	1/3919 (0.0%)	0.95	5/5311 (0.1%)
1	C	0.92	1/3919 (0.0%)	0.93	4/5311 (0.1%)
1	D	0.91	3/4042 (0.1%)	0.95	5/5477 (0.1%)
1	E	0.84	0/3974	0.92	6/5385 (0.1%)
1	F	0.87	2/3911 (0.1%)	0.96	5/5299 (0.1%)
All	All	0.91	7/23693 (0.0%)	0.94	28/32106 (0.1%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	485	TYR	N-CA	8.77	1.57	1.46
1	F	486	ASN	N-CA	6.76	1.54	1.46
1	D	336	GLY	N-CA	6.26	1.51	1.45
1	D	218	PRO	CA-C	-5.99	1.48	1.52
1	C	218	PRO	CA-C	5.90	1.55	1.51
1	D	299	ILE	CA-C	-5.36	1.45	1.52
1	B	218	PRO	C-O	-5.09	1.20	1.25

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	485	TYR	N-CA-C	9.04	130.06	110.80
1	D	494	SER	N-CA-C	7.21	118.83	110.97
1	F	484	THR	N-CA-C	7.12	120.69	108.02
1	D	335	ALA	N-CA-C	6.95	122.42	113.88
1	E	201	MET	CG-SD-CE	6.89	116.06	100.90
1	C	132	THR	CB-CA-C	-6.58	95.92	109.94
1	B	217	ARG	CA-C-N	-6.28	115.08	119.66
1	B	217	ARG	C-N-CA	-6.28	115.08	119.66

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	252	TRP	CA-CB-CG	6.16	125.31	113.60
1	B	132	THR	CB-CA-C	-5.97	96.31	109.56
1	C	217	ARG	CB-CG-CD	5.96	125.00	111.30
1	B	198	TYR	CA-CB-CG	5.88	124.48	113.90
1	D	384	ILE	CA-CB-CG1	5.88	120.39	110.40
1	A	347	ASP	N-CA-C	5.71	117.50	111.28
1	E	252	TRP	CB-CA-C	5.65	120.64	111.26
1	F	201	MET	CG-SD-CE	5.64	113.30	100.90
1	F	153	ILE	CB-CA-C	5.62	119.33	111.34
1	A	217	ARG	CB-CG-CD	5.59	124.15	111.30
1	C	5	ILE	CB-CG1-CD1	5.56	125.48	113.80
1	B	389	THR	N-CA-CB	-5.52	101.26	111.53
1	F	489	LYS	N-CA-C	5.47	122.46	110.80
1	D	218	PRO	O-C-N	5.46	123.72	121.15
1	E	132	THR	CB-CA-C	-5.38	97.61	109.56
1	D	314	LYS	CA-CB-CG	5.20	124.50	114.10
1	C	203	THR	N-CA-CB	-5.14	103.10	111.22
1	E	481	LYS	CB-CG-CD	5.12	123.09	111.30
1	E	419	VAL	N-CA-CB	5.12	118.26	110.58
1	A	214	ILE	N-CA-C	5.04	115.60	109.30

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	3841	0	3701	55	0
1	B	3832	0	3693	49	0
1	C	3832	0	3691	32	0
1	D	3952	0	3819	65	1
1	E	3886	0	3746	76	0
1	F	3825	0	3687	71	0
2	G	28	0	25	0	0
2	H	28	0	25	0	0
2	I	28	0	25	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	J	28	0	25	0	0
3	A	14	0	13	0	0
3	B	14	0	13	1	0
3	C	42	0	39	2	0
3	D	28	0	26	0	0
3	E	28	0	26	0	0
4	A	226	0	0	4	0
4	B	219	0	0	8	0
4	C	175	0	0	5	0
4	D	212	0	0	15	0
4	E	85	0	0	16	0
4	F	107	0	0	4	0
All	All	24430	0	22554	315	1

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

All (315) 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:E:145:ARG:O	1:E:252:TRP:NE1	1.57	1.35
1:F:480:VAL:HG23	1:F:485:TYR:OH	1.47	1.13
1:A:447:HIS:CE1	1:A:451:LYS:HZ3	1.70	1.08
1:F:476:CYS:O	1:F:485:TYR:OH	1.75	1.04
1:A:447:HIS:CE1	1:A:451:LYS:NZ	2.28	1.01
1:E:241:ASN:O	4:E:701:HOH:O	1.86	0.93
1:D:2:LYS:O	4:D:701:HOH:O	1.85	0.92
1:F:479:SER:OG	1:F:485:TYR:CE1	2.22	0.91
1:D:118:PRO:O	1:D:121:THR:HG23	1.70	0.91
1:A:3:ILE:HD11	1:A:481:LYS:NZ	1.86	0.90
1:B:118:PRO:O	1:B:121:THR:HG23	1.71	0.90
1:B:457:ASN:ND2	1:B:485:TYR:OH	2.04	0.90
1:F:118:PRO:O	1:F:121:THR:HG23	1.71	0.90
1:A:451:LYS:HZ2	1:A:466:PHE:HZ	1.18	0.89
1:A:118:PRO:O	1:A:121:THR:HG23	1.71	0.89
1:E:252:TRP:CD1	1:E:253:TYR:HD2	1.89	0.89
1:E:202:GLY:N	4:E:701:HOH:O	1.86	0.88
1:D:355:GLU:N	4:D:701:HOH:O	2.05	0.88
1:F:459:LYS:HE3	1:F:469:TRP:CZ2	2.08	0.86
1:F:480:VAL:CG2	1:F:485:TYR:OH	2.24	0.86
1:D:306:LYS:HE3	1:D:391:PHE:H	1.40	0.86

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:214:ILE:O	1:B:200:ARG:NH1	2.08	0.86
1:B:453:GLN:NE2	4:B:701:HOH:O	2.10	0.84
1:E:125:VAL:HG11	1:E:161:ILE:HD11	1.59	0.84
1:B:203:THR:HG22	1:B:205:SER:H	1.44	0.83
1:A:434:ARG:HE	1:B:434:ARG:HH22	1.23	0.82
1:A:497:ASN:O	1:A:498:ARG:HG3	1.80	0.81
1:D:358:GLN:NE2	4:D:703:HOH:O	2.12	0.81
1:F:459:LYS:HE3	1:F:469:TRP:CH2	2.16	0.81
1:A:203:THR:HG22	1:A:205:SER:H	1.45	0.81
1:D:491:GLN:HE21	1:F:498:ARG:NE	1.78	0.81
1:E:497:ASN:O	1:E:498:ARG:HG3	1.80	0.81
1:B:445:ASN:OD1	1:B:449:LYS:NZ	2.14	0.80
1:D:476:CYS:SG	1:D:477:ILE:N	2.56	0.79
1:E:213:GLU:HB3	1:F:209:ALA:HB3	1.64	0.78
1:F:309:LYS:HG3	1:F:417:LEU:HD21	1.66	0.78
1:C:486:ASN:N	4:C:702:HOH:O	2.17	0.78
1:C:203:THR:HG22	1:C:205:SER:H	1.47	0.77
1:D:320:ARG:NH1	4:D:704:HOH:O	2.17	0.77
1:F:479:SER:OG	1:F:485:TYR:CZ	2.33	0.77
1:B:200:ARG:NE	1:B:209:ALA:HB1	2.00	0.77
1:E:188:GLN:HE22	1:E:247:ASN:HD21	1.33	0.76
1:A:58:GLU:OE1	4:A:701:HOH:O	2.02	0.76
1:D:393:ALA:O	4:D:702:HOH:O	2.02	0.75
1:B:450:VAL:HG13	1:B:466:PHE:HE2	1.49	0.75
1:D:473:ASP:O	1:D:476:CYS:SG	2.45	0.75
1:A:434:ARG:HH22	1:C:434:ARG:HH11	1.35	0.75
1:E:122:TRP:HD1	1:E:161:ILE:CG2	2.00	0.74
1:D:492:GLU:HG2	1:F:498:ARG:NH2	2.03	0.73
1:F:457:ASN:OD1	1:F:487:TYR:CE1	2.41	0.73
1:B:201:MET:HE1	1:B:242:VAL:HG13	1.70	0.72
1:D:306:LYS:HD3	1:D:390:GLN:HA	1.71	0.71
1:A:400:ASN:OD1	4:A:702:HOH:O	2.10	0.70
1:A:434:ARG:NH2	1:C:434:ARG:HH11	1.91	0.69
1:B:75:SER:HB3	4:B:880:HOH:O	1.93	0.69
1:F:459:LYS:NZ	1:F:467:GLU:OE1	2.26	0.69
1:A:3:ILE:HD11	1:A:481:LYS:HZ2	1.57	0.68
1:C:395:GLU:OE1	4:C:701:HOH:O	2.12	0.68
1:B:123:THR:OG1	4:B:702:HOH:O	2.12	0.67
1:B:200:ARG:HD3	1:B:209:ALA:CB	2.25	0.67
1:B:498:ARG:HH11	1:B:498:ARG:HG3	1.60	0.67
1:B:198:TYR:CD1	1:B:200:ARG:HG2	2.31	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:5:ILE:HD11	1:F:446:LEU:HB2	1.77	0.66
1:F:471:LYS:H	1:F:471:LYS:HD3	1.60	0.66
1:F:459:LYS:HD2	1:F:469:TRP:CZ2	2.31	0.65
1:E:122:TRP:HD1	1:E:161:ILE:HG21	1.61	0.65
1:E:122:TRP:CD1	1:E:161:ILE:HG21	2.31	0.65
1:E:252:TRP:HD1	1:E:253:TYR:N	1.93	0.65
1:D:492:GLU:HG2	1:F:498:ARG:HH21	1.62	0.65
1:A:3:ILE:CD1	1:A:481:LYS:NZ	2.59	0.65
1:F:480:VAL:HG22	1:F:485:TYR:CE2	2.32	0.64
1:E:145:ARG:O	1:E:252:TRP:CE2	2.46	0.64
1:F:461:LEU:HG	1:F:463:ASN:OD1	1.97	0.64
1:A:207:ASN:OD1	1:C:217:ARG:NH1	2.32	0.63
1:B:201:MET:CE	1:B:242:VAL:HG13	2.28	0.63
1:F:457:ASN:OD1	1:F:487:TYR:CD1	2.51	0.63
1:E:172:SER:OG	1:E:233:VAL:CG1	2.46	0.63
1:E:437:ASP:HB3	4:E:773:HOH:O	1.98	0.62
1:E:201:MET:HA	4:E:701:HOH:O	1.99	0.62
1:B:309:LYS:HE2	1:B:417:LEU:HD13	1.80	0.62
1:E:209:ALA:HB3	1:D:213:GLU:CD	2.23	0.62
1:D:471:LYS:HD2	1:D:471:LYS:O	2.00	0.62
1:E:243:GLU:OE1	1:D:216:ASP:N	2.27	0.61
1:D:82:ARG:NH2	1:D:271:LEU:O	2.33	0.61
1:A:447:HIS:CE1	1:A:451:LYS:HZ1	2.16	0.61
1:A:82:ARG:NH2	1:A:271:LEU:O	2.34	0.61
1:E:201:MET:CA	4:E:701:HOH:O	2.48	0.61
1:F:492:GLU:OE2	1:F:493:GLU:OE2	2.19	0.61
1:F:469:TRP:NE1	1:F:494:SER:HG	1.98	0.61
1:A:451:LYS:HG2	1:A:466:PHE:HZ	1.64	0.61
1:F:82:ARG:NH2	1:F:271:LEU:O	2.32	0.60
1:D:334:ILE:HD12	1:D:334:ILE:C	2.27	0.60
1:F:490:TYR:O	1:F:493:GLU:OE1	2.18	0.60
1:A:3:ILE:HD11	1:A:481:LYS:HZ3	1.66	0.60
1:D:335:ALA:HB1	1:D:339:GLU:HG3	1.83	0.60
1:E:82:ARG:NH2	1:E:271:LEU:O	2.35	0.60
1:E:44:VAL:HG21	1:E:301:ILE:CD1	2.31	0.59
1:C:292:THR:HG21	1:C:384:ILE:HG12	1.85	0.59
1:F:459:LYS:HD2	1:F:469:TRP:CE2	2.38	0.59
1:F:459:LYS:CE	1:F:469:TRP:CZ2	2.84	0.59
1:E:252:TRP:CD1	1:E:253:TYR:CD2	2.82	0.59
1:E:252:TRP:HD1	1:E:253:TYR:H	1.50	0.58
1:A:292:THR:HG21	1:A:384:ILE:HG12	1.85	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:44:VAL:HG21	1:E:301:ILE:HD11	1.85	0.58
1:D:491:GLN:HE21	1:F:498:ARG:CZ	2.16	0.58
1:F:292:THR:HG21	1:F:384:ILE:HG12	1.85	0.58
1:C:82:ARG:NH2	1:C:271:LEU:O	2.36	0.58
1:D:58:GLU:OE1	4:D:705:HOH:O	2.17	0.58
1:B:82:ARG:NH2	1:B:271:LEU:O	2.37	0.58
1:B:292:THR:HG21	1:B:384:ILE:HG12	1.86	0.58
1:E:214:ILE:O	1:F:200:ARG:HD3	2.04	0.58
1:E:215:ALA:HA	1:F:200:ARG:HD3	1.86	0.58
1:E:292:THR:HG21	1:E:384:ILE:HG12	1.86	0.57
1:D:474:ASN:HA	1:D:477:ILE:HG12	1.85	0.57
1:B:433:GLU:OE1	1:C:434:ARG:NH2	2.37	0.57
1:B:200:ARG:CD	1:B:209:ALA:CB	2.82	0.57
1:C:96:LYS:HG3	1:C:230:TYR:CE1	2.40	0.57
1:C:459:LYS:HD2	1:C:469:TRP:CZ2	2.39	0.57
1:D:11:ASN:ND2	4:D:712:HOH:O	2.37	0.57
1:E:368:SER:N	4:E:702:HOH:O	2.05	0.56
1:D:349:TRP:CH2	1:D:373:ILE:HD13	2.39	0.56
1:B:451:LYS:NZ	1:B:460:ASP:OD1	2.29	0.56
1:E:145:ARG:O	1:E:252:TRP:CD1	2.50	0.56
1:E:365:ASP:CG	4:E:702:HOH:O	2.47	0.56
1:D:2:LYS:HG3	4:D:701:HOH:O	2.04	0.56
1:D:395:GLU:HB2	4:D:739:HOH:O	2.05	0.56
1:A:20:LEU:HD12	1:A:433:GLU:OE2	2.06	0.56
1:D:472:CYS:C	1:D:476:CYS:SG	2.89	0.56
1:F:492:GLU:OE2	1:F:493:GLU:CD	2.48	0.56
1:D:334:ILE:HG12	1:D:353:HIS:CE1	2.41	0.56
1:A:451:LYS:NZ	1:A:466:PHE:CZ	2.58	0.55
1:D:354:HIS:CD2	1:D:477:ILE:HD13	2.41	0.55
1:B:349:TRP:CH2	1:B:373:ILE:HD13	2.42	0.55
1:E:349:TRP:CH2	1:E:373:ILE:HD13	2.41	0.55
1:C:357:SER:OG	1:C:471:LYS:HE2	2.07	0.55
1:A:456:ASP:OD1	1:A:487:TYR:OH	2.23	0.54
1:E:20:LEU:HD12	1:E:433:GLU:OE2	2.08	0.54
1:D:20:LEU:HD12	1:D:433:GLU:OE2	2.06	0.54
1:F:20:LEU:HD12	1:F:433:GLU:OE2	2.07	0.54
1:F:459:LYS:CD	1:F:469:TRP:CE2	2.91	0.54
1:F:469:TRP:CD1	1:F:494:SER:HG	2.25	0.54
1:E:84:ASP:O	1:E:86:GLN:OE1	2.24	0.54
1:D:460:ASP:O	1:D:465:CYS:O	2.26	0.54
1:E:451:LYS:NZ	1:E:460:ASP:OD1	2.28	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:66:ARG:CZ	1:A:66:ARG:HB3	2.37	0.54
1:F:156:ASP:CG	1:F:157:PRO:HD2	2.33	0.54
1:B:434:ARG:HD3	4:B:771:HOH:O	2.08	0.54
1:D:392:GLU:O	1:F:411:ARG:HD2	2.08	0.54
1:B:154:ARG:NH1	1:B:190:ASN:OD1	2.40	0.54
1:C:486:ASN:ND2	1:C:489:LYS:HB2	2.23	0.53
1:C:311:LYS:O	3:C:605:NAG:H82	2.08	0.53
1:E:122:TRP:CZ3	1:E:148:LEU:HD23	2.43	0.53
1:A:451:LYS:HE3	1:A:460:ASP:OD1	2.09	0.53
1:E:240:LEU:HD12	4:E:701:HOH:O	2.08	0.53
1:B:200:ARG:HD3	1:B:209:ALA:HB2	1.91	0.52
1:E:216:ASP:HB3	1:F:243:GLU:OE2	2.10	0.52
1:E:460:ASP:O	1:E:465:CYS:O	2.28	0.52
1:D:334:ILE:HD11	1:D:353:HIS:ND1	2.25	0.52
1:D:206:MET:HG2	1:D:207:ASN:N	2.24	0.52
1:A:447:HIS:HE1	1:A:451:LYS:NZ	2.03	0.52
1:D:8:HIS:CD2	1:D:9:ALA:O	2.63	0.52
1:F:459:LYS:CD	1:F:469:TRP:CZ2	2.94	0.52
1:A:486:ASN:ND2	1:A:489:LYS:HB2	2.26	0.51
1:B:495:ARG:NH1	4:B:709:HOH:O	2.42	0.51
1:B:357:SER:HB3	1:B:471:LYS:HE2	1.91	0.51
1:F:259:SER:O	1:F:261:ARG:NH1	2.44	0.51
1:B:207:ASN:ND2	4:B:712:HOH:O	2.44	0.51
1:B:460:ASP:O	1:B:465:CYS:O	2.28	0.51
1:C:102:LYS:NZ	4:C:714:HOH:O	2.42	0.51
1:C:460:ASP:O	1:C:465:CYS:O	2.28	0.51
1:A:479:SER:OG	1:A:485:TYR:HA	2.11	0.51
1:D:479:SER:OG	1:D:485:TYR:HA	2.11	0.51
1:F:457:ASN:OD1	1:F:457:ASN:N	2.44	0.50
1:A:460:ASP:O	1:A:465:CYS:O	2.28	0.50
1:C:479:SER:OG	1:C:485:TYR:HA	2.12	0.50
1:B:15:GLN:OE1	3:B:601:NAG:H82	2.12	0.50
1:E:252:TRP:CD1	1:E:253:TYR:N	2.77	0.50
1:E:456:ASP:OD1	1:E:487:TYR:OH	2.24	0.50
1:F:184:ASP:OD1	1:F:186:VAL:HG13	2.11	0.50
1:E:479:SER:OG	1:E:485:TYR:HA	2.12	0.50
1:F:122:TRP:CZ3	1:F:148:LEU:HD23	2.47	0.49
1:E:240:LEU:CD1	4:E:701:HOH:O	2.61	0.49
1:F:456:ASP:OD1	1:F:487:TYR:OH	2.24	0.49
1:E:243:GLU:HB2	4:D:706:HOH:O	2.12	0.49
1:B:200:ARG:CD	1:B:209:ALA:HB1	2.43	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:374:ASP:O	1:C:377:THR:HG22	2.12	0.49
1:D:306:LYS:CE	1:D:391:PHE:H	2.19	0.49
1:A:66:ARG:HD3	4:A:755:HOH:O	2.13	0.49
1:F:96:LYS:HG3	1:F:230:TYR:CE1	2.47	0.49
1:F:309:LYS:CG	1:F:417:LEU:HD21	2.42	0.49
1:F:457:ASN:OD1	1:F:487:TYR:HE1	1.88	0.49
1:E:2:LYS:NZ	1:E:334:ILE:O	2.43	0.48
1:D:456:ASP:OD1	1:D:487:TYR:OH	2.25	0.48
1:F:122:TRP:NE1	4:F:2115:HOH:O	2.46	0.48
1:B:200:ARG:HE	1:B:209:ALA:HB1	1.73	0.48
1:E:43:ARG:NH2	1:E:277:ASP:OD1	2.46	0.48
1:A:130:GLY:HA3	1:A:149:TRP:HB3	1.94	0.48
1:A:207:ASN:CG	1:C:217:ARG:HH11	2.21	0.48
1:A:207:ASN:CG	1:C:217:ARG:NH1	2.72	0.48
1:F:460:ASP:O	1:F:465:CYS:O	2.31	0.48
1:E:209:ALA:CB	1:D:213:GLU:HB3	2.44	0.48
1:B:203:THR:HB	1:B:206:MET:HG3	1.96	0.48
1:C:203:THR:HB	1:C:206:MET:HG3	1.95	0.48
1:D:216:ASP:O	4:D:706:HOH:O	2.20	0.48
1:E:92:PRO:HA	4:E:718:HOH:O	2.14	0.47
1:D:306:LYS:NZ	4:D:726:HOH:O	2.47	0.47
1:F:340:GLY:N	4:F:2114:HOH:O	2.45	0.47
1:A:187:GLU:OE1	4:A:703:HOH:O	2.20	0.47
1:B:45:LEU:O	1:B:46:ASN:HB2	2.14	0.47
1:B:479:SER:OG	1:B:485:TYR:HA	2.13	0.47
1:E:122:TRP:CZ3	1:E:148:LEU:CD2	2.97	0.47
1:D:78:TYR:CD2	1:D:301:ILE:HD11	2.50	0.47
1:A:411:ARG:HD2	1:B:392:GLU:O	2.15	0.47
1:E:214:ILE:O	1:F:200:ARG:CD	2.62	0.47
1:D:130:GLY:HA3	1:D:149:TRP:HB3	1.97	0.47
1:D:268:ARG:NH1	4:D:725:HOH:O	2.47	0.47
1:F:456:ASP:OD1	1:F:487:TYR:CE1	2.67	0.47
1:B:213:GLU:HB3	1:C:209:ALA:CB	2.45	0.47
1:B:413:GLU:OE1	4:B:703:HOH:O	2.19	0.47
1:D:362:TYR:HB2	4:D:715:HOH:O	2.14	0.46
1:E:125:VAL:CG1	1:E:161:ILE:HD11	2.39	0.46
1:E:459:LYS:HG3	1:F:455:ARG:NH2	2.30	0.46
1:A:203:THR:HB	1:A:206:MET:HG3	1.96	0.46
1:A:213:GLU:HB2	4:B:712:HOH:O	2.15	0.46
1:E:58:GLU:HG2	1:E:95:LEU:HD12	1.98	0.46
1:E:172:SER:OG	1:E:233:VAL:HG13	2.14	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:45:LEU:HB2	4:C:797:HOH:O	2.14	0.46
1:E:130:GLY:HA3	1:E:149:TRP:HB3	1.98	0.46
1:E:241:ASN:HD22	1:D:217:ARG:HA	1.81	0.46
1:E:252:TRP:CD1	1:E:253:TYR:H	2.31	0.46
1:F:130:GLY:HA3	1:F:149:TRP:HB3	1.96	0.46
1:A:46:ASN:HD21	1:D:312:SER:HB2	1.81	0.46
1:B:433:GLU:CD	1:C:434:ARG:NH2	2.74	0.46
1:A:46:ASN:ND2	1:D:312:SER:HB2	2.31	0.46
1:A:434:ARG:HE	1:B:434:ARG:NH2	2.01	0.45
1:B:5:ILE:HG13	1:B:447:HIS:HA	1.97	0.45
1:C:182:PRO:O	1:C:217:ARG:NH2	2.50	0.45
1:E:44:VAL:HG21	1:E:301:ILE:HD12	1.99	0.45
1:B:130:GLY:HA3	1:B:149:TRP:HB3	1.99	0.45
1:E:118:PRO:HA	4:E:708:HOH:O	2.16	0.45
1:A:453:GLN:HG2	1:A:485:TYR:CB	2.46	0.45
1:C:130:GLY:HA3	1:C:149:TRP:HB3	1.98	0.45
1:E:5:ILE:HG13	1:E:447:HIS:HA	1.98	0.45
1:E:136:THR:OG1	4:E:703:HOH:O	2.21	0.45
1:F:342:TRP:CD1	4:F:2123:HOH:O	2.70	0.45
1:F:122:TRP:CZ3	1:F:148:LEU:CD2	3.01	0.44
1:A:451:LYS:NZ	1:A:466:PHE:HZ	2.01	0.44
1:F:408:LEU:C	1:F:408:LEU:HD23	2.43	0.44
1:C:58:GLU:HG2	1:C:95:LEU:HD12	2.00	0.44
1:A:3:ILE:CD1	1:A:481:LYS:HZ3	2.27	0.44
1:F:217:ARG:HB2	1:F:218:PRO:HD2	2.00	0.44
1:B:13:THR:O	1:B:13:THR:HG22	2.18	0.43
3:C:601:NAG:O7	3:C:601:NAG:O3	2.28	0.43
1:F:480:VAL:HG22	1:F:485:TYR:HE2	1.77	0.43
1:D:5:ILE:HG13	1:D:447:HIS:HA	2.01	0.43
1:B:166:THR:HG23	1:B:239:THR:HG22	1.99	0.43
1:F:469:TRP:CG	1:F:494:SER:HG	2.35	0.43
1:E:241:ASN:ND2	1:D:218:PRO:HD3	2.34	0.43
1:D:86:GLN:HG3	4:D:875:HOH:O	2.19	0.43
1:E:200:ARG:NH2	1:D:213:GLU:HA	2.34	0.43
1:E:386:LYS:NZ	4:E:705:HOH:O	2.26	0.43
1:A:5:ILE:HG13	1:A:447:HIS:HA	2.01	0.43
1:E:246:GLY:C	1:E:247:ASN:HD22	2.27	0.43
1:D:334:ILE:HD12	1:D:334:ILE:O	2.18	0.43
1:F:47:LYS:HA	1:F:47:LYS:HD3	1.85	0.43
1:B:200:ARG:CD	1:B:209:ALA:HB2	2.46	0.43
1:F:13:THR:HG22	1:F:13:THR:O	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:386:LYS:HA	1:E:386:LYS:HD3	1.85	0.42
1:D:8:HIS:CD2	1:D:9:ALA:N	2.87	0.42
1:A:64:ASN:OD1	1:A:64:ASN:C	2.62	0.42
1:F:309:LYS:HG3	1:F:417:LEU:CD2	2.43	0.42
1:A:78:TYR:CD2	1:A:301:ILE:HD11	2.54	0.42
1:F:480:VAL:CG2	1:F:485:TYR:CZ	3.01	0.42
1:D:470:HIS:NE2	1:D:485:TYR:OH	2.52	0.42
1:C:217:ARG:HB2	1:C:218:PRO:HD2	2.01	0.42
1:E:392:GLU:O	1:D:411:ARG:HD2	2.20	0.42
1:F:5:ILE:HG21	1:F:447:HIS:HB2	2.01	0.42
1:A:451:LYS:CE	1:A:460:ASP:OD1	2.68	0.42
1:E:122:TRP:CE3	1:E:148:LEU:HD23	2.55	0.42
1:D:166:THR:HG23	1:D:239:THR:HG22	2.02	0.42
1:A:391:PHE:CZ	1:A:412:MET:HE3	2.55	0.41
1:D:6:GLY:HA2	1:D:337:PHE:HB3	2.02	0.41
1:D:487:TYR:N	1:D:488:PRO:HD2	2.35	0.41
1:A:487:TYR:N	1:A:488:PRO:HD2	2.35	0.41
1:C:444:LYS:O	1:C:444:LYS:HG3	2.18	0.41
1:E:217:ARG:HB2	1:E:218:PRO:HD2	2.01	0.41
1:E:241:ASN:CG	1:D:218:PRO:HD3	2.45	0.41
1:C:487:TYR:N	1:C:488:PRO:HD2	2.35	0.41
1:F:78:TYR:CD2	1:F:301:ILE:HD11	2.55	0.41
1:D:261:ARG:CZ	1:D:261:ARG:HB3	2.50	0.41
1:F:95:LEU:HD12	1:F:229:TYR:HB2	2.03	0.41
1:A:365:ASP:OD1	1:A:446:LEU:HD21	2.20	0.41
1:C:486:ASN:CA	4:C:702:HOH:O	2.65	0.41
1:D:477:ILE:HG13	1:D:478:ASN:N	2.36	0.41
1:F:342:TRP:NE1	4:F:2123:HOH:O	2.53	0.41
1:E:6:GLY:HA2	1:E:337:PHE:HB3	2.03	0.41
1:E:487:TYR:N	1:E:488:PRO:HD2	2.36	0.41
1:D:476:CYS:SG	1:D:477:ILE:HG23	2.61	0.41
1:F:391:PHE:CZ	1:F:412:MET:HE3	2.56	0.41
1:A:453:GLN:HG2	1:A:485:TYR:HB3	2.03	0.41
1:C:78:TYR:CD2	1:C:301:ILE:HD11	2.56	0.41
1:B:90:CYS:HB2	1:B:134:ALA:O	2.21	0.40
1:E:200:ARG:NH1	1:D:214:ILE:O	2.53	0.40
1:A:408:LEU:C	1:A:408:LEU:HD23	2.46	0.40
1:E:90:CYS:HB2	1:E:134:ALA:O	2.21	0.40
1:E:186:VAL:N	4:E:710:HOH:O	2.41	0.40
1:F:5:ILE:HG22	1:F:464:GLY:O	2.20	0.40
1:A:182:PRO:O	1:A:217:ARG:NH2	2.54	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:386:LYS:HA	1:B:386:LYS:HD3	1.91	0.40
1:E:119:LYS:N	4:E:708:HOH:O	2.38	0.40
1:E:498:ARG:N	4:E:717:HOH:O	2.54	0.40
1:A:177:TRP:CG	1:A:201:MET:HE2	2.56	0.40
1:D:81:GLU:O	1:D:268:ARG:HA	2.22	0.40
1:F:391:PHE:HZ	1:F:412:MET:HE3	1.87	0.40
1:B:78:TYR:CD2	1:B:301:ILE:HD11	2.56	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:137:TYR:OH	1:D:137:TYR:OH[2_555]	2.00	0.20

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	479/514 (93%)	464 (97%)	14 (3%)	1 (0%)	43	63
1	B	478/514 (93%)	464 (97%)	13 (3%)	1 (0%)	43	63
1	C	478/514 (93%)	465 (97%)	12 (2%)	1 (0%)	43	63
1	D	496/514 (96%)	479 (97%)	15 (3%)	2 (0%)	30	49
1	E	485/514 (94%)	472 (97%)	12 (2%)	1 (0%)	43	63
1	F	477/514 (93%)	461 (97%)	14 (3%)	2 (0%)	30	49
All	All	2893/3084 (94%)	2805 (97%)	80 (3%)	8 (0%)	36	55

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	486	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	497	ASN
1	D	346	VAL
1	A	346	VAL
1	E	346	VAL
1	F	346	VAL
1	B	346	VAL
1	C	346	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	421/443 (95%)	402 (96%)	19 (4%)	24	49
1	B	420/443 (95%)	398 (95%)	22 (5%)	21	42
1	C	420/443 (95%)	401 (96%)	19 (4%)	24	49
1	D	431/443 (97%)	407 (94%)	24 (6%)	19	39
1	E	425/443 (96%)	409 (96%)	16 (4%)	29	56
1	F	419/443 (95%)	398 (95%)	21 (5%)	22	44
All	All	2536/2658 (95%)	2415 (95%)	121 (5%)	23	46

All (121) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	LEU
1	A	37	LYS
1	A	71	LEU
1	A	82	ARG
1	A	95	LEU
1	A	121	THR
1	A	152	LYS
1	A	155	SER
1	A	194	LEU
1	A	203	THR
1	A	217	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	239	THR
1	A	290	ASN
1	A	322	VAL
1	A	417	LEU
1	A	426	LEU
1	A	445	ASN
1	A	479	SER
1	A	484	THR
1	B	32	LEU
1	B	37	LYS
1	B	71	LEU
1	B	82	ARG
1	B	95	LEU
1	B	96	LYS
1	B	121	THR
1	B	132	THR
1	B	147	LEU
1	B	152	LYS
1	B	159	SER
1	B	203	THR
1	B	217	ARG
1	B	239	THR
1	B	243	GLU
1	B	389	THR
1	B	417	LEU
1	B	426	LEU
1	B	475	GLU
1	B	479	SER
1	B	489	LYS
1	B	495	ARG
1	C	37	LYS
1	C	71	LEU
1	C	75	SER
1	C	82	ARG
1	C	95	LEU
1	C	132	THR
1	C	136	THR
1	C	147	LEU
1	C	152	LYS
1	C	154	ARG
1	C	159	SER
1	C	203	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	206	MET
1	C	217	ARG
1	C	417	LEU
1	C	419	VAL
1	C	426	LEU
1	C	454	LEU
1	C	479	SER
1	E	37	LYS
1	E	82	ARG
1	E	94	VAL
1	E	95	LEU
1	E	132	THR
1	E	152	LYS
1	E	214	ILE
1	E	217	ARG
1	E	252	TRP
1	E	301	ILE
1	E	317	THR
1	E	339	GLU
1	E	417	LEU
1	E	419	VAL
1	E	426	LEU
1	E	479	SER
1	D	37	LYS
1	D	71	LEU
1	D	82	ARG
1	D	95	LEU
1	D	121	THR
1	D	147	LEU
1	D	152	LYS
1	D	159	SER
1	D	194	LEU
1	D	206	MET
1	D	217	ARG
1	D	239	THR
1	D	327	THR
1	D	330	LEU
1	D	334	ILE
1	D	384	ILE
1	D	419	VAL
1	D	426	LEU
1	D	454	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	457	ASN
1	D	463	ASN
1	D	471	LYS
1	D	479	SER
1	D	489	LYS
1	F	5	ILE
1	F	37	LYS
1	F	71	LEU
1	F	82	ARG
1	F	121	THR
1	F	147	LEU
1	F	152	LYS
1	F	153	ILE
1	F	159	SER
1	F	186	VAL
1	F	214	ILE
1	F	217	ARG
1	F	419	VAL
1	F	426	LEU
1	F	438	MET
1	F	457	ASN
1	F	459	LYS
1	F	463	ASN
1	F	471	LYS
1	F	479	SER
1	F	490	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	GLN
1	A	46	ASN
1	A	447	HIS
1	B	36	GLN
1	B	353	HIS
1	B	457	ASN
1	E	15	GLN
1	E	86	GLN
1	E	241	ASN
1	E	247	ASN
1	E	396	HIS
1	E	445	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	8	HIS
1	D	15	GLN
1	D	491	GLN
1	F	23	ASN
1	F	87	ASN
1	F	262	HIS
1	F	288	ASN
1	F	353	HIS
1	F	354	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

17 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	NAG	A	601	1	14,14,15	0.70	0	17,19,21	1.59	5 (29%)
2	NAG	I	1	2,1	14,14,15	0.81	1 (7%)	17,19,21	1.09	1 (5%)
3	NAG	E	602	1	14,14,15	0.52	0	17,19,21	1.58	1 (5%)
3	NAG	D	601	1	14,14,15	0.77	0	17,19,21	2.10	5 (29%)
3	NAG	E	601	1	14,14,15	0.82	0	17,19,21	2.43	6 (35%)
3	NAG	C	601	1	14,14,15	1.04	1 (7%)	17,19,21	3.01	6 (35%)
2	NAG	G	1	2,1	14,14,15	0.81	1 (7%)	17,19,21	2.04	7 (41%)
2	NAG	H	1	2,1	14,14,15	0.74	1 (7%)	17,19,21	1.86	5 (29%)
2	NAG	H	2	2	14,14,15	0.74	0	17,19,21	1.49	2 (11%)
2	NAG	I	2	2	14,14,15	0.71	0	17,19,21	1.96	3 (17%)
2	NAG	J	1	2,1	14,14,15	0.92	1 (7%)	17,19,21	1.49	5 (29%)
3	NAG	B	601	1	14,14,15	0.67	0	17,19,21	2.65	7 (41%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	J	2	2	14,14,15	0.68	0	17,19,21	2.15	3 (17%)
3	NAG	D	602	1	14,14,15	0.65	0	17,19,21	1.76	1 (5%)
2	NAG	G	2	2	14,14,15	0.62	0	17,19,21	1.22	2 (11%)
3	NAG	C	602	1	14,14,15	0.78	1 (7%)	17,19,21	1.70	4 (23%)
3	NAG	C	605	1	14,14,15	1.03	1 (7%)	17,19,21	1.70	5 (29%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	A	601	1	1/1/5/7	2/6/23/26	0/1/1/1
2	NAG	I	1	2,1	-	2/6/23/26	0/1/1/1
3	NAG	E	602	1	-	2/6/23/26	0/1/1/1
3	NAG	E	601	1	1/1/5/7	3/6/23/26	0/1/1/1
3	NAG	C	601	1	-	4/6/23/26	0/1/1/1
2	NAG	G	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	H	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	H	2	2	-	2/6/23/26	0/1/1/1
2	NAG	I	2	2	-	0/6/23/26	0/1/1/1
2	NAG	J	1	2,1	-	2/6/23/26	0/1/1/1
3	NAG	B	601	1	1/1/5/7	1/6/23/26	0/1/1/1
2	NAG	J	2	2	-	2/6/23/26	0/1/1/1
3	NAG	D	602	1	1/1/5/7	1/6/23/26	0/1/1/1
2	NAG	G	2	2	-	2/6/23/26	0/1/1/1
3	NAG	C	602	1	-	0/6/23/26	0/1/1/1
3	NAG	C	605	1	1/1/5/7	3/6/23/26	0/1/1/1
3	NAG	D	601	1	1/1/5/7	1/6/23/26	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	601	NAG	C1-C2	2.91	1.56	1.52
3	C	602	NAG	C1-C2	2.42	1.55	1.52
2	G	1	NAG	C1-C2	2.37	1.55	1.52
3	C	605	NAG	C1-C2	2.27	1.55	1.52
2	J	1	NAG	C1-C2	2.24	1.55	1.52
2	H	1	NAG	C1-C2	2.16	1.55	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	1	NAG	O5-C1	-2.11	1.40	1.43

All (68) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	601	NAG	C1-O5-C5	9.72	125.21	112.19
3	B	601	NAG	C1-O5-C5	8.55	123.65	112.19
3	D	602	NAG	O5-C1-C2	-6.42	101.36	111.29
2	J	2	NAG	C1-O5-C5	6.33	120.67	112.19
2	I	2	NAG	C1-O5-C5	6.07	120.32	112.19
3	D	601	NAG	O5-C1-C2	-5.93	102.12	111.29
3	E	601	NAG	O5-C1-C2	-5.27	103.13	111.29
3	E	602	NAG	C1-O5-C5	5.16	119.10	112.19
3	E	601	NAG	C4-C3-C2	5.11	118.51	111.02
2	G	1	NAG	C1-C2-N2	4.69	117.82	110.43
3	C	601	NAG	O5-C5-C6	4.37	116.16	107.66
3	D	601	NAG	C4-C3-C2	4.33	117.36	111.02
2	H	2	NAG	C4-C3-C2	4.20	117.17	111.02
3	C	602	NAG	C1-O5-C5	3.95	117.48	112.19
2	H	2	NAG	C3-C4-C5	3.65	116.85	110.23
2	H	1	NAG	O5-C1-C2	-3.65	105.65	111.29
2	J	2	NAG	C1-C2-N2	3.37	115.75	110.43
3	E	601	NAG	O5-C5-C4	-3.31	102.78	110.83
3	E	601	NAG	C1-O5-C5	-3.26	107.81	112.19
2	H	1	NAG	C1-C2-N2	3.23	115.52	110.43
2	G	2	NAG	C1-O5-C5	3.14	116.39	112.19
3	E	601	NAG	O5-C5-C6	3.11	113.72	107.66
3	C	605	NAG	O5-C1-C2	-3.07	106.55	111.29
2	I	1	NAG	O5-C1-C2	-2.99	106.67	111.29
3	A	601	NAG	C2-N2-C7	2.99	126.90	122.90
2	G	1	NAG	C1-O5-C5	2.75	115.88	112.19
2	G	1	NAG	O5-C5-C6	2.69	112.89	107.66
3	A	601	NAG	O7-C7-C8	-2.68	117.28	122.05
2	H	1	NAG	O5-C5-C6	2.66	112.84	107.66
3	C	601	NAG	O7-C7-C8	-2.61	117.40	122.05
3	B	601	NAG	O7-C7-C8	-2.60	117.43	122.05
2	H	1	NAG	O3-C3-C2	-2.56	104.08	109.40
2	I	2	NAG	O7-C7-C8	-2.56	117.50	122.05
3	B	601	NAG	O5-C5-C6	2.55	112.62	107.66
2	G	1	NAG	O7-C7-C8	-2.53	117.56	122.05
2	J	1	NAG	O5-C5-C6	2.49	112.50	107.66
2	G	1	NAG	O5-C1-C2	-2.45	107.50	111.29

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	2	NAG	C1-C2-N2	-2.44	106.58	110.43
3	C	605	NAG	O5-C5-C4	-2.43	104.90	110.83
3	C	602	NAG	C6-C5-C4	-2.41	107.10	113.02
2	I	2	NAG	C2-N2-C7	2.41	126.12	122.90
2	J	2	NAG	O5-C1-C2	2.39	114.99	111.29
3	B	601	NAG	C4-C3-C2	-2.36	107.56	111.02
3	C	602	NAG	O5-C5-C6	2.34	112.22	107.66
2	J	1	NAG	O4-C4-C3	-2.34	104.87	110.38
2	G	1	NAG	C3-C4-C5	2.31	114.42	110.23
3	A	601	NAG	O5-C5-C6	2.29	112.13	107.66
3	A	601	NAG	O7-C7-N2	2.26	125.98	121.98
3	B	601	NAG	C1-C2-N2	2.26	113.99	110.43
3	D	601	NAG	O3-C3-C4	-2.24	105.09	110.38
3	B	601	NAG	C6-C5-C4	-2.23	107.55	113.02
3	C	602	NAG	O5-C1-C2	-2.22	107.85	111.29
3	A	601	NAG	C4-C3-C2	-2.21	107.78	111.02
2	J	1	NAG	C2-N2-C7	2.21	125.86	122.90
3	C	601	NAG	C6-C5-C4	-2.21	107.60	113.02
3	C	601	NAG	C2-N2-C7	2.20	125.85	122.90
3	C	605	NAG	C8-C7-N2	2.20	119.77	116.12
3	B	601	NAG	C3-C4-C5	-2.19	106.26	110.23
3	D	601	NAG	C3-C4-C5	2.15	114.14	110.23
2	J	1	NAG	O7-C7-N2	2.14	125.76	121.98
3	C	601	NAG	C4-C3-C2	-2.14	107.88	111.02
3	C	605	NAG	C2-N2-C7	-2.13	120.04	122.90
3	E	601	NAG	C2-N2-C7	2.13	125.76	122.90
3	D	601	NAG	O7-C7-C8	-2.11	118.30	122.05
3	C	605	NAG	O7-C7-C8	-2.09	118.33	122.05
2	H	1	NAG	O7-C7-C8	-2.06	118.39	122.05
2	G	1	NAG	C8-C7-N2	2.03	119.48	116.12
2	J	1	NAG	O7-C7-C8	-2.02	118.46	122.05

All (6) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	601	NAG	C1
3	B	601	NAG	C1
3	C	605	NAG	C1
3	E	601	NAG	C1
3	D	601	NAG	C1
3	D	602	NAG	C1

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	601	NAG	C3-C2-N2-C7
2	J	1	NAG	O5-C5-C6-O6
3	C	601	NAG	O5-C5-C6-O6
2	I	1	NAG	O5-C5-C6-O6
3	A	601	NAG	O5-C5-C6-O6
3	C	605	NAG	C4-C5-C6-O6
3	C	605	NAG	O5-C5-C6-O6
2	J	1	NAG	C4-C5-C6-O6
2	G	2	NAG	O5-C5-C6-O6
3	E	601	NAG	O5-C5-C6-O6
3	A	601	NAG	C4-C5-C6-O6
2	G	2	NAG	C4-C5-C6-O6
2	I	1	NAG	C4-C5-C6-O6
3	E	602	NAG	C4-C5-C6-O6
3	E	601	NAG	C4-C5-C6-O6
2	H	1	NAG	C4-C5-C6-O6
3	C	601	NAG	C4-C5-C6-O6
2	H	1	NAG	O5-C5-C6-O6
3	E	602	NAG	O5-C5-C6-O6
3	C	601	NAG	C3-C2-N2-C7
3	D	601	NAG	O5-C5-C6-O6
2	J	2	NAG	C4-C5-C6-O6
2	H	2	NAG	C4-C5-C6-O6
2	H	2	NAG	C1-C2-N2-C7
3	C	601	NAG	C1-C2-N2-C7
3	D	602	NAG	C1-C2-N2-C7
3	C	605	NAG	C3-C2-N2-C7
2	J	2	NAG	O5-C5-C6-O6
3	B	601	NAG	O5-C5-C6-O6

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	601	NAG	1	0
3	B	601	NAG	1	0
3	C	605	NAG	1	0

5.5 Carbohydrates

8 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	G	1	2,1	14,14,15	0.81	1 (7%)	17,19,21	2.04	7 (41%)
2	NAG	G	2	2	14,14,15	0.62	0	17,19,21	1.22	2 (11%)
2	NAG	H	1	2,1	14,14,15	0.74	1 (7%)	17,19,21	1.86	5 (29%)
2	NAG	H	2	2	14,14,15	0.74	0	17,19,21	1.49	2 (11%)
2	NAG	I	1	2,1	14,14,15	0.81	1 (7%)	17,19,21	1.09	1 (5%)
2	NAG	I	2	2	14,14,15	0.71	0	17,19,21	1.96	3 (17%)
2	NAG	J	1	2,1	14,14,15	0.92	1 (7%)	17,19,21	1.49	5 (29%)
2	NAG	J	2	2	14,14,15	0.68	0	17,19,21	2.15	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
2	NAG	G	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	G	2	2	-	2/6/23/26	0/1/1/1
2	NAG	H	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	H	2	2	-	2/6/23/26	0/1/1/1
2	NAG	I	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	I	2	2	-	0/6/23/26	0/1/1/1
2	NAG	J	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	J	2	2	-	2/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	1	NAG	C1-C2	2.37	1.55	1.52
2	J	1	NAG	C1-C2	2.24	1.55	1.52
2	H	1	NAG	C1-C2	2.16	1.55	1.52
2	I	1	NAG	O5-C1	-2.11	1.40	1.43

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	2	NAG	C1-O5-C5	6.33	120.67	112.19
2	I	2	NAG	C1-O5-C5	6.07	120.32	112.19
2	G	1	NAG	C1-C2-N2	4.69	117.82	110.43
2	H	2	NAG	C4-C3-C2	4.20	117.17	111.02
2	H	2	NAG	C3-C4-C5	3.65	116.85	110.23
2	H	1	NAG	O5-C1-C2	-3.65	105.65	111.29
2	J	2	NAG	C1-C2-N2	3.37	115.75	110.43
2	H	1	NAG	C1-C2-N2	3.23	115.52	110.43
2	G	2	NAG	C1-O5-C5	3.14	116.39	112.19
2	I	1	NAG	O5-C1-C2	-2.99	106.67	111.29
2	G	1	NAG	C1-O5-C5	2.75	115.88	112.19
2	G	1	NAG	O5-C5-C6	2.69	112.89	107.66
2	H	1	NAG	O5-C5-C6	2.66	112.84	107.66
2	H	1	NAG	O3-C3-C2	-2.56	104.08	109.40
2	I	2	NAG	O7-C7-C8	-2.56	117.50	122.05
2	G	1	NAG	O7-C7-C8	-2.53	117.56	122.05
2	J	1	NAG	O5-C5-C6	2.49	112.50	107.66
2	G	1	NAG	O5-C1-C2	-2.45	107.50	111.29
2	G	2	NAG	C1-C2-N2	-2.44	106.58	110.43
2	I	2	NAG	C2-N2-C7	2.41	126.12	122.90
2	J	2	NAG	O5-C1-C2	2.39	114.99	111.29
2	J	1	NAG	O4-C4-C3	-2.34	104.87	110.38
2	G	1	NAG	C3-C4-C5	2.31	114.42	110.23
2	J	1	NAG	C2-N2-C7	2.21	125.86	122.90
2	J	1	NAG	O7-C7-N2	2.14	125.76	121.98
2	H	1	NAG	O7-C7-C8	-2.06	118.39	122.05
2	G	1	NAG	C8-C7-N2	2.03	119.48	116.12
2	J	1	NAG	O7-C7-C8	-2.02	118.46	122.05

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	J	1	NAG	O5-C5-C6-O6
2	I	1	NAG	O5-C5-C6-O6
2	J	1	NAG	C4-C5-C6-O6
2	G	2	NAG	O5-C5-C6-O6
2	G	2	NAG	C4-C5-C6-O6
2	I	1	NAG	C4-C5-C6-O6
2	H	1	NAG	C4-C5-C6-O6
2	H	1	NAG	O5-C5-C6-O6

Continued on next page...

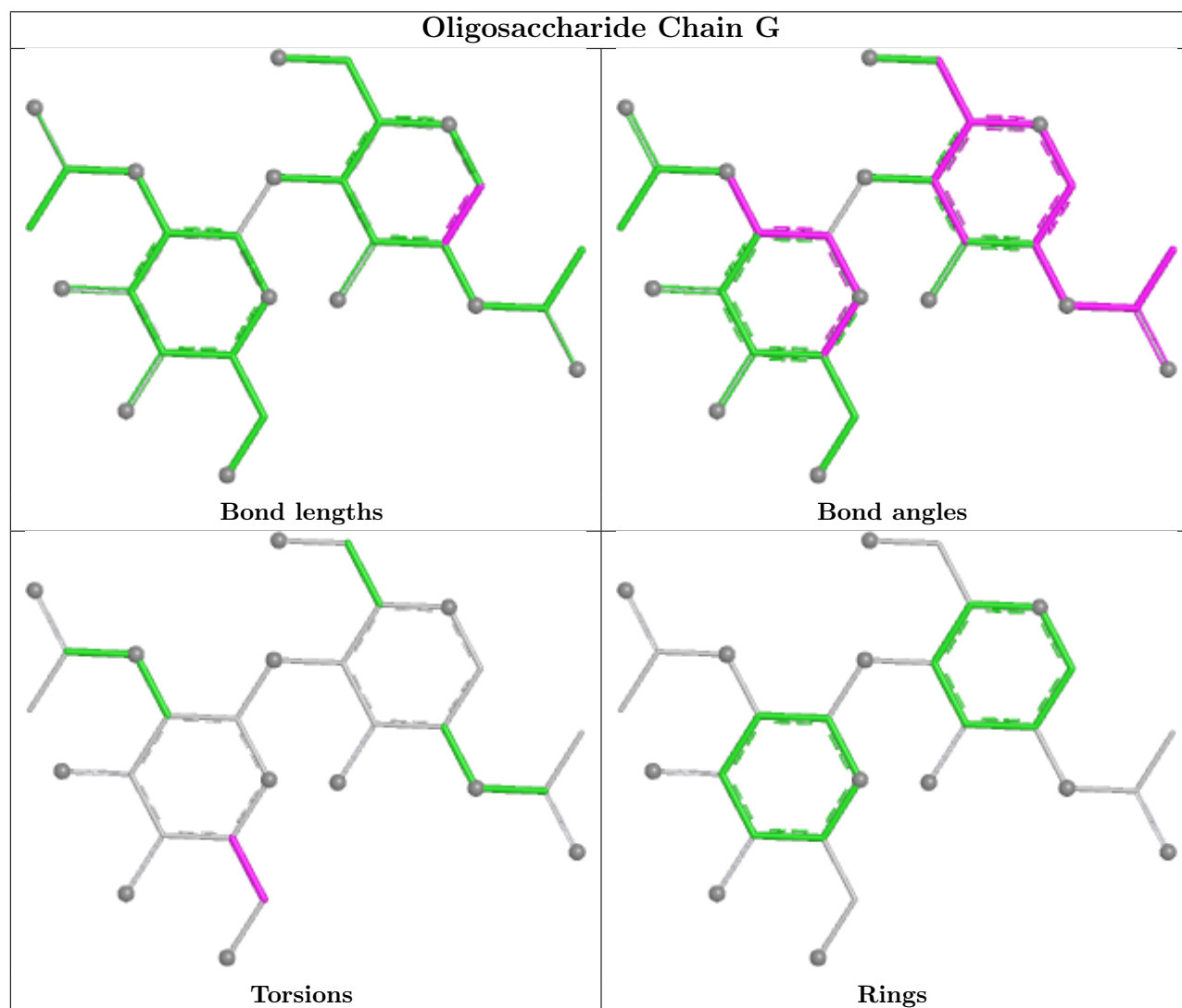
Continued from previous page...

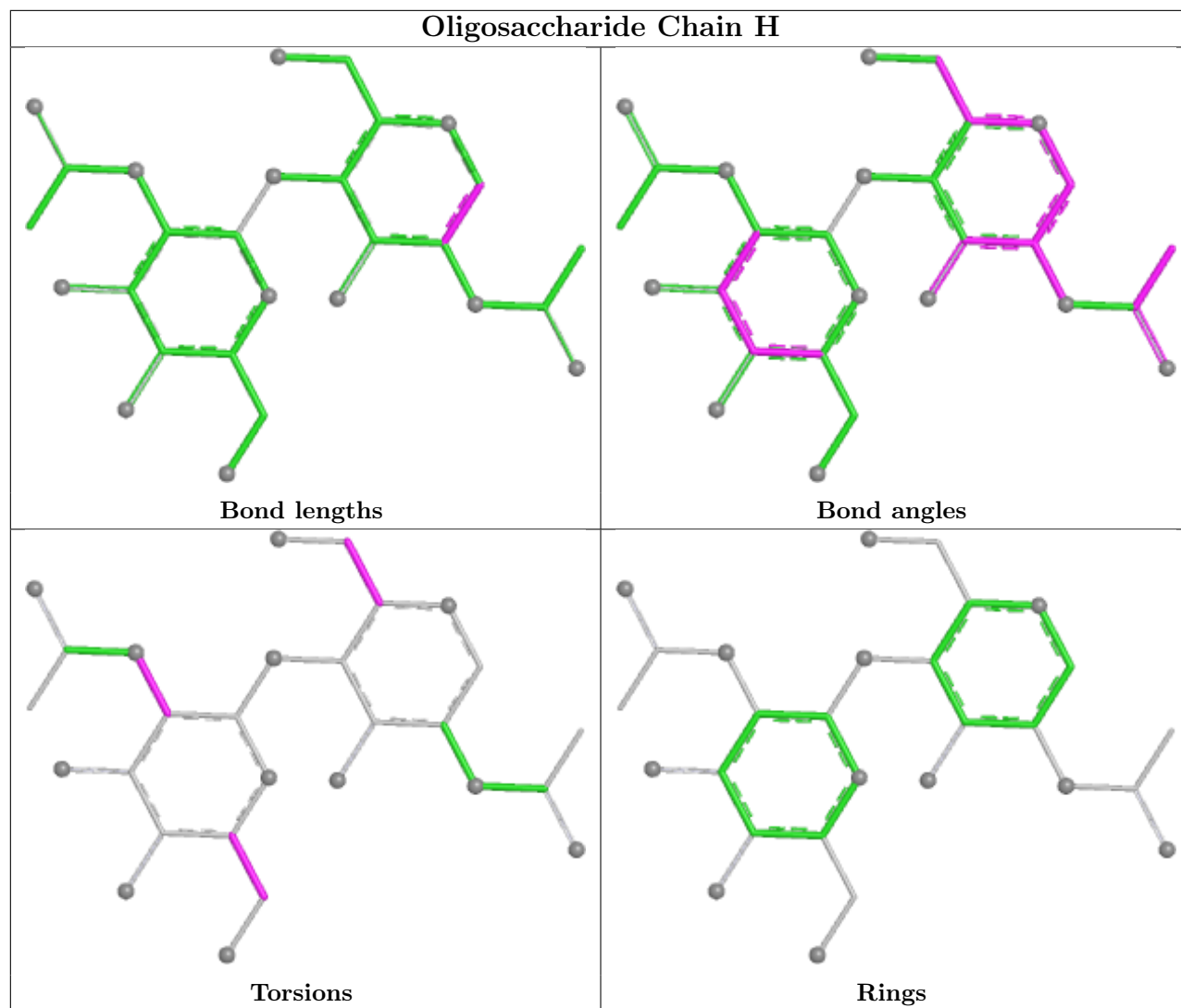
Mol	Chain	Res	Type	Atoms
2	J	2	NAG	C4-C5-C6-O6
2	H	2	NAG	C4-C5-C6-O6
2	H	2	NAG	C1-C2-N2-C7
2	J	2	NAG	O5-C5-C6-O6

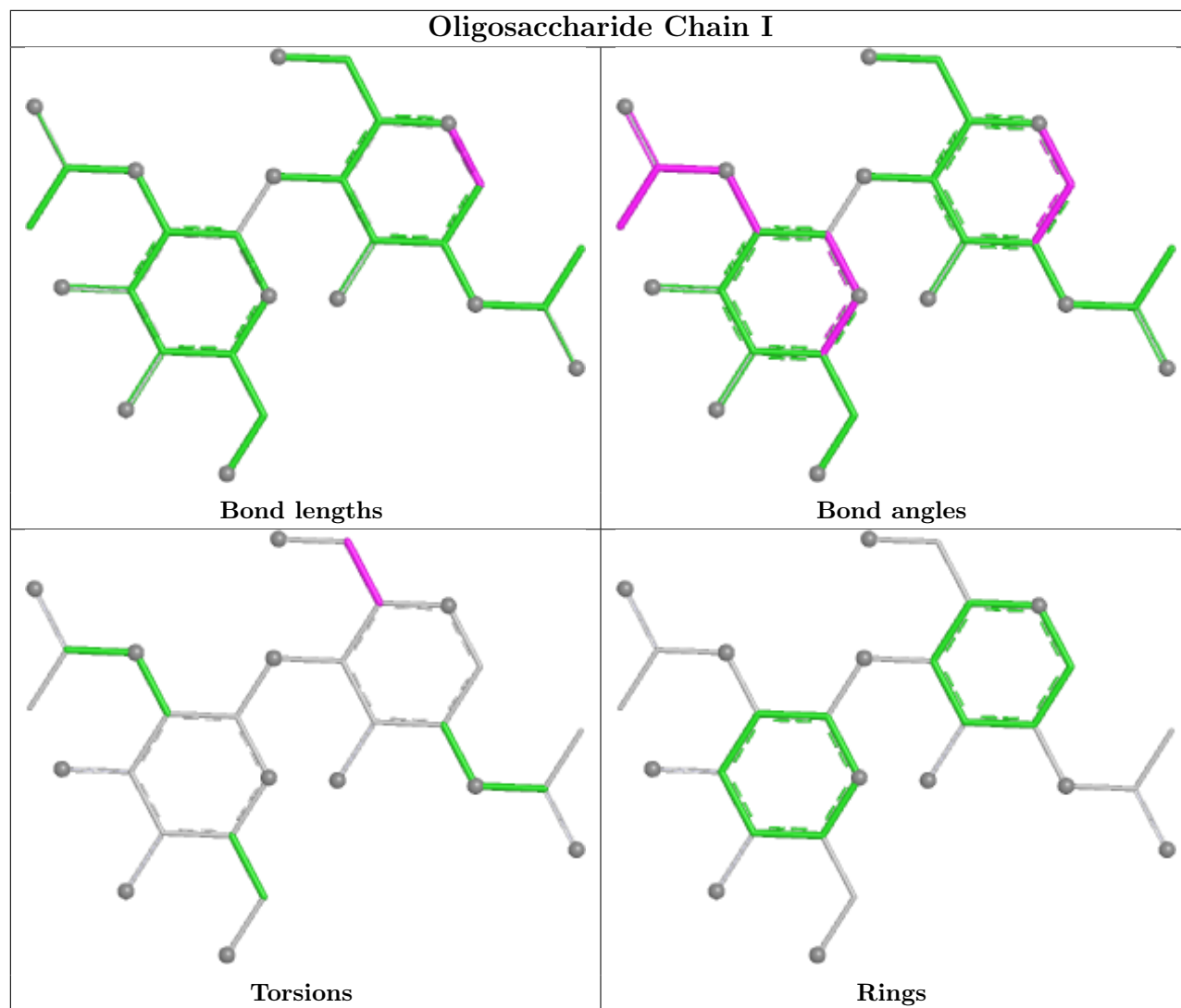
There are no ring outliers.

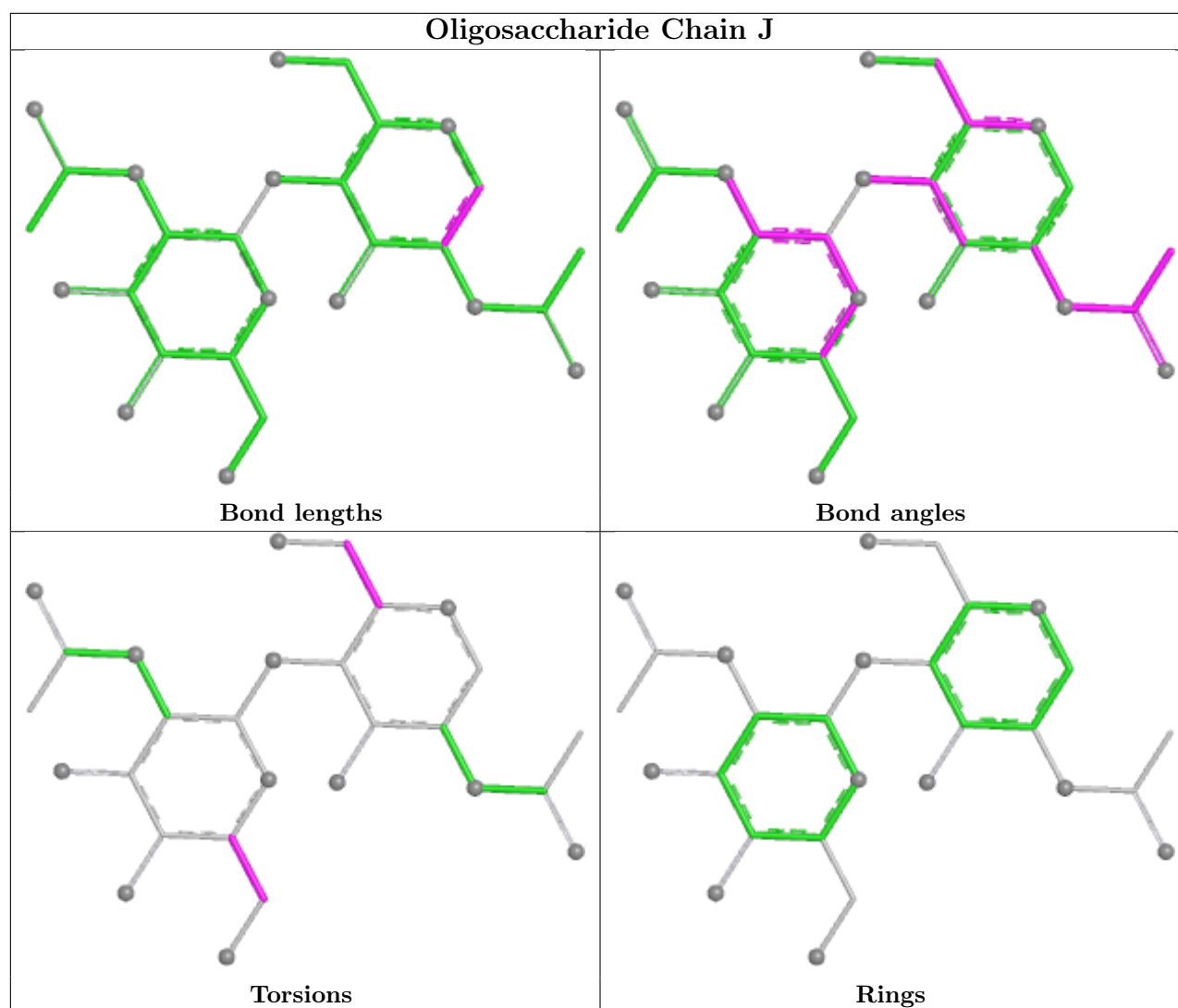
No monomer is involved in short contacts.

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









5.6 Ligand geometry [i](#)

9 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	$\# Z > 2$
3	NAG	A	601	1	14,14,15	0.70	0	17,19,21	1.59	5 (29%)
3	NAG	E	602	1	14,14,15	0.52	0	17,19,21	1.58	1 (5%)
3	NAG	D	601	1	14,14,15	0.77	0	17,19,21	2.10	5 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	E	601	1	14,14,15	0.82	0	17,19,21	2.43	6 (35%)
3	NAG	C	601	1	14,14,15	1.04	1 (7%)	17,19,21	3.01	6 (35%)
3	NAG	B	601	1	14,14,15	0.67	0	17,19,21	2.65	7 (41%)
3	NAG	D	602	1	14,14,15	0.65	0	17,19,21	1.76	1 (5%)
3	NAG	C	602	1	14,14,15	0.78	1 (7%)	17,19,21	1.70	4 (23%)
3	NAG	C	605	1	14,14,15	1.03	1 (7%)	17,19,21	1.70	5 (29%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	A	601	1	1/1/5/7	2/6/23/26	0/1/1/1
3	NAG	E	602	1	-	2/6/23/26	0/1/1/1
3	NAG	E	601	1	1/1/5/7	3/6/23/26	0/1/1/1
3	NAG	C	601	1	-	4/6/23/26	0/1/1/1
3	NAG	B	601	1	1/1/5/7	1/6/23/26	0/1/1/1
3	NAG	D	602	1	1/1/5/7	1/6/23/26	0/1/1/1
3	NAG	C	602	1	-	0/6/23/26	0/1/1/1
3	NAG	C	605	1	1/1/5/7	3/6/23/26	0/1/1/1
3	NAG	D	601	1	1/1/5/7	1/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	601	NAG	C1-C2	2.91	1.56	1.52
3	C	602	NAG	C1-C2	2.42	1.55	1.52
3	C	605	NAG	C1-C2	2.27	1.55	1.52

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	601	NAG	C1-O5-C5	9.72	125.21	112.19
3	B	601	NAG	C1-O5-C5	8.55	123.65	112.19
3	D	602	NAG	O5-C1-C2	-6.42	101.36	111.29
3	D	601	NAG	O5-C1-C2	-5.93	102.12	111.29
3	E	601	NAG	O5-C1-C2	-5.27	103.13	111.29
3	E	602	NAG	C1-O5-C5	5.16	119.10	112.19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	601	NAG	C4-C3-C2	5.11	118.51	111.02
3	C	601	NAG	O5-C5-C6	4.37	116.16	107.66
3	D	601	NAG	C4-C3-C2	4.33	117.36	111.02
3	C	602	NAG	C1-O5-C5	3.95	117.48	112.19
3	E	601	NAG	O5-C5-C4	-3.31	102.78	110.83
3	E	601	NAG	C1-O5-C5	-3.26	107.81	112.19
3	E	601	NAG	O5-C5-C6	3.11	113.72	107.66
3	C	605	NAG	O5-C1-C2	-3.07	106.55	111.29
3	A	601	NAG	C2-N2-C7	2.99	126.90	122.90
3	A	601	NAG	O7-C7-C8	-2.68	117.28	122.05
3	C	601	NAG	O7-C7-C8	-2.61	117.40	122.05
3	B	601	NAG	O7-C7-C8	-2.60	117.43	122.05
3	B	601	NAG	O5-C5-C6	2.55	112.62	107.66
3	C	605	NAG	O5-C5-C4	-2.43	104.90	110.83
3	C	602	NAG	C6-C5-C4	-2.41	107.10	113.02
3	B	601	NAG	C4-C3-C2	-2.36	107.56	111.02
3	C	602	NAG	O5-C5-C6	2.34	112.22	107.66
3	A	601	NAG	O5-C5-C6	2.29	112.13	107.66
3	A	601	NAG	O7-C7-N2	2.26	125.98	121.98
3	B	601	NAG	C1-C2-N2	2.26	113.99	110.43
3	D	601	NAG	O3-C3-C4	-2.24	105.09	110.38
3	B	601	NAG	C6-C5-C4	-2.23	107.55	113.02
3	C	602	NAG	O5-C1-C2	-2.22	107.85	111.29
3	A	601	NAG	C4-C3-C2	-2.21	107.78	111.02
3	C	601	NAG	C6-C5-C4	-2.21	107.60	113.02
3	C	601	NAG	C2-N2-C7	2.20	125.85	122.90
3	C	605	NAG	C8-C7-N2	2.20	119.77	116.12
3	B	601	NAG	C3-C4-C5	-2.19	106.26	110.23
3	D	601	NAG	C3-C4-C5	2.15	114.14	110.23
3	C	601	NAG	C4-C3-C2	-2.14	107.88	111.02
3	C	605	NAG	C2-N2-C7	-2.13	120.04	122.90
3	E	601	NAG	C2-N2-C7	2.13	125.76	122.90
3	D	601	NAG	O7-C7-C8	-2.11	118.30	122.05
3	C	605	NAG	O7-C7-C8	-2.09	118.33	122.05

All (6) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	601	NAG	C1
3	B	601	NAG	C1
3	C	605	NAG	C1
3	E	601	NAG	C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
3	D	601	NAG	C1
3	D	602	NAG	C1

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	601	NAG	C3-C2-N2-C7
3	C	601	NAG	O5-C5-C6-O6
3	A	601	NAG	O5-C5-C6-O6
3	C	605	NAG	C4-C5-C6-O6
3	C	605	NAG	O5-C5-C6-O6
3	E	601	NAG	O5-C5-C6-O6
3	A	601	NAG	C4-C5-C6-O6
3	E	602	NAG	C4-C5-C6-O6
3	E	601	NAG	C4-C5-C6-O6
3	C	601	NAG	C4-C5-C6-O6
3	E	602	NAG	O5-C5-C6-O6
3	C	601	NAG	C3-C2-N2-C7
3	D	601	NAG	O5-C5-C6-O6
3	C	601	NAG	C1-C2-N2-C7
3	D	602	NAG	C1-C2-N2-C7
3	C	605	NAG	C3-C2-N2-C7
3	B	601	NAG	O5-C5-C6-O6

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	601	NAG	1	0
3	B	601	NAG	1	0
3	C	605	NAG	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

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	483/514 (93%)	0.12	28 (5%) 29 25	29, 47, 101, 126	0
1	B	482/514 (93%)	0.25	30 (6%) 26 23	30, 51, 125, 173	0
1	C	482/514 (93%)	0.15	16 (3%) 49 45	31, 53, 104, 133	0
1	D	498/514 (96%)	0.42	37 (7%) 20 18	31, 59, 151, 182	0
1	E	489/514 (95%)	0.79	54 (11%) 10 8	39, 73, 112, 140	0
1	F	481/514 (93%)	0.70	59 (12%) 8 7	36, 72, 146, 195	0
All	All	2915/3084 (94%)	0.41	224 (7%) 19 17	29, 60, 126, 195	0

All (224) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	252	TRP	7.1
1	A	481	LYS	5.9
1	F	3	ILE	5.2
1	F	322	VAL	5.1
1	E	160	LEU	4.8
1	C	323	PRO	4.5
1	A	477	ILE	4.3
1	B	5	ILE	4.3
1	D	330	LEU	4.2
1	D	3	ILE	4.2
1	A	498	ARG	4.1
1	E	158	TYR	4.1
1	A	480	VAL	4.1
1	D	496	LEU	4.0
1	D	137	TYR	4.0
1	E	244	SER	4.0
1	E	130	GLY	3.8
1	B	466	PHE	3.8
1	D	468	PHE	3.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	127	THR	3.7
1	E	323	PRO	3.6
1	E	192	TYR	3.6
1	D	5	ILE	3.6
1	F	488	PRO	3.6
1	A	462	GLY	3.5
1	F	215	ALA	3.5
1	B	477	ILE	3.5
1	E	148	LEU	3.5
1	E	153	ILE	3.5
1	F	151	ILE	3.4
1	E	188	GLN	3.3
1	F	191	LEU	3.3
1	F	490	TYR	3.3
1	F	122	TRP	3.3
1	F	149	TRP	3.3
1	A	456	ASP	3.2
1	F	466	PHE	3.2
1	A	352	TYR	3.2
1	C	492	GLU	3.2
1	B	3	ILE	3.2
1	E	161	ILE	3.2
1	F	2	LYS	3.2
1	D	325	VAL	3.2
1	F	198	TYR	3.2
1	E	179	VAL	3.1
1	D	352	TYR	3.1
1	B	496	LEU	3.1
1	E	191	LEU	3.1
1	E	242	VAL	3.1
1	F	472	CYS	3.1
1	A	2	LYS	3.1
1	E	182	PRO	3.1
1	C	496	LEU	3.1
1	F	496	LEU	3.1
1	E	199	VAL	3.1
1	A	467	GLU	3.0
1	F	485	TYR	3.0
1	A	482	ASN	3.0
1	E	322	VAL	3.0
1	F	183	PRO	3.0
1	B	323	PRO	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	469	TRP	2.9
1	B	457	ASN	2.9
1	F	5	ILE	2.9
1	A	461	LEU	2.9
1	B	2	LYS	2.8
1	D	477	ILE	2.8
1	E	488	PRO	2.8
1	F	158	TYR	2.8
1	E	125	VAL	2.8
1	F	214	ILE	2.8
1	F	153	ILE	2.8
1	D	346	VAL	2.8
1	D	461	LEU	2.7
1	F	13	THR	2.7
1	F	468	PHE	2.7
1	F	477	ILE	2.7
1	E	496	LEU	2.7
1	D	454	LEU	2.7
1	E	189	ALA	2.7
1	E	209	ALA	2.7
1	D	364	ALA	2.7
1	B	472	CYS	2.7
1	F	361	GLY	2.7
1	B	357	SER	2.7
1	B	485	TYR	2.7
1	B	4	CYS	2.7
1	B	464	GLY	2.7
1	F	351	GLY	2.7
1	D	485	TYR	2.7
1	A	483	GLY	2.6
1	D	138	ASN	2.6
1	F	497	ASN	2.6
1	F	319	LEU	2.6
1	C	369	THR	2.6
1	A	471	LYS	2.6
1	F	6	GLY	2.6
1	E	249	ILE	2.6
1	F	192	TYR	2.6
1	C	348	GLY	2.6
1	A	496	LEU	2.6
1	E	485	TYR	2.6
1	D	490	TYR	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	451	LYS	2.6
1	C	340	GLY	2.6
1	E	454	LEU	2.6
1	B	322	VAL	2.6
1	D	457	ASN	2.6
1	A	363	ALA	2.6
1	B	495	ARG	2.5
1	B	453	GLN	2.5
1	B	459	LYS	2.5
1	F	157	PRO	2.5
1	E	149	TRP	2.5
1	E	151	ILE	2.5
1	E	469	TRP	2.5
1	F	469	TRP	2.5
1	B	498	ARG	2.5
1	F	349	TRP	2.5
1	A	454	LEU	2.5
1	F	194	LEU	2.5
1	D	2	LYS	2.5
1	F	217	ARG	2.5
1	B	456	ASP	2.5
1	C	160	LEU	2.5
1	E	122	TRP	2.5
1	E	180	HIS	2.5
1	F	340	GLY	2.4
1	C	366	LYS	2.4
1	D	1	ASP	2.4
1	D	459	LYS	2.4
1	D	466	PHE	2.4
1	F	129	SER	2.4
1	E	178	GLY	2.4
1	B	469	TRP	2.4
1	F	344	GLY	2.4
1	A	3	ILE	2.4
1	A	216	ASP	2.4
1	E	186	VAL	2.4
1	F	458	ALA	2.4
1	A	449	LYS	2.4
1	F	130	GLY	2.4
1	F	216	ASP	2.4
1	C	159	SER	2.3
1	E	142	SER	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	155	SER	2.3
1	E	163	GLY	2.3
1	D	387	MET	2.3
1	E	466	PHE	2.3
1	D	362	TYR	2.3
1	D	391	PHE	2.3
1	E	138	ASN	2.3
1	F	209	ALA	2.3
1	A	469	TRP	2.3
1	B	450	VAL	2.3
1	E	433	GLU	2.3
1	E	498	ARG	2.3
1	A	459	LYS	2.3
1	F	247	ASN	2.3
1	F	353	HIS	2.3
1	F	454	LEU	2.3
1	E	449	LYS	2.3
1	D	392	GLU	2.3
1	C	480	VAL	2.3
1	A	485	TYR	2.3
1	C	498	ARG	2.3
1	E	157	PRO	2.3
1	F	487	TYR	2.3
1	E	324	GLN	2.2
1	F	354	HIS	2.2
1	B	468	PHE	2.2
1	B	352	TYR	2.2
1	A	19	ILE	2.2
1	A	452	SER	2.2
1	E	214	ILE	2.2
1	F	150	ILE	2.2
1	B	455	ARG	2.2
1	C	268	ARG	2.2
1	F	226	ARG	2.2
1	D	458	ALA	2.2
1	F	352	TYR	2.2
1	F	471	LYS	2.2
1	D	480	VAL	2.2
1	C	438	MET	2.2
1	E	222	GLY	2.2
1	D	446	LEU	2.2
1	C	153	ILE	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	468	PHE	2.2
1	F	171	GLN	2.1
1	C	4	CYS	2.1
1	C	495	ARG	2.1
1	F	29	SER	2.1
1	E	183	PRO	2.1
1	E	176	PHE	2.1
1	F	450	VAL	2.1
1	E	220	ALA	2.1
1	A	6	GLY	2.1
1	F	343	THR	2.1
1	F	348	GLY	2.1
1	D	363	ALA	2.1
1	B	461	LEU	2.1
1	E	248	LEU	2.1
1	A	5	ILE	2.1
1	D	395	GLU	2.1
1	E	185	ASP	2.1
1	E	489	LYS	2.1
1	D	488	PRO	2.1
1	F	491	GLN	2.1
1	D	450	VAL	2.1
1	E	250	ALA	2.1
1	F	342	TRP	2.1
1	B	433	GLU	2.1
1	D	493	GLU	2.1
1	B	471	LYS	2.1
1	B	481	LYS	2.1
1	B	198	TYR	2.1
1	E	216	ASP	2.1
1	D	487	TYR	2.1
1	E	154	ARG	2.0
1	F	498	ARG	2.0
1	B	153	ILE	2.0
1	D	354	HIS	2.0
1	E	197	ARG	2.0
1	D	389	THR	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NAG	H	2	14/15	0.46	0.14	104,115,119,121	0
3	NAG	D	602	14/15	0.48	0.17	102,130,143,148	0
3	NAG	C	601	14/15	0.50	0.15	99,105,113,114	0
2	NAG	I	2	14/15	0.52	0.14	105,124,129,130	0
3	NAG	B	601	14/15	0.52	0.16	117,125,140,143	0
3	NAG	D	601	14/15	0.53	0.16	127,140,146,151	0
2	NAG	I	1	14/15	0.62	0.12	95,108,115,124	0
3	NAG	A	601	14/15	0.65	0.12	87,105,115,115	0
3	NAG	E	601	14/15	0.66	0.15	61,88,96,124	0
3	NAG	C	602	14/15	0.70	0.13	106,118,123,131	0
2	NAG	G	2	14/15	0.71	0.11	87,96,100,105	0
3	NAG	E	602	14/15	0.71	0.13	101,111,115,119	0
2	NAG	J	2	14/15	0.77	0.12	86,95,101,102	0
3	NAG	C	605	14/15	0.82	0.12	61,80,98,109	0
2	NAG	H	1	14/15	0.83	0.12	78,86,92,99	0
2	NAG	J	1	14/15	0.90	0.09	60,72,76,81	0
2	NAG	G	1	14/15	0.90	0.09	63,71,78,86	0

6.3 Carbohydrates

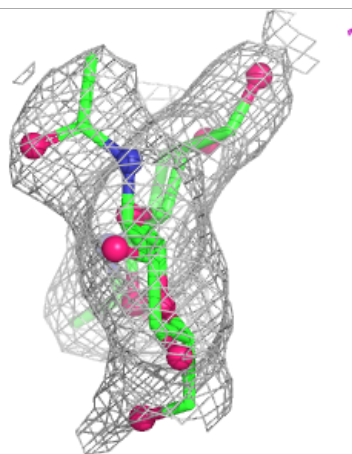
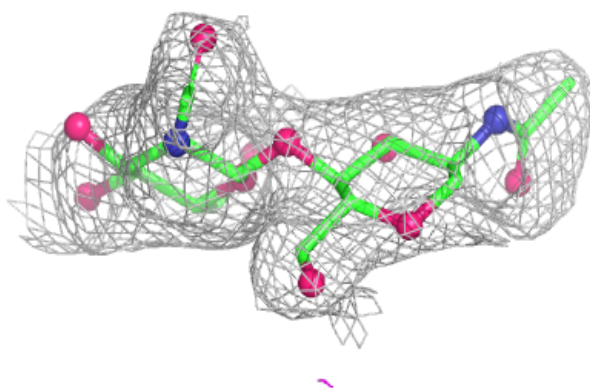
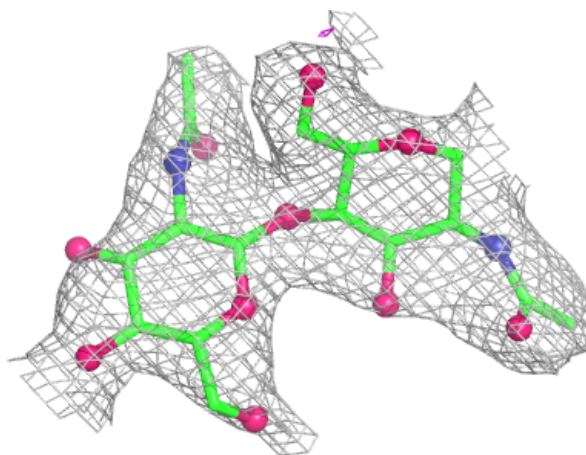
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NAG	H	2	14/15	0.46	0.14	104,115,119,121	0
2	NAG	I	2	14/15	0.52	0.14	105,124,129,130	0
2	NAG	I	1	14/15	0.62	0.12	95,108,115,124	0
2	NAG	G	2	14/15	0.71	0.11	87,96,100,105	0
2	NAG	J	2	14/15	0.77	0.12	86,95,101,102	0
2	NAG	H	1	14/15	0.83	0.12	78,86,92,99	0
2	NAG	J	1	14/15	0.90	0.09	60,72,76,81	0
2	NAG	G	1	14/15	0.90	0.09	63,71,78,86	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.

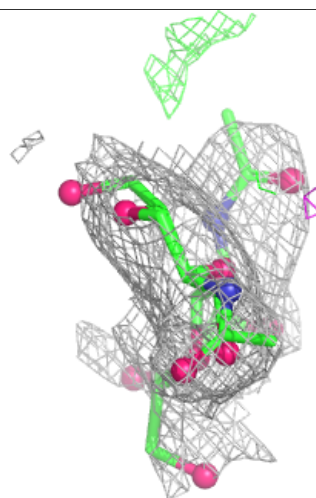
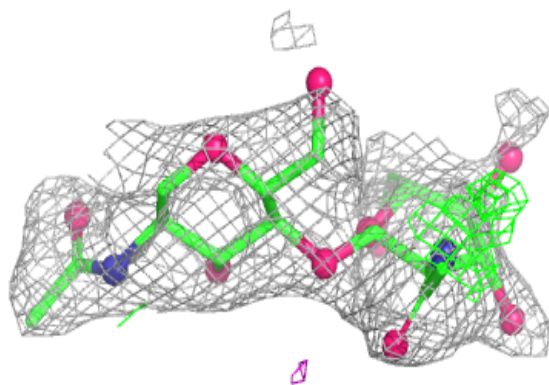
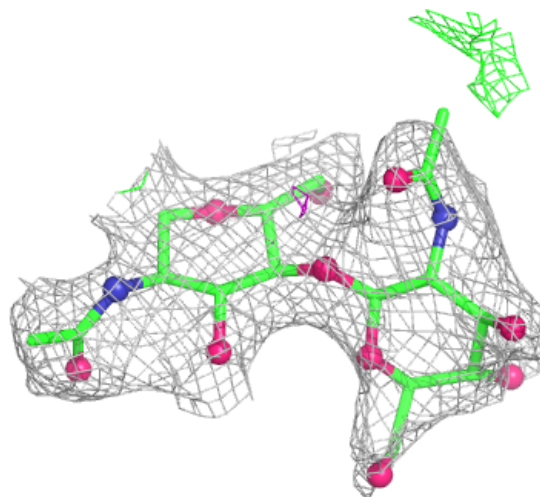
Electron density around Chain G:

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



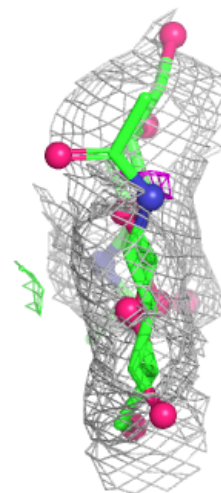
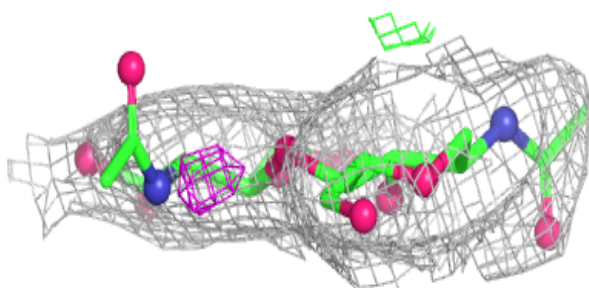
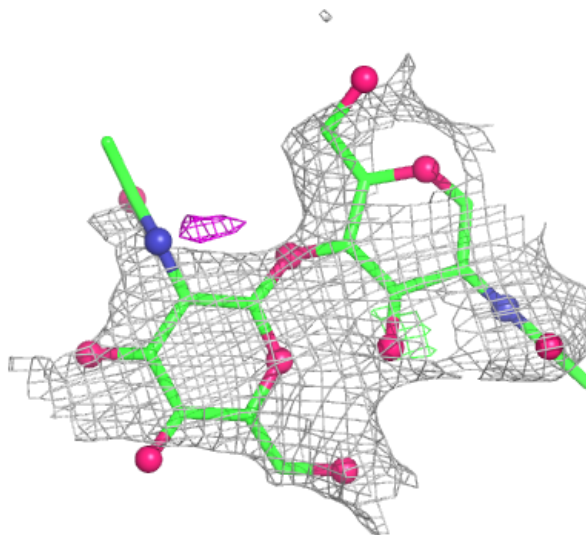
Electron density around Chain H:

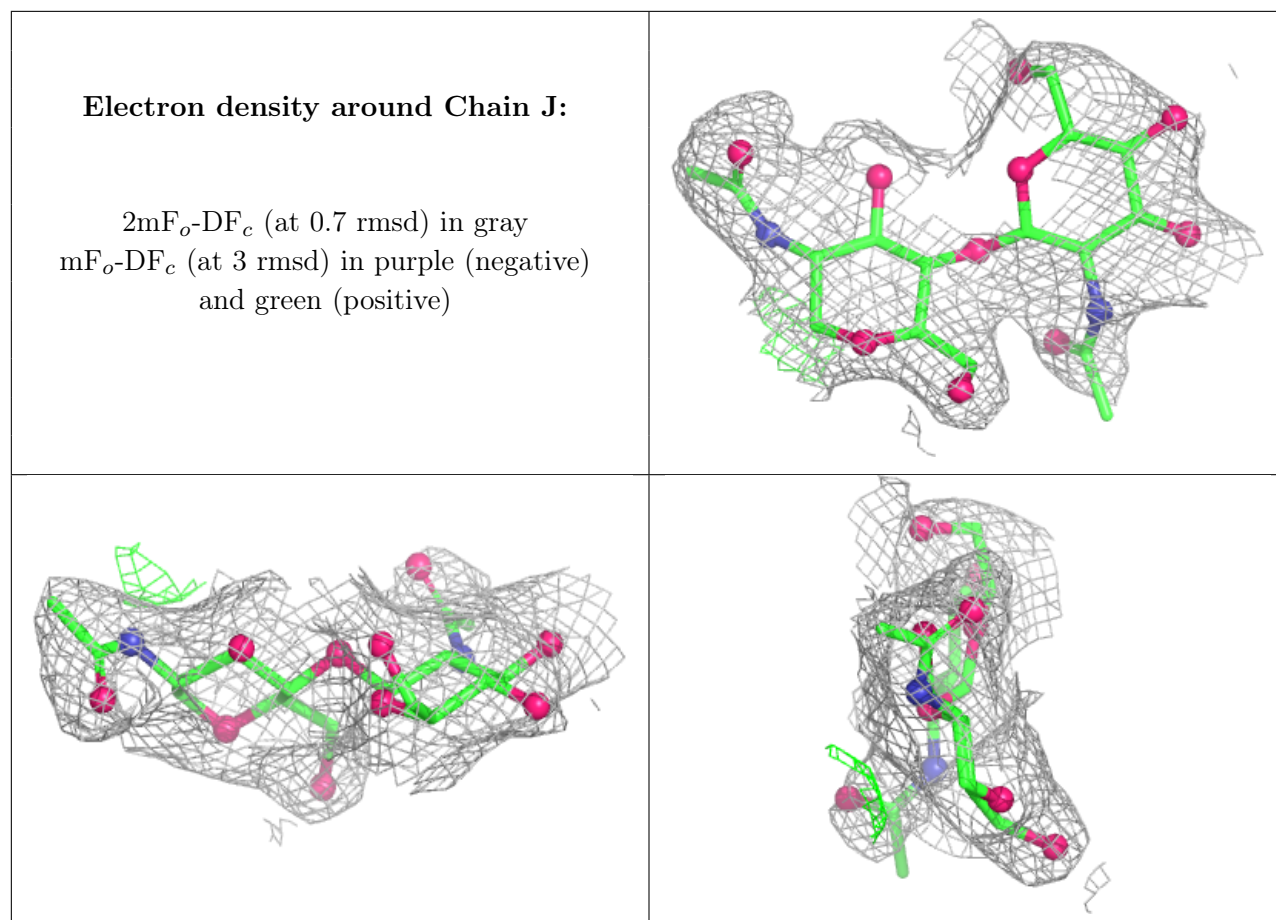
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain I:

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





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
3	NAG	D	602	14/15	0.48	0.17	102,130,143,148	0
3	NAG	C	601	14/15	0.50	0.15	99,105,113,114	0
3	NAG	B	601	14/15	0.52	0.16	117,125,140,143	0
3	NAG	D	601	14/15	0.53	0.16	127,140,146,151	0
3	NAG	A	601	14/15	0.65	0.12	87,105,115,115	0
3	NAG	E	601	14/15	0.66	0.15	61,88,96,124	0
3	NAG	C	602	14/15	0.70	0.13	106,118,123,131	0
3	NAG	E	602	14/15	0.71	0.13	101,111,115,119	0
3	NAG	C	605	14/15	0.82	0.12	61,80,98,109	0

6.5 Other polymers [i](#)

There are no such residues in this entry.