



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 15, 2026 – 01:39 PM UTC

PDB ID : 1INH / pdb_00001inh
Title : INFLUENZA A SUBTYPE N2 NEURAMINIDASE COMPLEXED WITH AROMATIC BANA111 INHIBITOR
Authors : Jedrzejewski, M.J.; Luo, M.
Deposited on : 1995-07-07
Resolution : 2.40 Å(reported)

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

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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
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
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

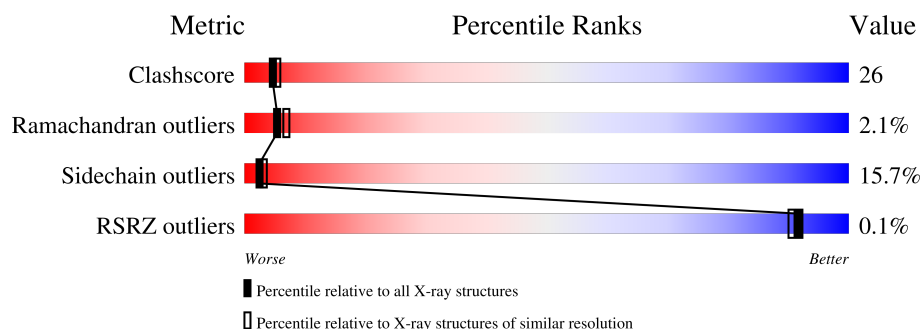
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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))
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	388	
1	B	388	
2	C	2	
2	F	2	
2	G	2	
2	J	2	
3	D	4	

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Mol	Chain	Length	Quality of chain
4	E	6	 100%
5	H	4	 50% 50%
6	I	6	 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
4	MAN	E	4	-	-	X	-
4	BMA	E	5	X	-	X	-
5	FUC	H	4	X	-	-	-
6	NAG	I	1	-	-	X	-
6	MAN	I	4	-	-	X	-
6	MAN	I	5	-	-	X	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 8232 atoms, of which 1796 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 INFLUENZA A SUBTYPE N2 NEURAMINIDASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	388	Total	C	H	N	O	S	0	0	0
			3745	1866	723	545	588	23			
1	B	388	Total	C	H	N	O	S	0	0	0
			3745	1866	723	545	588	23			

There are 2 discrepancies between the modelled and reference sequences:

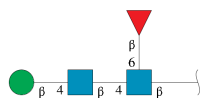
Chain	Residue	Modelled	Actual	Comment	Reference
A	339	ASP	ASN	conflict	UNP P06820
B	339	ASP	ASN	conflict	UNP P06820

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



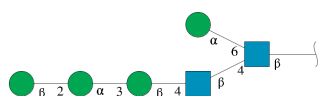
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	C	2	Total	C	H	N	O		0	0	0
			55	16	27	2	10				
2	F	2	Total	C	H	N	O		0	0	0
			55	16	27	2	10				
2	G	2	Total	C	H	N	O		0	0	0
			55	16	27	2	10				
2	J	2	Total	C	H	N	O		0	0	0
			55	16	27	2	10				

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



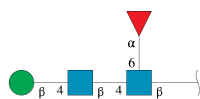
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	4	Total	C	H	N	O	0	0	0
			96	28	47	2	19			

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



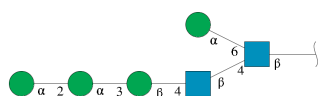
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	6	Total	C	H	N	O	0	0	0
			139	40	67	2	30			

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	H	4	Total	C	H	N	O	0	0	0
			96	28	47	2	19			

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

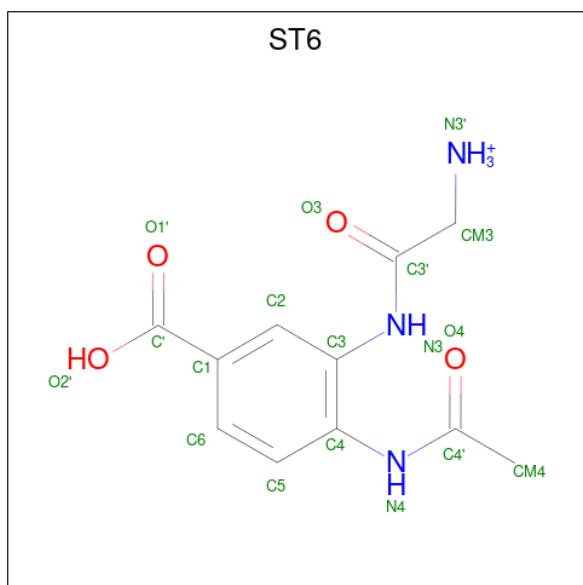


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	I	6	Total	C	H	N	O	0	0	0
			139	40	67	2	30			

- Molecule 7 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

- Molecule 8 is 4-(ACETYLAMINO)-3-[(AMINOACETYL)AMINO]BENZOIC ACID (CCD ID: ST6) (formula: C₁₁H₁₄N₃O₄).

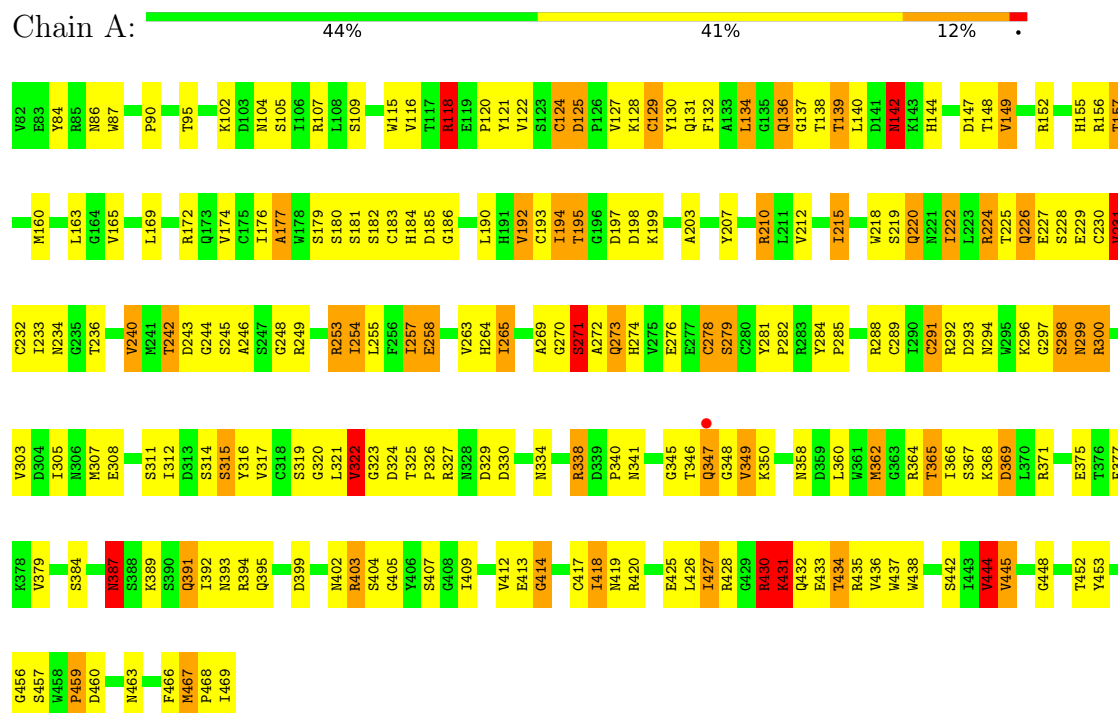


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	A	1	Total	C	H	N	O	0	0
			25	11	7	3	4		
8	B	1	Total	C	H	N	O	0	0
			25	11	7	3	4		

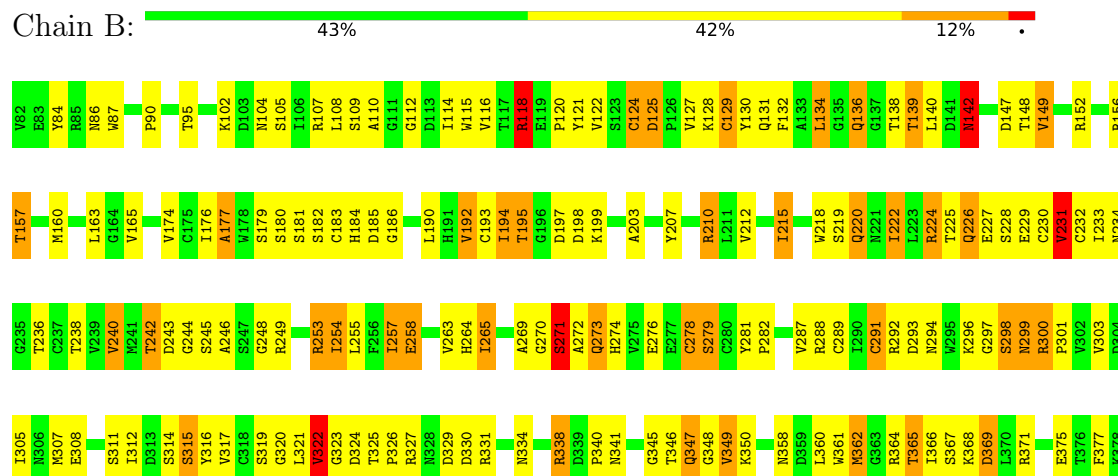
3 Residue-property plots

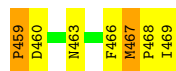
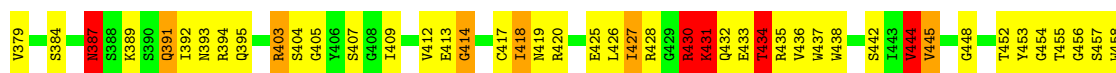
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: INFLUENZA A SUBTYPE N2 NEURAMINIDASE



• Molecule 1: INFLUENZA A SUBTYPE N2 NEURAMINIDASE





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

Chain C:  100%



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

Chain F:  100%

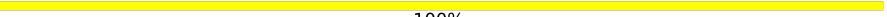


- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:  100%



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

Chain J:  100%



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

Chain D:  50%



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

Chain E:  100%

NAG1
NAG2
BMA3
MAN4
BMA5
MAN6

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

Chain H:

50%

50%

NAG1
NAG2
BMA3
FUC4

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

Chain I:

100%

NAG1
NAG2
BMA3
MAN4
MAN5
MAN6

4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	119.74Å 141.02Å 141.78Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	6.50 – 2.40 6.50 – 2.43	Depositor EDS
% Data completeness (in resolution range)	(Not available) (6.50-2.40) 42.5 (6.50-2.43)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.67 (at 2.44Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.184 , (Not available) 0.214 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	16.0	Xtriage
Anisotropy	1.500	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 56.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	8232	wwPDB-VP
Average B, all atoms (Å ²)	12.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.04% 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: FUL, ST6, FUC, CA, NAG, MAN, BMA

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.80	3/3092 (0.1%)	1.31	48/4194 (1.1%)
1	B	0.80	3/3092 (0.1%)	1.31	48/4194 (1.1%)
All	All	0.80	6/6184 (0.1%)	1.31	96/8388 (1.1%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	254	ILE	CA-CB	5.48	1.61	1.53
1	B	254	ILE	CA-CB	5.48	1.61	1.53
1	A	139	THR	CA-CB	5.36	1.62	1.53
1	B	139	THR	CA-CB	5.36	1.62	1.53
1	A	362	MET	SD-CE	5.29	1.92	1.79
1	B	362	MET	SD-CE	5.29	1.92	1.79

All (96) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	248	GLY	N-CA-C	-9.08	97.47	110.63
1	B	248	GLY	N-CA-C	-9.08	97.47	110.63
1	A	271	SER	N-CA-C	8.97	123.83	113.15
1	B	271	SER	N-CA-C	8.97	123.83	113.15
1	A	430	ARG	N-CA-C	8.62	121.44	110.24
1	B	430	ARG	N-CA-C	8.62	121.44	110.24
1	A	180	SER	N-CA-C	8.13	119.35	108.38
1	B	180	SER	N-CA-C	8.13	119.35	108.38
1	A	467	MET	N-CA-C	7.22	117.90	109.60
1	B	467	MET	N-CA-C	7.22	117.90	109.60
1	A	297	GLY	N-CA-C	7.05	122.85	110.80
1	B	297	GLY	N-CA-C	7.05	122.85	110.80
1	A	365	THR	N-CA-C	-6.95	101.17	110.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	365	THR	N-CA-C	-6.95	101.17	110.55
1	A	391	GLN	N-CA-C	6.85	120.99	109.76
1	B	391	GLN	N-CA-C	6.85	120.99	109.76
1	A	212	VAL	CB-CA-C	-6.77	105.10	111.06
1	B	212	VAL	CB-CA-C	-6.77	105.10	111.06
1	A	320	GLY	N-CA-C	-6.76	104.32	113.37
1	B	320	GLY	N-CA-C	-6.76	104.32	113.37
1	A	125	ASP	N-CA-C	-6.70	102.42	110.13
1	B	125	ASP	N-CA-C	-6.70	102.42	110.13
1	A	300	ARG	CA-C-N	6.60	126.51	119.85
1	A	300	ARG	C-N-CA	6.60	126.51	119.85
1	B	300	ARG	CA-C-N	6.60	126.51	119.85
1	B	300	ARG	C-N-CA	6.60	126.51	119.85
1	A	194	ILE	N-CA-C	6.57	117.35	107.75
1	B	194	ILE	N-CA-C	6.57	117.35	107.75
1	A	105	SER	N-CA-C	6.56	119.27	111.33
1	B	105	SER	N-CA-C	6.56	119.27	111.33
1	A	115	TRP	N-CA-C	6.39	119.04	110.35
1	B	115	TRP	N-CA-C	6.39	119.04	110.35
1	A	258	GLU	N-CA-C	6.37	119.11	108.73
1	B	258	GLU	N-CA-C	6.37	119.11	108.73
1	A	369	ASP	N-CA-C	6.36	119.16	111.40
1	B	369	ASP	N-CA-C	6.36	119.16	111.40
1	A	225	THR	N-CA-C	6.34	117.80	108.86
1	B	225	THR	N-CA-C	6.34	117.80	108.86
1	A	278	CYS	N-CA-C	6.30	119.42	109.96
1	B	278	CYS	N-CA-C	6.30	119.42	109.96
1	A	367	SER	N-CA-C	5.89	119.42	109.76
1	B	367	SER	N-CA-C	5.89	119.42	109.76
1	A	431	LYS	N-CA-C	-5.86	98.32	110.80
1	B	431	LYS	N-CA-C	-5.86	98.32	110.80
1	A	291	CYS	N-CA-C	5.84	123.23	110.80
1	B	291	CYS	N-CA-C	5.84	123.23	110.80
1	A	177	ALA	N-CA-C	5.77	117.28	108.52
1	A	298	SER	N-CA-C	-5.77	106.08	113.23
1	B	177	ALA	N-CA-C	5.77	117.28	108.52
1	B	298	SER	N-CA-C	-5.77	106.08	113.23
1	A	142	ASN	N-CA-C	-5.76	100.58	109.52
1	B	142	ASN	N-CA-C	-5.76	100.58	109.52
1	A	87	TRP	N-CA-C	5.75	119.56	111.52
1	B	87	TRP	N-CA-C	5.75	119.56	111.52
1	A	273	GLN	N-CA-C	5.70	120.37	112.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	273	GLN	N-CA-C	5.70	120.37	112.90
1	A	127	VAL	N-CA-C	5.66	117.05	111.67
1	B	127	VAL	N-CA-C	5.66	117.05	111.67
1	A	296	LYS	N-CA-C	5.55	120.94	113.72
1	B	296	LYS	N-CA-C	5.55	120.94	113.72
1	A	324	ASP	N-CA-C	-5.54	98.41	108.65
1	B	324	ASP	N-CA-C	-5.54	98.41	108.65
1	A	222	ILE	N-CA-C	5.52	120.81	109.34
1	B	222	ILE	N-CA-C	5.52	120.81	109.34
1	A	387	ASN	N-CA-C	5.48	119.13	111.90
1	B	387	ASN	N-CA-C	5.48	119.13	111.90
1	A	136	GLN	N-CA-C	5.42	119.62	111.81
1	B	136	GLN	N-CA-C	5.42	119.62	111.81
1	A	212	VAL	N-CA-C	5.30	118.26	112.96
1	B	212	VAL	N-CA-C	5.30	118.26	112.96
1	A	152	ARG	N-CA-C	5.21	117.57	108.76
1	B	152	ARG	N-CA-C	5.21	117.57	108.76
1	A	174	VAL	N-CA-C	5.19	117.53	111.05
1	B	174	VAL	N-CA-C	5.19	117.53	111.05
1	A	292	ARG	N-CA-C	5.16	117.40	107.44
1	B	292	ARG	N-CA-C	5.16	117.40	107.44
1	A	231	VAL	N-CA-C	5.16	115.55	108.12
1	B	231	VAL	N-CA-C	5.16	115.55	108.12
1	A	338	ARG	N-CA-C	5.13	119.75	112.93
1	B	338	ARG	N-CA-C	5.13	119.75	112.93
1	A	279	SER	N-CA-C	-5.13	99.43	108.20
1	B	279	SER	N-CA-C	-5.13	99.43	108.20
1	A	434	THR	N-CA-C	5.12	120.52	113.97
1	B	434	THR	N-CA-C	5.12	120.52	113.97
1	A	414	GLY	N-CA-C	-5.08	104.55	112.58
1	B	414	GLY	N-CA-C	-5.08	104.55	112.58
1	A	444	VAL	N-CA-C	-5.08	100.47	108.90
1	B	444	VAL	N-CA-C	-5.08	100.47	108.90
1	A	456	GLY	N-CA-C	5.06	117.42	110.69
1	B	456	GLY	N-CA-C	5.06	117.42	110.69
1	A	102	LYS	N-CA-C	-5.02	100.83	108.76
1	B	102	LYS	N-CA-C	-5.02	100.83	108.76
1	A	220	GLN	N-CA-C	5.00	118.96	112.86
1	A	265	ILE	N-CA-C	-5.00	101.27	108.42
1	B	220	GLN	N-CA-C	5.00	118.96	112.86
1	B	265	ILE	N-CA-C	-5.00	101.27	108.42

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	3022	723	2851	143	63
1	B	3022	723	2849	178	9
2	C	28	27	25	0	0
2	F	28	27	25	0	0
2	G	28	27	25	0	0
2	J	28	27	25	0	0
3	D	49	47	43	1	0
4	E	72	67	52	42	0
5	H	49	47	43	1	0
6	I	72	67	60	6	63
7	A	1	0	0	0	0
7	B	1	0	0	0	0
8	A	18	7	13	1	0
8	B	18	7	13	1	0
All	All	6436	1796	6024	321	72

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 26.

All (321) 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:B:391:GLN:OE1	4:E:4:MAN:C4	1.68	1.39
1:B:395:GLN:HG3	4:E:5:BMA:C5	1.62	1.29
1:B:377:PHE:CB	4:E:4:MAN:H3	1.64	1.27
1:B:395:GLN:CG	4:E:5:BMA:H5	1.67	1.25
1:B:453:TYR:OH	4:E:5:BMA:H4	1.32	1.23
1:B:391:GLN:CD	4:E:4:MAN:C4	2.24	1.08
1:B:377:PHE:CB	4:E:4:MAN:C3	2.38	1.02
1:B:377:PHE:HB3	4:E:4:MAN:H3	1.03	1.01
1:B:391:GLN:O	4:E:4:MAN:H62	1.42	1.01
1:B:393:ASN:HD22	4:E:5:BMA:H3	1.22	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:393:ASN:ND2	4:E:5:BMA:H3	1.70	0.99
1:A:323:GLY:HA2	1:A:327:ARG:HD3	1.48	0.95
1:B:323:GLY:HA2	1:B:327:ARG:HD3	1.48	0.94
1:B:377:PHE:HB2	4:E:4:MAN:C3	1.97	0.93
1:B:453:TYR:OH	4:E:5:BMA:C4	2.18	0.89
1:B:377:PHE:HB3	4:E:4:MAN:C3	1.97	0.87
1:B:361:TRP:HZ3	4:E:5:BMA:O6	1.59	0.85
6:I:1:NAG:H5	6:I:6:MAN:H2	1.62	0.82
1:B:377:PHE:HB2	4:E:4:MAN:O3	1.80	0.81
4:E:1:NAG:H5	4:E:6:MAN:H2	1.62	0.81
1:B:395:GLN:HG3	4:E:5:BMA:H5	0.86	0.81
1:B:394:ARG:HD3	4:E:3:BMA:H2	1.63	0.80
1:B:391:GLN:OE1	4:E:4:MAN:O4	1.99	0.79
1:B:393:ASN:O	4:E:5:BMA:O6	1.99	0.79
1:B:395:GLN:OE1	4:E:5:BMA:H61	1.83	0.78
1:A:134:LEU:HB3	1:A:156:ARG:NH1	2.00	0.77
1:B:319:SER:O	1:B:322:VAL:HB	1.86	0.76
1:B:134:LEU:HB3	1:B:156:ARG:NH1	2.00	0.75
1:A:254:ILE:HG21	1:A:305:ILE:HG12	1.69	0.75
1:B:254:ILE:HG21	1:B:305:ILE:HG12	1.69	0.75
1:A:319:SER:O	1:A:322:VAL:HB	1.86	0.74
1:B:218:TRP:CE2	1:B:253:ARG:HD3	2.24	0.72
1:A:218:TRP:CE2	1:A:253:ARG:HD3	2.24	0.72
1:A:222:ILE:O	1:A:224:ARG:HG3	1.90	0.72
1:B:454:GLY:O	4:E:1:NAG:C7	2.36	0.72
1:B:298:SER:HB2	1:B:341:ASN:HD21	1.55	0.72
1:B:393:ASN:O	4:E:5:BMA:C6	2.39	0.71
1:B:222:ILE:O	1:B:224:ARG:HG3	1.90	0.71
1:A:334:ASN:HA	1:A:387:ASN:HD21	1.55	0.71
1:A:298:SER:HB2	1:A:341:ASN:HD21	1.55	0.70
1:B:334:ASN:HA	1:B:387:ASN:HD21	1.55	0.70
1:B:453:TYR:HH	4:E:5:BMA:H4	1.56	0.69
1:B:104:ASN:HD22	1:B:107:ARG:HD3	1.58	0.69
1:A:254:ILE:HD13	1:A:312:ILE:HG12	1.76	0.67
1:B:254:ILE:HD13	1:B:312:ILE:HG12	1.76	0.67
1:B:395:GLN:CD	4:E:5:BMA:H5	2.18	0.67
1:A:104:ASN:HD22	1:A:107:ARG:HD3	1.58	0.66
1:A:142:ASN:HD21	1:B:110:ALA:HB3	1.60	0.66
1:B:276:GLU:O	1:B:291:CYS:HB3	1.96	0.65
1:B:311:SER:C	1:B:312:ILE:HD12	2.21	0.65
1:A:311:SER:C	1:A:312:ILE:HD12	2.21	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:176:ILE:HG22	1:B:195:THR:HG21	1.79	0.64
1:A:169:LEU:HD22	1:B:114:ILE:HD11	1.78	0.64
1:B:198:ASP:HB3	1:B:222:ILE:HG12	1.80	0.64
1:A:169:LEU:HD11	1:B:112:GLY:HA3	1.79	0.64
1:A:276:GLU:O	1:A:291:CYS:HB3	1.96	0.64
1:A:155:HIS:HB3	1:B:104:ASN:HD21	1.63	0.63
1:A:403:ARG:HH21	1:A:433:GLU:HG3	1.63	0.63
1:A:176:ILE:HG22	1:A:195:THR:HG21	1.79	0.63
1:B:403:ARG:HH21	1:B:433:GLU:HG3	1.63	0.62
1:B:177:ALA:HB2	1:B:193:CYS:HB3	1.82	0.62
1:A:198:ASP:HB3	1:A:222:ILE:HG12	1.80	0.62
1:B:228:SER:HB3	1:B:350:LYS:HE2	1.82	0.61
1:B:131:GLN:HE21	1:B:163:LEU:HD12	1.65	0.61
1:A:321:LEU:HD12	1:A:379:VAL:HG22	1.83	0.60
1:B:418:ILE:O	1:B:418:ILE:HG13	2.01	0.60
1:A:131:GLN:HE21	1:A:163:LEU:HD12	1.65	0.60
1:A:177:ALA:HB2	1:A:193:CYS:HB3	1.82	0.60
1:B:218:TRP:CZ2	1:B:253:ARG:HD3	2.37	0.60
1:A:228:SER:HB3	1:A:350:LYS:HE2	1.82	0.60
1:B:419:ASN:ND2	1:B:420:ARG:H	2.00	0.59
1:A:418:ILE:O	1:A:418:ILE:HG13	2.01	0.59
1:B:391:GLN:O	4:E:4:MAN:C6	2.26	0.59
1:B:321:LEU:HD12	1:B:379:VAL:HG22	1.83	0.59
1:A:419:ASN:ND2	1:A:420:ARG:H	2.00	0.59
1:A:218:TRP:CZ2	1:A:253:ARG:HD3	2.37	0.59
1:B:300:ARG:NH2	1:B:349:VAL:O	2.36	0.58
1:B:392:ILE:C	4:E:4:MAN:O3	2.46	0.58
1:A:300:ARG:NH2	1:A:349:VAL:O	2.36	0.58
1:A:272:ALA:HA	1:A:316:TYR:HE1	1.68	0.58
1:A:139:THR:HG23	1:B:108:LEU:HD23	1.85	0.58
1:B:272:ALA:HA	1:B:316:TYR:HE1	1.68	0.58
1:A:190:LEU:HD11	1:A:257:ILE:HD13	1.86	0.57
1:B:326:PRO:HA	1:B:368:LYS:O	2.03	0.57
1:A:326:PRO:HA	1:A:368:LYS:O	2.03	0.57
1:B:190:LEU:HD11	1:B:257:ILE:HD13	1.86	0.57
1:A:84:TYR:HE1	1:A:185:ASP:OD2	1.88	0.57
1:A:323:GLY:HA2	1:A:327:ARG:CD	2.30	0.57
1:B:246:ALA:O	1:B:274:HIS:NE2	2.38	0.57
1:A:273:GLN:HG3	1:A:340:PRO:HG3	1.87	0.57
4:E:1:NAG:H5	4:E:6:MAN:C2	2.32	0.57
1:A:86:ASN:HB2	1:A:234:ASN:OD1	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:I:1:NAG:H5	6:I:6:MAN:C2	2.32	0.56
1:B:84:TYR:HE1	1:B:185:ASP:OD2	1.88	0.56
1:A:325:THR:O	1:A:348:GLY:HA2	2.06	0.56
1:B:299:ASN:H	1:B:299:ASN:ND2	2.03	0.56
1:B:317:VAL:HG23	1:B:322:VAL:HG23	1.87	0.56
1:A:278:CYS:HB3	1:A:289:CYS:HB3	1.87	0.56
1:B:86:ASN:HB2	1:B:234:ASN:OD1	2.05	0.56
1:B:391:GLN:CD	4:E:4:MAN:O4	2.48	0.56
1:A:270:GLY:HA3	1:A:314:SER:H	1.71	0.56
1:B:273:GLN:HG3	1:B:340:PRO:HG3	1.87	0.56
1:A:300:ARG:NH1	1:A:323:GLY:O	2.39	0.56
1:B:278:CYS:HB3	1:B:289:CYS:HB3	1.87	0.56
1:B:325:THR:O	1:B:348:GLY:HA2	2.06	0.56
1:A:172:ARG:NH2	1:B:163:LEU:O	2.38	0.55
1:A:246:ALA:O	1:A:274:HIS:NE2	2.38	0.55
1:B:125:ASP:OD1	1:B:130:TYR:HE1	1.89	0.55
1:B:270:GLY:HA3	1:B:314:SER:H	1.71	0.55
1:A:236:THR:HA	1:A:258:GLU:HB3	1.88	0.55
1:A:125:ASP:OD1	1:A:130:TYR:HE1	1.89	0.55
1:A:289:CYS:HB2	1:A:303:VAL:HB	1.88	0.55
1:B:300:ARG:NH1	1:B:323:GLY:O	2.39	0.55
1:A:317:VAL:HG23	1:A:322:VAL:HG23	1.87	0.55
1:B:226:GLN:NE2	1:B:240:VAL:H	2.05	0.55
1:B:236:THR:HA	1:B:258:GLU:HB3	1.88	0.55
1:B:455:THR:OG1	4:E:6:MAN:H3	2.06	0.55
1:A:245:SER:O	1:A:274:HIS:HE1	1.90	0.55
1:A:226:GLN:NE2	1:A:240:VAL:H	2.05	0.55
1:B:263:VAL:O	1:B:264:HIS:HB2	2.07	0.55
1:A:299:ASN:ND2	1:A:299:ASN:H	2.03	0.54
1:A:463:ASN:HB3	1:A:466:PHE:CD2	2.43	0.54
1:B:245:SER:O	1:B:274:HIS:HE1	1.90	0.54
1:B:463:ASN:HB3	1:B:466:PHE:CD2	2.43	0.54
6:I:1:NAG:O7	6:I:1:NAG:H3	2.08	0.54
1:B:184:HIS:HD2	1:B:186:GLY:H	1.55	0.54
1:B:289:CYS:HB2	1:B:303:VAL:HB	1.88	0.54
1:A:184:HIS:HD2	1:A:186:GLY:H	1.55	0.53
1:B:233:ILE:CD1	1:B:307:MET:HE2	2.38	0.53
1:B:349:VAL:HB	1:B:371:ARG:HE	1.73	0.53
1:B:430:ARG:HA	1:B:433:GLU:O	2.09	0.53
1:B:95:THR:O	1:B:95:THR:HG22	2.08	0.53
1:B:334:ASN:HA	1:B:387:ASN:ND2	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:144:HIS:CE1	1:B:107:ARG:HA	2.44	0.53
1:B:394:ARG:O	4:E:5:BMA:O5	1.98	0.53
1:B:394:ARG:HB2	4:E:4:MAN:O4	2.09	0.53
1:A:124:CYS:HA	1:A:129:CYS:HA	1.91	0.53
1:B:224:ARG:HD2	1:B:242:THR:O	2.09	0.53
1:A:263:VAL:O	1:A:264:HIS:HB2	2.07	0.53
1:A:233:ILE:CD1	1:A:307:MET:HE2	2.38	0.53
1:B:361:TRP:CZ3	4:E:5:BMA:O6	2.51	0.53
1:A:224:ARG:HD2	1:A:242:THR:O	2.09	0.52
1:A:349:VAL:HB	1:A:371:ARG:HE	1.73	0.52
1:A:368:LYS:HG3	1:A:369:ASP:N	2.25	0.52
1:A:430:ARG:HA	1:A:433:GLU:O	2.09	0.52
1:B:271:SER:HB2	1:B:338:ARG:O	2.10	0.52
1:A:95:THR:HG22	1:A:95:THR:O	2.08	0.52
1:A:144:HIS:HD2	1:B:466:PHE:HD2	1.55	0.52
1:A:271:SER:HB2	1:A:338:ARG:O	2.10	0.52
1:A:437:TRP:H	1:A:469:ILE:HG21	1.75	0.52
4:E:1:NAG:H3	4:E:1:NAG:O7	2.08	0.52
1:A:274:HIS:O	1:A:293:ASP:HA	2.10	0.52
1:B:274:HIS:O	1:B:293:ASP:HA	2.10	0.52
1:B:437:TRP:H	1:B:469:ILE:HG21	1.75	0.52
1:B:453:TYR:CZ	4:E:5:BMA:H4	2.38	0.52
1:A:413:GLU:HG3	1:A:418:ILE:HG22	1.92	0.52
1:A:203:ALA:HB3	1:A:215:ILE:HG22	1.92	0.52
1:B:368:LYS:HG3	1:B:369:ASP:N	2.25	0.52
1:B:413:GLU:HG3	1:B:418:ILE:HG22	1.92	0.51
1:A:181:SER:HB3	1:A:192:VAL:HG22	1.92	0.51
1:A:299:ASN:HA	1:A:322:VAL:CG2	2.41	0.51
1:B:183:CYS:SG	1:B:232:CYS:SG	3.08	0.51
1:B:203:ALA:HB3	1:B:215:ILE:HG22	1.92	0.51
1:B:124:CYS:HA	1:B:129:CYS:HA	1.91	0.51
5:H:2:NAG:H5	5:H:3:BMA:O5	2.11	0.51
1:A:334:ASN:HA	1:A:387:ASN:ND2	2.23	0.51
1:B:299:ASN:HA	1:B:322:VAL:CG2	2.41	0.51
1:A:183:CYS:SG	1:A:232:CYS:SG	3.08	0.51
4:E:1:NAG:C5	4:E:6:MAN:H2	2.37	0.51
1:A:139:THR:O	1:A:142:ASN:HB2	2.11	0.50
1:B:181:SER:HB3	1:B:192:VAL:HG22	1.92	0.50
1:B:139:THR:O	1:B:142:ASN:HB2	2.11	0.50
1:B:233:ILE:HD12	1:B:307:MET:HE2	1.93	0.50
3:D:2:NAG:H5	3:D:3:BMA:O5	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:274:HIS:HD2	1:A:294:ASN:H	1.59	0.50
1:A:233:ILE:HD12	1:A:307:MET:HE2	1.93	0.50
1:A:377:PHE:HA	1:A:393:ASN:O	2.12	0.50
1:A:299:ASN:HA	1:A:322:VAL:HG21	1.95	0.49
1:B:315:SER:O	1:B:316:TYR:CD1	2.66	0.49
1:B:274:HIS:HD2	1:B:294:ASN:H	1.59	0.49
1:B:377:PHE:HA	1:B:393:ASN:O	2.12	0.49
1:A:315:SER:O	1:A:316:TYR:CD1	2.66	0.49
1:B:323:GLY:HA2	1:B:327:ARG:CD	2.30	0.49
1:A:224:ARG:NH1	1:A:243:ASP:HA	2.28	0.49
1:B:299:ASN:HA	1:B:322:VAL:HG21	1.95	0.49
1:A:413:GLU:HG2	1:A:414:GLY:O	2.13	0.49
1:B:323:GLY:HA3	1:B:364:ARG:HD2	1.95	0.48
6:I:1:NAG:C5	6:I:6:MAN:H2	2.37	0.48
1:B:224:ARG:NH1	1:B:243:ASP:HA	2.28	0.48
1:A:349:VAL:HG22	1:A:350:LYS:O	2.13	0.48
1:B:349:VAL:HG22	1:B:350:LYS:O	2.13	0.48
1:B:436:VAL:HB	1:B:438:TRP:NE1	2.29	0.48
1:B:346:THR:O	1:B:347:GLN:HG2	2.14	0.48
1:B:413:GLU:HG2	1:B:414:GLY:O	2.13	0.48
1:A:176:ILE:CG2	1:A:195:THR:HG21	2.44	0.48
1:A:444:VAL:C	1:A:445:VAL:HG12	2.39	0.48
1:A:157:THR:HG22	1:A:176:ILE:HA	1.95	0.47
1:B:444:VAL:C	1:B:445:VAL:HG12	2.39	0.47
1:A:323:GLY:HA3	1:A:364:ARG:HD2	1.95	0.47
1:B:120:PRO:CG	1:B:425:GLU:HB2	2.44	0.47
1:A:226:GLN:HE21	1:A:240:VAL:HG13	1.79	0.47
1:A:346:THR:O	1:A:347:GLN:HG2	2.14	0.47
1:B:157:THR:HG22	1:B:176:ILE:HA	1.95	0.47
1:A:169:LEU:CD2	1:B:114:ILE:HD11	2.45	0.47
1:A:182:SER:HA	1:A:190:LEU:O	2.15	0.47
1:A:436:VAL:HB	1:A:438:TRP:NE1	2.29	0.47
1:B:184:HIS:CD2	1:B:186:GLY:H	2.33	0.47
1:A:120:PRO:CG	1:A:425:GLU:HB2	2.44	0.47
1:B:182:SER:HA	1:B:190:LEU:O	2.15	0.46
1:A:118:ARG:HD2	1:A:427:ILE:HD12	1.98	0.46
1:A:279:SER:HB3	1:A:409:ILE:HG22	1.98	0.46
1:B:276:GLU:OE1	8:B:489:ST6:N3'	2.45	0.46
1:B:226:GLN:HE21	1:B:240:VAL:HG13	1.79	0.46
1:B:299:ASN:ND2	1:B:299:ASN:N	2.64	0.46
6:I:2:NAG:H3	6:I:3:BMA:O2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:137:GLY:O	1:B:107:ARG:NE	2.47	0.46
1:A:184:HIS:CD2	1:A:186:GLY:H	2.33	0.46
1:A:468:PRO:O	1:A:469:ILE:HB	2.16	0.46
1:A:195:THR:HB	1:B:458:TRP:HE1	1.81	0.46
1:A:362:MET:HE2	1:A:377:PHE:CZ	2.52	0.46
1:B:300:ARG:HA	1:B:301:PRO:HD2	1.80	0.46
1:B:118:ARG:HD2	1:B:427:ILE:HD12	1.98	0.45
1:B:362:MET:HE2	1:B:377:PHE:CZ	2.52	0.45
1:B:136:GLN:O	1:B:138:THR:HG22	2.17	0.45
1:B:393:ASN:O	4:E:5:BMA:C5	2.64	0.45
4:E:2:NAG:H3	4:E:3:BMA:O2	2.16	0.45
1:A:329:ASP:OD1	1:A:330:ASP:N	2.50	0.45
1:B:176:ILE:CG2	1:B:195:THR:HG21	2.44	0.45
1:A:136:GLN:O	1:A:138:THR:HG22	2.17	0.45
1:A:366:ILE:HA	1:A:375:GLU:OE2	2.17	0.45
1:B:90:PRO:O	1:B:417:CYS:HB2	2.17	0.45
1:B:226:GLN:HG2	1:B:278:CYS:O	2.17	0.45
1:B:329:ASP:OD1	1:B:330:ASP:N	2.50	0.45
1:A:120:PRO:O	1:A:121:TYR:HB3	2.17	0.45
1:B:366:ILE:HA	1:B:375:GLU:OE2	2.17	0.45
1:A:299:ASN:ND2	1:A:299:ASN:N	2.64	0.45
1:B:134:LEU:HB3	1:B:156:ARG:HH12	1.80	0.45
1:A:176:ILE:HG22	1:A:195:THR:CG2	2.47	0.45
1:A:435:ARG:NH2	1:A:467:MET:O	2.50	0.45
1:B:395:GLN:OE1	4:E:5:BMA:H5	2.16	0.45
1:A:231:VAL:HG21	1:A:282:PRO:HB3	1.99	0.44
1:B:419:ASN:HD21	1:B:448:GLY:HA3	1.82	0.44
1:B:468:PRO:O	1:B:469:ILE:HB	2.16	0.44
1:A:169:LEU:HD21	1:B:108:LEU:HD22	1.99	0.44
1:B:231:VAL:HG21	1:B:282:PRO:HB3	1.99	0.44
1:B:279:SER:HB3	1:B:409:ILE:HG22	1.98	0.44
1:A:199:LYS:O	1:A:220:GLN:HA	2.18	0.44
1:A:90:PRO:O	1:A:417:CYS:HB2	2.17	0.44
1:A:419:ASN:HD21	1:A:448:GLY:HA3	1.82	0.44
1:B:392:ILE:O	4:E:4:MAN:O3	2.35	0.44
1:A:109:SER:HB3	1:A:140:LEU:HD22	2.00	0.44
1:A:142:ASN:ND2	1:B:110:ALA:HB3	2.30	0.44
1:B:264:HIS:ND1	1:B:265:ILE:O	2.51	0.44
1:A:264:HIS:ND1	1:A:265:ILE:O	2.51	0.44
1:B:109:SER:HB3	1:B:140:LEU:HD22	2.00	0.44
1:B:435:ARG:NH2	1:B:467:MET:O	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:226:GLN:HG2	1:A:278:CYS:O	2.17	0.43
1:A:276:GLU:OE1	8:A:471:ST6:N3'	2.45	0.43
1:B:358:ASN:OD1	1:B:384:SER:HB2	2.18	0.43
1:A:269:ALA:HB3	1:A:312:ILE:O	2.18	0.43
1:A:218:TRP:NE1	1:A:243:ASP:HB3	2.34	0.43
1:B:132:PHE:CZ	1:B:160:MET:HE3	2.54	0.43
1:A:120:PRO:HD2	1:A:425:GLU:OE1	2.19	0.43
1:B:199:LYS:O	1:B:220:GLN:HA	2.18	0.43
1:B:176:ILE:HG22	1:B:195:THR:CG2	2.47	0.43
1:B:233:ILE:HD13	1:B:307:MET:HG3	2.00	0.43
1:A:132:PHE:CZ	1:A:160:MET:HE3	2.54	0.43
1:A:233:ILE:HD13	1:A:307:MET:HG3	2.00	0.43
1:A:149:VAL:HG11	1:A:431:LYS:HD2	2.01	0.43
1:A:224:ARG:HH12	1:A:244:GLY:H	1.67	0.43
1:B:120:PRO:HD2	1:B:425:GLU:OE1	2.19	0.43
1:B:185:ASP:OD1	1:B:207:TYR:HE2	2.02	0.43
1:A:284:TYR:HA	1:A:285:PRO:HA	1.88	0.42
1:A:358:ASN:OD1	1:A:384:SER:HB2	2.18	0.42
1:B:224:ARG:HH12	1:B:244:GLY:H	1.67	0.42
1:A:403:ARG:NH2	1:A:432:GLN:HB3	2.35	0.42
1:B:149:VAL:HG11	1:B:431:LYS:HD2	2.01	0.42
1:A:86:ASN:OD1	1:A:86:ASN:C	2.63	0.42
1:A:183:CYS:HB3	1:A:230:CYS:O	2.19	0.42
1:B:183:CYS:HB3	1:B:230:CYS:O	2.19	0.42
1:B:254:ILE:HD12	1:B:254:ILE:N	2.35	0.42
1:B:269:ALA:HB3	1:B:312:ILE:O	2.18	0.42
1:B:319:SER:OG	1:B:322:VAL:N	2.53	0.42
1:A:312:ILE:HD12	1:A:312:ILE:N	2.35	0.42
1:B:120:PRO:O	1:B:121:TYR:HB3	2.17	0.42
1:A:185:ASP:OD1	1:A:207:TYR:HE2	2.02	0.42
1:A:272:ALA:H	1:A:314:SER:CB	2.33	0.42
1:B:218:TRP:NE1	1:B:243:ASP:HB3	2.34	0.42
1:B:322:VAL:O	1:B:327:ARG:HD3	2.20	0.42
1:B:371:ARG:HD3	1:B:405:GLY:HA2	2.01	0.42
1:A:322:VAL:O	1:A:327:ARG:HD3	2.20	0.42
1:B:457:SER:O	1:B:459:PRO:HD3	2.20	0.42
1:A:254:ILE:N	1:A:254:ILE:HD12	2.35	0.41
1:A:319:SER:OG	1:A:322:VAL:N	2.53	0.41
1:A:457:SER:O	1:A:459:PRO:HD3	2.20	0.41
1:A:371:ARG:HD3	1:A:405:GLY:HA2	2.01	0.41
1:B:179:SER:HB3	1:B:194:ILE:HB	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:271:SER:N	1:B:314:SER:HB2	2.35	0.41
1:B:404:SER:O	1:B:427:ILE:HG22	2.20	0.41
1:A:179:SER:HB3	1:A:194:ILE:HB	2.03	0.41
1:B:403:ARG:NH2	1:B:432:GLN:HB3	2.35	0.41
1:A:134:LEU:HB3	1:A:156:ARG:HH12	1.80	0.41
1:A:271:SER:N	1:A:314:SER:HB2	2.35	0.41
1:B:86:ASN:OD1	1:B:86:ASN:C	2.63	0.41
1:B:272:ALA:H	1:B:314:SER:CB	2.33	0.41
1:A:399:ASP:O	1:A:402:ASN:HB2	2.21	0.41
1:B:281:TYR:OH	1:B:288:ARG:HD2	2.21	0.41
1:B:312:ILE:HD12	1:B:312:ILE:N	2.35	0.41
6:I:2:NAG:C4	6:I:3:BMA:O2	2.69	0.41
1:A:120:PRO:HG3	1:A:425:GLU:HB2	2.02	0.41
1:A:321:LEU:HD23	1:A:321:LEU:HA	1.85	0.41
4:E:2:NAG:C4	4:E:3:BMA:O2	2.69	0.41
1:A:269:ALA:H	1:A:312:ILE:HG22	1.86	0.40
1:A:144:HIS:CD2	1:B:466:PHE:HD2	2.37	0.40
1:A:404:SER:O	1:A:427:ILE:HG22	2.20	0.40
1:B:264:HIS:ND1	1:B:265:ILE:N	2.70	0.40
1:A:210:ARG:H	1:A:210:ARG:HD2	1.86	0.40
1:A:281:TYR:OH	1:A:288:ARG:HD2	2.21	0.40
1:B:269:ALA:H	1:B:312:ILE:HG22	1.86	0.40
1:B:210:ARG:H	1:B:210:ARG:HD2	1.86	0.40
1:B:238:THR:HG21	1:B:287:VAL:HG21	2.03	0.40

All (72) 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:B:331:ARG:NH2	1:B:434:THR:CG2[3_654]	0.72	1.48
1:A:394:ARG:N	6:I:5:MAN:C1[4_555]	0.73	1.47
1:A:393:ASN:CA	6:I:5:MAN:O2[4_555]	0.84	1.36
1:A:394:ARG:N	6:I:4:MAN:O2[4_555]	0.84	1.36
1:A:393:ASN:CB	6:I:5:MAN:HO3[4_555]	0.26	1.34
1:A:393:ASN:CB	6:I:5:MAN:O3[4_555]	0.86	1.34
1:A:393:ASN:C	6:I:5:MAN:C1[4_555]	0.90	1.30
1:A:391:GLN:CG	6:I:4:MAN:H61[4_555]	0.32	1.28
1:A:393:ASN:N	6:I:5:MAN:O2[4_555]	0.93	1.27
1:A:394:ARG:CA	6:I:4:MAN:O2[4_555]	0.99	1.21
1:A:391:GLN:CB	6:I:4:MAN:O6[4_555]	1.01	1.19

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:331:ARG:CZ	1:B:434:THR:CG2[3_654]	1.12	1.08
1:A:393:ASN:CA	6:I:5:MAN:C2[4_555]	1.20	1.00
1:A:391:GLN:CG	6:I:4:MAN:C6[4_555]	1.26	0.94
1:A:391:GLN:CB	6:I:4:MAN:C6[4_555]	1.28	0.92
1:A:393:ASN:O	6:I:5:MAN:H1[4_555]	0.72	0.88
1:B:331:ARG:NH2	1:B:434:THR:CB[3_654]	1.33	0.87
1:A:393:ASN:C	6:I:5:MAN:C2[4_555]	1.36	0.84
1:A:393:ASN:C	6:I:5:MAN:H1[4_555]	0.90	0.70
1:A:393:ASN:H	6:I:5:MAN:HO2[4_555]	0.93	0.67
1:A:391:GLN:CA	6:I:4:MAN:O6[4_555]	1.57	0.63
1:A:394:ARG:CB	6:I:4:MAN:O2[4_555]	1.62	0.58
1:B:331:ARG:HH21	1:B:434:THR:CB[3_654]	1.03	0.57
1:A:393:ASN:O	6:I:5:MAN:C1[4_555]	1.65	0.55
1:A:394:ARG:C	6:I:5:MAN:O5[4_555]	1.65	0.55
1:A:391:GLN:OE1	6:I:4:MAN:H4[4_555]	1.06	0.54
1:B:331:ARG:HH21	1:B:434:THR:CG2[3_654]	1.06	0.54
1:A:394:ARG:CA	6:I:5:MAN:C1[4_555]	1.67	0.53
1:A:391:GLN:OE1	6:I:4:MAN:C4[4_555]	1.68	0.52
1:A:394:ARG:N	6:I:5:MAN:C2[4_555]	1.69	0.51
1:A:393:ASN:HD22	6:I:5:MAN:H3[4_555]	1.10	0.50
1:A:453:TYR:CD1	6:I:1:NAG:C8[4_555]	1.73	0.47
1:A:393:ASN:CB	6:I:5:MAN:C3[4_555]	1.75	0.45
1:A:394:ARG:CB	6:I:4:MAN:C2[4_555]	1.75	0.45
1:A:394:ARG:CB	6:I:4:MAN:H2[4_555]	1.16	0.44
1:A:453:TYR:OH	6:I:5:MAN:H4[4_555]	1.18	0.42
1:A:393:ASN:CA	6:I:5:MAN:C3[4_555]	1.80	0.40
1:B:331:ARG:NE	1:B:434:THR:CG2[3_654]	1.80	0.40
1:A:393:ASN:N	6:I:5:MAN:HO2[4_555]	1.24	0.36
1:A:394:ARG:H	6:I:4:MAN:O2[4_555]	1.25	0.35
1:A:394:ARG:N	6:I:5:MAN:O5[4_555]	1.86	0.34
1:A:394:ARG:CA	6:I:5:MAN:O5[4_555]	1.87	0.33
1:A:391:GLN:CB	6:I:4:MAN:H61[4_555]	1.28	0.32
1:A:393:ASN:CG	6:I:5:MAN:O3[4_555]	1.88	0.32
1:A:393:ASN:C	6:I:5:MAN:O2[4_555]	1.89	0.31
1:A:453:TYR:CE1	6:I:1:NAG:C8[4_555]	1.91	0.29
1:A:391:GLN:O	6:I:4:MAN:H62[4_555]	1.32	0.28
1:A:391:GLN:CA	6:I:4:MAN:C6[4_555]	1.93	0.27
1:A:391:GLN:C	6:I:4:MAN:O6[4_555]	1.94	0.26
1:A:393:ASN:CG	6:I:5:MAN:HO3[4_555]	1.34	0.26
1:A:394:ARG:O	6:I:5:MAN:O5[4_555]	1.98	0.22
1:A:391:GLN:OE1	6:I:4:MAN:O4[4_555]	1.99	0.21

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:393:ASN:O	6:I:5:MAN:O6[4_555]	1.99	0.21
1:A:453:TYR:CE1	6:I:1:NAG:H82[4_555]	1.39	0.21
1:A:453:TYR:CD1	6:I:1:NAG:H83[4_555]	1.39	0.21
1:A:393:ASN:O	6:I:5:MAN:HO6[4_555]	1.40	0.20
1:A:394:ARG:N	6:I:4:MAN:C2[4_555]	2.03	0.17
1:A:393:ASN:H	6:I:5:MAN:O2[4_555]	1.44	0.16
1:A:395:GLN:CG	6:I:5:MAN:H5[4_555]	1.45	0.15
1:B:331:ARG:NH2	1:B:434:THR:CA[3_654]	2.06	0.14
1:A:391:GLN:C	6:I:4:MAN:C6[4_555]	2.07	0.13
1:A:393:ASN:C	6:I:4:MAN:O2[4_555]	2.07	0.13
1:A:393:ASN:CA	6:I:5:MAN:O3[4_555]	2.07	0.13
1:B:331:ARG:HH22	1:B:434:THR:CB[3_654]	1.49	0.11
1:B:331:ARG:NH2	1:B:434:THR:C[3_654]	2.10	0.10
1:A:392:ILE:C	6:I:5:MAN:O2[4_555]	2.14	0.06
1:A:391:GLN:C	6:I:4:MAN:H62[4_555]	1.55	0.05
1:A:391:GLN:CG	6:I:4:MAN:C5[4_555]	2.18	0.02
1:A:453:TYR:OH	6:I:5:MAN:C4[4_555]	2.18	0.02
1:A:391:GLN:CD	6:I:4:MAN:C5[4_555]	2.19	0.01
1:A:393:ASN:C	6:I:5:MAN:O5[4_555]	2.19	0.01
1:A:377:PHE:CB	6:I:4:MAN:H3[4_555]	1.60	0.00

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%)	325 (84%)	53 (14%)	8 (2%)	5	7
1	B	386/388 (100%)	325 (84%)	53 (14%)	8 (2%)	5	7
All	All	772/776 (100%)	650 (84%)	106 (14%)	16 (2%)	5	7

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	322	VAL
1	A	431	LYS
1	B	322	VAL
1	B	431	LYS
1	A	345	GLY
1	A	460	ASP
1	B	345	GLY
1	B	460	ASP
1	A	226	GLN
1	B	226	GLN
1	A	219	SER
1	B	219	SER
1	A	118	ARG
1	B	118	ARG
1	A	459	PRO
1	B	459	PRO

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	338/338 (100%)	285 (84%)	53 (16%)	2	3
1	B	338/338 (100%)	285 (84%)	53 (16%)	2	3
All	All	676/676 (100%)	570 (84%)	106 (16%)	2	3

All (106) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	116	VAL
1	A	118	ARG
1	A	122	VAL
1	A	124	CYS
1	A	128	LYS
1	A	129	CYS
1	A	134	LEU
1	A	142	ASN

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Mol	Chain	Res	Type
1	A	147	ASP
1	A	148	THR
1	A	149	VAL
1	A	157	THR
1	A	165	VAL
1	A	192	VAL
1	A	195	THR
1	A	197	ASP
1	A	210	ARG
1	A	215	ILE
1	A	224	ARG
1	A	227	GLU
1	A	229	GLU
1	A	231	VAL
1	A	240	VAL
1	A	242	THR
1	A	249	ARG
1	A	253	ARG
1	A	255	LEU
1	A	257	ILE
1	A	271	SER
1	A	299	ASN
1	A	308	GLU
1	A	315	SER
1	A	322	VAL
1	A	347	GLN
1	A	349	VAL
1	A	360	LEU
1	A	365	THR
1	A	387	ASN
1	A	389	LYS
1	A	403	ARG
1	A	407	SER
1	A	412	VAL
1	A	418	ILE
1	A	426	LEU
1	A	427	ILE
1	A	428	ARG
1	A	430	ARG
1	A	431	LYS
1	A	434	THR
1	A	442	SER

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Mol	Chain	Res	Type
1	A	444	VAL
1	A	445	VAL
1	A	452	THR
1	B	116	VAL
1	B	118	ARG
1	B	122	VAL
1	B	124	CYS
1	B	128	LYS
1	B	129	CYS
1	B	134	LEU
1	B	142	ASN
1	B	147	ASP
1	B	148	THR
1	B	149	VAL
1	B	157	THR
1	B	165	VAL
1	B	192	VAL
1	B	195	THR
1	B	197	ASP
1	B	210	ARG
1	B	215	ILE
1	B	224	ARG
1	B	227	GLU
1	B	229	GLU
1	B	231	VAL
1	B	240	VAL
1	B	242	THR
1	B	249	ARG
1	B	253	ARG
1	B	255	LEU
1	B	257	ILE
1	B	271	SER
1	B	299	ASN
1	B	308	GLU
1	B	315	SER
1	B	322	VAL
1	B	347	GLN
1	B	349	VAL
1	B	360	LEU
1	B	365	THR
1	B	387	ASN
1	B	389	LYS

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Mol	Chain	Res	Type
1	B	403	ARG
1	B	407	SER
1	B	412	VAL
1	B	418	ILE
1	B	426	LEU
1	B	427	ILE
1	B	428	ARG
1	B	430	ARG
1	B	431	LYS
1	B	434	THR
1	B	442	SER
1	B	444	VAL
1	B	445	VAL
1	B	452	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	104	ASN
1	A	131	GLN
1	A	136	GLN
1	A	142	ASN
1	A	144	HIS
1	A	226	GLN
1	A	273	GLN
1	A	274	HIS
1	A	387	ASN
1	A	393	ASN
1	A	402	ASN
1	A	419	ASN
1	B	104	ASN
1	B	131	GLN
1	B	226	GLN
1	B	273	GLN
1	B	274	HIS
1	B	387	ASN
1	B	393	ASN
1	B	402	ASN
1	B	419	ASN
1	B	465	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 ⓘ

28 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	C	1	2,1	14,14,15	1.19	2 (14%)	17,19,21	2.88	7 (41%)
2	NAG	C	2	2	14,14,15	2.25	4 (28%)	17,19,21	3.28	7 (41%)
3	NAG	D	1	3,1	14,14,15	1.49	3 (21%)	17,19,21	3.47	8 (47%)
3	NAG	D	2	3	14,14,15	2.96	6 (42%)	17,19,21	2.30	6 (35%)
3	BMA	D	3	3	11,11,12	2.17	4 (36%)	15,15,17	2.55	8 (53%)
3	FUL	D	4	3	10,10,11	3.39	6 (60%)	14,14,16	2.59	4 (28%)
4	NAG	E	1	4,1	14,14,15	3.56	8 (57%)	17,19,21	3.15	8 (47%)
4	NAG	E	2	4	14,14,15	3.87	9 (64%)	17,19,21	4.15	11 (64%)
4	BMA	E	3	4	11,11,12	4.96	5 (45%)	15,15,17	3.04	10 (66%)
4	MAN	E	4	4	11,11,12	2.63	4 (36%)	15,15,17	3.22	3 (20%)
4	BMA	E	5	4	11,11,12	2.49	4 (36%)	15,15,17	2.56	7 (46%)
4	MAN	E	6	4	11,11,12	3.42	5 (45%)	15,15,17	2.92	2 (13%)
2	NAG	F	1	2,1	14,14,15	1.57	3 (21%)	17,19,21	2.99	5 (29%)
2	NAG	F	2	2	14,14,15	2.33	7 (50%)	17,19,21	1.91	4 (23%)
2	NAG	G	1	2,1	14,14,15	1.19	2 (14%)	17,19,21	2.88	7 (41%)
2	NAG	G	2	2	14,14,15	2.25	4 (28%)	17,19,21	3.28	7 (41%)
5	NAG	H	1	1,5	14,14,15	1.49	3 (21%)	17,19,21	3.47	8 (47%)
5	NAG	H	2	5	14,14,15	2.96	6 (42%)	17,19,21	2.30	6 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	BMA	H	3	5	11,11,12	2.17	4 (36%)	15,15,17	2.55	8 (53%)
5	FUC	H	4	5	10,10,11	3.39	6 (60%)	14,14,16	2.59	4 (28%)
6	NAG	I	1	6,1	14,14,15	3.56	8 (57%)	17,19,21	3.15	8 (47%)
6	NAG	I	2	6	14,14,15	3.87	9 (64%)	17,19,21	4.15	11 (64%)
6	BMA	I	3	6	11,11,12	4.96	5 (45%)	15,15,17	3.04	10 (66%)
6	MAN	I	4	6	11,11,12	2.63	4 (36%)	15,15,17	3.22	3 (20%)
6	MAN	I	5	6	11,11,12	2.49	4 (36%)	15,15,17	2.56	7 (46%)
6	MAN	I	6	6	11,11,12	3.42	5 (45%)	15,15,17	2.92	2 (13%)
2	NAG	J	1	2,1	14,14,15	1.57	3 (21%)	17,19,21	2.99	5 (29%)
2	NAG	J	2	2	14,14,15	2.33	7 (50%)	17,19,21	1.91	4 (23%)

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	C	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	C	2	2	-	3/6/23/26	0/1/1/1
3	NAG	D	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	D	2	3	-	1/6/23/26	0/1/1/1
3	BMA	D	3	3	-	1/2/19/22	0/1/1/1
3	FUL	D	4	3	-	-	0/1/1/1
4	NAG	E	1	4,1	-	3/6/23/26	0/1/1/1
4	NAG	E	2	4	-	1/6/23/26	0/1/1/1
4	BMA	E	3	4	-	1/2/19/22	1/1/1/1
4	MAN	E	4	4	-	0/2/19/22	1/1/1/1
4	BMA	E	5	4	1/1/5/5	2/2/19/22	0/1/1/1
4	MAN	E	6	4	-	0/2/19/22	0/1/1/1
2	NAG	F	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	F	2	2	-	3/6/23/26	0/1/1/1
2	NAG	G	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	G	2	2	-	3/6/23/26	0/1/1/1
5	NAG	H	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	H	2	5	-	1/6/23/26	0/1/1/1
5	BMA	H	3	5	-	1/2/19/22	0/1/1/1
5	FUC	H	4	5	1/1/5/5	-	0/1/1/1
6	NAG	I	1	6,1	-	3/6/23/26	0/1/1/1

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

All (140) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	3	BMA	C2-C3	11.72	1.70	1.52
6	I	3	BMA	C2-C3	11.72	1.70	1.52
4	E	1	NAG	C1-C2	10.90	1.67	1.52
6	I	1	NAG	C1-C2	10.90	1.67	1.52
4	E	3	BMA	O5-C1	8.92	1.58	1.43
6	I	3	BMA	O5-C1	8.92	1.58	1.43
3	D	4	FUL	C2-C3	6.59	1.62	1.52
5	H	4	FUC	C2-C3	6.59	1.62	1.52
4	E	2	NAG	C4-C3	6.56	1.69	1.52
6	I	2	NAG	C4-C3	6.56	1.69	1.52
3	D	2	NAG	C1-C2	6.43	1.61	1.52
5	H	2	NAG	C1-C2	6.43	1.61	1.52
4	E	2	NAG	C3-C2	6.19	1.65	1.52
6	I	2	NAG	C3-C2	6.19	1.65	1.52
4	E	2	NAG	C6-C5	5.99	1.71	1.51
6	I	2	NAG	C6-C5	5.99	1.71	1.51
4	E	6	MAN	C4-C5	5.77	1.65	1.53
6	I	6	MAN	C4-C5	5.77	1.65	1.53
3	D	2	NAG	C4-C5	5.59	1.64	1.53
5	H	2	NAG	C4-C5	5.59	1.64	1.53
4	E	6	MAN	O5-C5	5.50	1.54	1.43
6	I	6	MAN	O5-C5	5.50	1.54	1.43
3	D	4	FUL	C1-C2	5.49	1.65	1.52
5	H	4	FUC	C1-C2	5.49	1.65	1.52
4	E	6	MAN	C2-C3	5.33	1.60	1.52
6	I	6	MAN	C2-C3	5.33	1.60	1.52
4	E	5	BMA	C2-C3	5.29	1.60	1.52
6	I	5	MAN	C2-C3	5.29	1.60	1.52
4	E	4	MAN	C1-C2	5.21	1.64	1.52
6	I	4	MAN	C1-C2	5.21	1.64	1.52
2	C	2	NAG	C4-C3	5.14	1.65	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	2	NAG	C4-C3	5.14	1.65	1.52
2	F	2	NAG	C3-C2	5.01	1.63	1.52
2	J	2	NAG	C3-C2	5.01	1.63	1.52
4	E	2	NAG	C1-C2	5.00	1.59	1.52
6	I	2	NAG	C1-C2	5.00	1.59	1.52
3	D	2	NAG	C3-C2	4.99	1.63	1.52
5	H	2	NAG	C3-C2	4.99	1.63	1.52
2	C	2	NAG	C1-C2	4.73	1.58	1.52
2	G	2	NAG	C1-C2	4.73	1.58	1.52
4	E	2	NAG	O4-C4	4.71	1.54	1.43
6	I	2	NAG	O4-C4	4.71	1.54	1.43
3	D	3	BMA	C4-C5	4.50	1.62	1.53
5	H	3	BMA	C4-C5	4.50	1.62	1.53
4	E	4	MAN	O5-C5	4.33	1.51	1.43
6	I	4	MAN	O5-C5	4.33	1.51	1.43
4	E	3	BMA	C4-C3	4.30	1.63	1.52
6	I	3	BMA	C4-C3	4.30	1.63	1.52
4	E	3	BMA	O5-C5	4.28	1.51	1.43
6	I	3	BMA	O5-C5	4.28	1.51	1.43
3	D	3	BMA	C1-C2	4.17	1.62	1.52
5	H	3	BMA	C1-C2	4.17	1.62	1.52
4	E	6	MAN	O5-C1	3.96	1.50	1.43
6	I	6	MAN	O5-C1	3.96	1.50	1.43
4	E	5	BMA	C4-C5	3.62	1.60	1.53
6	I	5	MAN	C4-C5	3.62	1.60	1.53
3	D	4	FUL	O5-C1	3.58	1.49	1.43
5	H	4	FUC	O5-C1	3.58	1.49	1.43
4	E	1	NAG	C4-C5	3.54	1.60	1.53
6	I	1	NAG	C4-C5	3.54	1.60	1.53
2	F	1	NAG	C4-C3	3.53	1.61	1.52
2	J	1	NAG	C4-C3	3.53	1.61	1.52
4	E	2	NAG	C8-C7	3.50	1.57	1.50
6	I	2	NAG	C8-C7	3.50	1.57	1.50
4	E	4	MAN	O2-C2	3.48	1.50	1.43
6	I	4	MAN	O2-C2	3.48	1.50	1.43
4	E	3	BMA	C4-C5	3.47	1.60	1.53
6	I	3	BMA	C4-C5	3.47	1.60	1.53
4	E	6	MAN	C1-C2	3.47	1.60	1.52
6	I	6	MAN	C1-C2	3.47	1.60	1.52
3	D	4	FUL	C4-C5	3.42	1.60	1.52
5	H	4	FUC	C4-C5	3.42	1.60	1.52
4	E	1	NAG	O4-C4	3.32	1.51	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	I	1	NAG	O4-C4	3.32	1.51	1.43
4	E	5	BMA	C6-C5	3.31	1.62	1.51
6	I	5	MAN	C6-C5	3.31	1.62	1.51
4	E	2	NAG	O5-C5	3.30	1.49	1.43
6	I	2	NAG	O5-C5	3.30	1.49	1.43
4	E	2	NAG	C4-C5	3.28	1.60	1.53
6	I	2	NAG	C4-C5	3.28	1.60	1.53
4	E	1	NAG	C8-C7	3.27	1.57	1.50
6	I	1	NAG	C8-C7	3.27	1.57	1.50
2	F	2	NAG	C4-C5	3.11	1.59	1.53
2	J	2	NAG	C4-C5	3.11	1.59	1.53
2	F	2	NAG	C6-C5	3.04	1.62	1.51
2	J	2	NAG	C6-C5	3.04	1.62	1.51
2	C	2	NAG	C8-C7	2.98	1.56	1.50
2	G	2	NAG	C8-C7	2.98	1.56	1.50
2	C	1	NAG	C4-C5	2.85	1.59	1.53
2	G	1	NAG	C4-C5	2.85	1.59	1.53
4	E	5	BMA	C4-C3	2.80	1.59	1.52
6	I	5	MAN	C4-C3	2.80	1.59	1.52
2	F	2	NAG	O5-C5	2.79	1.48	1.43
2	J	2	NAG	O5-C5	2.79	1.48	1.43
2	F	1	NAG	O5-C5	-2.79	1.38	1.43
2	J	1	NAG	O5-C5	-2.79	1.38	1.43
3	D	1	NAG	C3-C2	2.76	1.58	1.52
5	H	1	NAG	C3-C2	2.76	1.58	1.52
2	F	2	NAG	C4-C3	2.72	1.59	1.52
2	J	2	NAG	C4-C3	2.72	1.59	1.52
3	D	4	FUL	C6-C5	2.71	1.58	1.51
5	H	4	FUC	C6-C5	2.71	1.58	1.51
3	D	2	NAG	C4-C3	2.66	1.59	1.52
5	H	2	NAG	C4-C3	2.66	1.59	1.52
3	D	3	BMA	C4-C3	2.61	1.59	1.52
5	H	3	BMA	C4-C3	2.61	1.59	1.52
2	F	2	NAG	C1-C2	-2.60	1.48	1.52
2	J	2	NAG	C1-C2	-2.60	1.48	1.52
3	D	1	NAG	C2-N2	2.60	1.50	1.46
5	H	1	NAG	C2-N2	2.60	1.50	1.46
4	E	4	MAN	C2-C3	2.56	1.56	1.52
6	I	4	MAN	C2-C3	2.56	1.56	1.52
3	D	2	NAG	C6-C5	2.43	1.60	1.51
5	H	2	NAG	C6-C5	2.43	1.60	1.51
3	D	3	BMA	C6-C5	2.41	1.59	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	H	3	BMA	C6-C5	2.41	1.59	1.51
3	D	4	FUL	O5-C5	2.33	1.48	1.43
5	H	4	FUC	O5-C5	2.33	1.48	1.43
2	F	1	NAG	C6-C5	2.25	1.59	1.51
2	J	1	NAG	C6-C5	2.25	1.59	1.51
3	D	2	NAG	O4-C4	2.23	1.48	1.43
5	H	2	NAG	O4-C4	2.23	1.48	1.43
4	E	1	NAG	O3-C3	-2.21	1.37	1.43
6	I	1	NAG	O3-C3	-2.21	1.37	1.43
2	C	2	NAG	C3-C2	2.20	1.57	1.52
2	G	2	NAG	C3-C2	2.20	1.57	1.52
3	D	1	NAG	C4-C3	2.16	1.57	1.52
5	H	1	NAG	C4-C3	2.16	1.57	1.52
4	E	1	NAG	O5-C1	2.15	1.47	1.43
6	I	1	NAG	O5-C1	2.15	1.47	1.43
4	E	2	NAG	C2-N2	2.13	1.49	1.46
6	I	2	NAG	C2-N2	2.13	1.49	1.46
2	F	2	NAG	C8-C7	2.13	1.55	1.50
2	J	2	NAG	C8-C7	2.13	1.55	1.50
2	C	1	NAG	C1-C2	2.10	1.55	1.52
2	G	1	NAG	C1-C2	2.10	1.55	1.52
4	E	1	NAG	C6-C5	2.09	1.58	1.51
6	I	1	NAG	C6-C5	2.09	1.58	1.51
4	E	1	NAG	C2-N2	2.06	1.49	1.46
6	I	1	NAG	C2-N2	2.06	1.49	1.46

All (180) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1	NAG	C2-N2-C7	10.22	136.59	122.90
5	H	1	NAG	C2-N2-C7	10.22	136.59	122.90
4	E	2	NAG	C1-O5-C5	10.17	125.81	112.19
6	I	2	NAG	C1-O5-C5	10.17	125.81	112.19
4	E	6	MAN	C1-O5-C5	9.49	124.91	112.19
6	I	6	MAN	C1-O5-C5	9.49	124.91	112.19
4	E	4	MAN	C1-O5-C5	8.77	123.94	112.19
6	I	4	MAN	C1-O5-C5	8.77	123.94	112.19
2	F	1	NAG	C1-O5-C5	8.45	123.52	112.19
2	J	1	NAG	C1-O5-C5	8.45	123.52	112.19
4	E	2	NAG	O4-C4-C3	8.33	130.00	110.38
6	I	2	NAG	O4-C4-C3	8.33	130.00	110.38
4	E	1	NAG	C1-C2-N2	8.16	123.30	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	I	1	NAG	C1-C2-N2	8.16	123.30	110.43
2	C	2	NAG	O5-C1-C2	8.07	123.77	111.29
2	G	2	NAG	O5-C1-C2	8.07	123.77	111.29
2	C	1	NAG	C1-O5-C5	7.81	122.65	112.19
2	G	1	NAG	C1-O5-C5	7.81	122.65	112.19
4	E	4	MAN	O2-C2-C1	7.62	126.66	109.22
6	I	4	MAN	O2-C2-C1	7.62	126.66	109.22
4	E	2	NAG	C2-N2-C7	7.61	133.10	122.90
6	I	2	NAG	C2-N2-C7	7.61	133.10	122.90
2	C	2	NAG	C1-O5-C5	6.52	120.93	112.19
2	G	2	NAG	C1-O5-C5	6.52	120.93	112.19
3	D	4	FUL	C6-C5-C4	6.36	124.72	113.08
5	H	4	FUC	C6-C5-C4	6.36	124.72	113.08
3	D	3	BMA	C1-O5-C5	6.27	120.59	112.19
5	H	3	BMA	C1-O5-C5	6.27	120.59	112.19
4	E	1	NAG	C1-O5-C5	5.95	120.16	112.19
6	I	1	NAG	C1-O5-C5	5.95	120.16	112.19
4	E	3	BMA	C3-C4-C5	-5.91	99.51	110.23
6	I	3	BMA	C3-C4-C5	-5.91	99.51	110.23
2	F	1	NAG	C6-C5-C4	5.87	127.44	113.02
2	J	1	NAG	C6-C5-C4	5.87	127.44	113.02
3	D	2	NAG	C1-O5-C5	5.67	119.79	112.19
5	H	2	NAG	C1-O5-C5	5.67	119.79	112.19
3	D	1	NAG	C1-O5-C5	5.44	119.48	112.19
5	H	1	NAG	C1-O5-C5	5.44	119.48	112.19
2	C	2	NAG	C6-C5-C4	5.28	125.97	113.02
2	G	2	NAG	C6-C5-C4	5.28	125.97	113.02
4	E	5	BMA	C6-C5-C4	5.25	125.90	113.02
6	I	5	MAN	C6-C5-C4	5.25	125.90	113.02
3	D	4	FUL	C1-C2-C3	4.76	116.57	109.64
5	H	4	FUC	C1-C2-C3	4.76	116.57	109.64
2	C	1	NAG	O4-C4-C3	-4.70	99.29	110.38
2	G	1	NAG	O4-C4-C3	-4.70	99.29	110.38
2	C	1	NAG	C3-C4-C5	4.53	118.44	110.23
2	G	1	NAG	C3-C4-C5	4.53	118.44	110.23
2	F	2	NAG	C1-C2-N2	-4.52	103.31	110.43
2	J	2	NAG	C1-C2-N2	-4.52	103.31	110.43
2	F	1	NAG	O3-C3-C2	-4.24	100.60	109.40
2	J	1	NAG	O3-C3-C2	-4.24	100.60	109.40
3	D	1	NAG	C6-C5-C4	4.14	123.17	113.02
5	H	1	NAG	C6-C5-C4	4.14	123.17	113.02
4	E	5	BMA	C1-O5-C5	4.03	117.59	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	I	5	MAN	C1-O5-C5	4.03	117.59	112.19
4	E	5	BMA	C2-C3-C4	-3.98	103.85	110.86
6	I	5	MAN	C2-C3-C4	-3.98	103.85	110.86
4	E	3	BMA	O5-C5-C6	3.97	115.39	107.66
6	I	3	BMA	O5-C5-C6	3.97	115.39	107.66
4	E	6	MAN	O3-C3-C2	3.96	118.14	110.05
6	I	6	MAN	O3-C3-C2	3.96	118.14	110.05
4	E	3	BMA	O2-C2-C3	3.94	118.30	110.15
6	I	3	BMA	O2-C2-C3	3.94	118.30	110.15
4	E	1	NAG	C2-N2-C7	3.85	128.06	122.90
6	I	1	NAG	C2-N2-C7	3.85	128.06	122.90
2	F	2	NAG	O3-C3-C2	3.80	117.29	109.40
2	J	2	NAG	O3-C3-C2	3.80	117.29	109.40
4	E	5	BMA	O5-C5-C4	-3.76	101.69	110.83
6	I	5	MAN	O5-C5-C4	-3.76	101.69	110.83
2	C	2	NAG	O5-C5-C4	-3.67	101.91	110.83
2	G	2	NAG	O5-C5-C4	-3.67	101.91	110.83
4	E	3	BMA	O4-C4-C5	3.66	118.34	109.32
6	I	3	BMA	O4-C4-C5	3.66	118.34	109.32
3	D	2	NAG	O3-C3-C2	3.54	116.75	109.40
5	H	2	NAG	O3-C3-C2	3.54	116.75	109.40
4	E	4	MAN	C1-C2-C3	-3.52	104.51	109.64
6	I	4	MAN	C1-C2-C3	-3.52	104.51	109.64
4	E	1	NAG	C6-C5-C4	3.42	121.42	113.02
6	I	1	NAG	C6-C5-C4	3.42	121.42	113.02
4	E	3	BMA	O3-C3-C2	3.33	116.84	110.05
6	I	3	BMA	O3-C3-C2	3.33	116.84	110.05
4	E	3	BMA	C1-C2-C3	-3.29	104.85	109.64
6	I	3	BMA	C1-C2-C3	-3.29	104.85	109.64
4	E	2	NAG	C6-C5-C4	3.29	121.10	113.02
6	I	2	NAG	C6-C5-C4	3.29	121.10	113.02
4	E	3	BMA	O4-C4-C3	3.26	118.06	110.38
6	I	3	BMA	O4-C4-C3	3.26	118.06	110.38
3	D	1	NAG	O7-C7-C8	-3.19	116.37	122.05
5	H	1	NAG	O7-C7-C8	-3.19	116.37	122.05
3	D	3	BMA	C1-C2-C3	3.19	114.29	109.64
5	H	3	BMA	C1-C2-C3	3.19	114.29	109.64
3	D	1	NAG	C1-C2-N2	3.16	115.41	110.43
5	H	1	NAG	C1-C2-N2	3.16	115.41	110.43
4	E	3	BMA	O5-C5-C4	-3.12	103.23	110.83
6	I	3	BMA	O5-C5-C4	-3.12	103.23	110.83
3	D	3	BMA	O2-C2-C3	-3.10	103.73	110.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	H	3	BMA	O2-C2-C3	-3.10	103.73	110.15
3	D	1	NAG	O3-C3-C2	3.09	115.81	109.40
5	H	1	NAG	O3-C3-C2	3.09	115.81	109.40
3	D	4	FUL	O5-C5-C4	-3.03	104.09	109.55
5	H	4	FUC	O5-C5-C4	-3.03	104.09	109.55
2	C	2	NAG	O3-C3-C2	-3.01	103.14	109.40
2	G	2	NAG	O3-C3-C2	-3.01	103.14	109.40
2	F	2	NAG	C3-C4-C5	3.00	115.67	110.23
2	J	2	NAG	C3-C4-C5	3.00	115.67	110.23
4	E	1	NAG	C4-C3-C2	2.98	115.39	111.02
6	I	1	NAG	C4-C3-C2	2.98	115.39	111.02
3	D	2	NAG	C4-C3-C2	-2.97	106.66	111.02
5	H	2	NAG	C4-C3-C2	-2.97	106.66	111.02
2	C	1	NAG	C2-N2-C7	2.95	126.85	122.90
2	G	1	NAG	C2-N2-C7	2.95	126.85	122.90
4	E	2	NAG	O3-C3-C2	2.87	115.36	109.40
6	I	2	NAG	O3-C3-C2	2.87	115.36	109.40
4	E	2	NAG	O6-C6-C5	2.85	121.05	111.33
6	I	2	NAG	O6-C6-C5	2.85	121.05	111.33
3	D	3	BMA	C6-C5-C4	2.85	120.01	113.02
5	H	3	BMA	C6-C5-C4	2.85	120.01	113.02
4	E	2	NAG	O5-C5-C4	-2.84	103.93	110.83
6	I	2	NAG	O5-C5-C4	-2.84	103.93	110.83
4	E	2	NAG	C4-C3-C2	-2.79	106.93	111.02
6	I	2	NAG	C4-C3-C2	-2.79	106.93	111.02
2	F	1	NAG	C2-N2-C7	2.78	126.63	122.90
2	J	1	NAG	C2-N2-C7	2.78	126.63	122.90
4	E	1	NAG	O7-C7-C8	-2.73	117.19	122.05
6	I	1	NAG	O7-C7-C8	-2.73	117.19	122.05
3	D	3	BMA	O5-C5-C6	-2.70	102.40	107.66
5	H	3	BMA	O5-C5-C6	-2.70	102.40	107.66
3	D	3	BMA	O2-C2-C1	2.65	115.29	109.22
5	H	3	BMA	O2-C2-C1	2.65	115.29	109.22
3	D	3	BMA	C3-C4-C5	2.64	115.03	110.23
5	H	3	BMA	C3-C4-C5	2.64	115.03	110.23
4	E	5	BMA	C3-C4-C5	2.61	114.96	110.23
6	I	5	MAN	C3-C4-C5	2.61	114.96	110.23
3	D	1	NAG	C8-C7-N2	2.60	120.43	116.12
5	H	1	NAG	C8-C7-N2	2.60	120.43	116.12
2	C	1	NAG	O3-C3-C2	2.58	114.76	109.40
2	G	1	NAG	O3-C3-C2	2.58	114.76	109.40
3	D	2	NAG	C3-C4-C5	-2.52	105.66	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	H	2	NAG	C3-C4-C5	-2.52	105.66	110.23
4	E	2	NAG	O5-C5-C6	2.52	112.57	107.66
6	I	2	NAG	O5-C5-C6	2.52	112.57	107.66
4	E	2	NAG	O4-C4-C5	-2.49	103.19	109.32
6	I	2	NAG	O4-C4-C5	-2.49	103.19	109.32
3	D	2	NAG	O4-C4-C3	2.48	116.22	110.38
5	H	2	NAG	O4-C4-C3	2.48	116.22	110.38
3	D	1	NAG	O5-C5-C4	-2.45	104.88	110.83
5	H	1	NAG	O5-C5-C4	-2.45	104.88	110.83
3	D	3	BMA	O4-C4-C3	-2.44	104.62	110.38
5	H	3	BMA	O4-C4-C3	-2.44	104.62	110.38
3	D	4	FUL	O2-C2-C3	-2.41	105.15	110.15
5	H	4	FUC	O2-C2-C3	-2.41	105.15	110.15
4	E	1	NAG	O4-C4-C3	-2.39	104.75	110.38
6	I	1	NAG	O4-C4-C3	-2.39	104.75	110.38
4	E	5	BMA	O3-C3-C4	2.35	115.91	110.38
6	I	5	MAN	O3-C3-C4	2.35	115.91	110.38
2	C	2	NAG	O4-C4-C5	-2.28	103.72	109.32
2	G	2	NAG	O4-C4-C5	-2.28	103.72	109.32
4	E	2	NAG	C1-C2-N2	2.25	113.98	110.43
6	I	2	NAG	C1-C2-N2	2.25	113.98	110.43
4	E	3	BMA	C1-O5-C5	2.25	115.20	112.19
6	I	3	BMA	C1-O5-C5	2.25	115.20	112.19
3	D	2	NAG	O7-C7-C8	-2.25	118.05	122.05
5	H	2	NAG	O7-C7-C8	-2.25	118.05	122.05
2	C	2	NAG	C1-C2-N2	-2.23	106.92	110.43
2	G	2	NAG	C1-C2-N2	-2.23	106.92	110.43
4	E	1	NAG	C8-C7-N2	2.22	119.79	116.12
6	I	1	NAG	C8-C7-N2	2.22	119.79	116.12
2	F	2	NAG	C6-C5-C4	2.20	118.41	113.02
2	J	2	NAG	C6-C5-C4	2.20	118.41	113.02
4	E	3	BMA	O3-C3-C4	-2.10	105.43	110.38
6	I	3	BMA	O3-C3-C4	-2.10	105.43	110.38
2	C	1	NAG	O3-C3-C4	-2.09	105.45	110.38
2	G	1	NAG	O3-C3-C4	-2.09	105.45	110.38
2	C	1	NAG	C8-C7-N2	-2.05	112.71	116.12
2	G	1	NAG	C8-C7-N2	-2.05	112.71	116.12
4	E	5	BMA	O3-C3-C2	2.03	114.19	110.05
6	I	5	MAN	O3-C3-C2	2.03	114.19	110.05
2	F	1	NAG	O5-C5-C4	-2.02	105.92	110.83
2	J	1	NAG	O5-C5-C4	-2.02	105.92	110.83

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	E	5	BMA	C1
5	H	4	FUC	C1

All (42) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	2	NAG	C3-C2-N2-C7
2	F	2	NAG	C3-C2-N2-C7
2	G	2	NAG	C3-C2-N2-C7
2	J	2	NAG	C3-C2-N2-C7
4	E	1	NAG	C3-C2-N2-C7
4	E	2	NAG	C3-C2-N2-C7
6	I	1	NAG	C3-C2-N2-C7
6	I	2	NAG	C3-C2-N2-C7
2	C	1	NAG	C4-C5-C6-O6
2	G	1	NAG	C4-C5-C6-O6
2	C	1	NAG	O5-C5-C6-O6
2	G	1	NAG	O5-C5-C6-O6
3	D	1	NAG	O5-C5-C6-O6
5	H	1	NAG	O5-C5-C6-O6
2	F	1	NAG	C4-C5-C6-O6
2	J	1	NAG	C4-C5-C6-O6
2	C	2	NAG	O5-C5-C6-O6
2	G	2	NAG	O5-C5-C6-O6
2	F	1	NAG	O5-C5-C6-O6
2	J	1	NAG	O5-C5-C6-O6
2	C	2	NAG	C4-C5-C6-O6
2	G	2	NAG	C4-C5-C6-O6
3	D	1	NAG	C4-C5-C6-O6
5	H	1	NAG	C4-C5-C6-O6
4	E	1	NAG	C4-C5-C6-O6
6	I	1	NAG	C4-C5-C6-O6
2	F	2	NAG	O5-C5-C6-O6
2	J	2	NAG	O5-C5-C6-O6
3	D	3	BMA	O5-C5-C6-O6
5	H	3	BMA	O5-C5-C6-O6
3	D	2	NAG	O5-C5-C6-O6
5	H	2	NAG	O5-C5-C6-O6
4	E	1	NAG	O5-C5-C6-O6
6	I	1	NAG	O5-C5-C6-O6
4	E	5	BMA	C4-C5-C6-O6
6	I	5	MAN	C4-C5-C6-O6
4	E	3	BMA	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
6	I	3	BMA	O5-C5-C6-O6
4	E	5	BMA	O5-C5-C6-O6
6	I	5	MAN	O5-C5-C6-O6
2	F	2	NAG	C4-C5-C6-O6
2	J	2	NAG	C4-C5-C6-O6

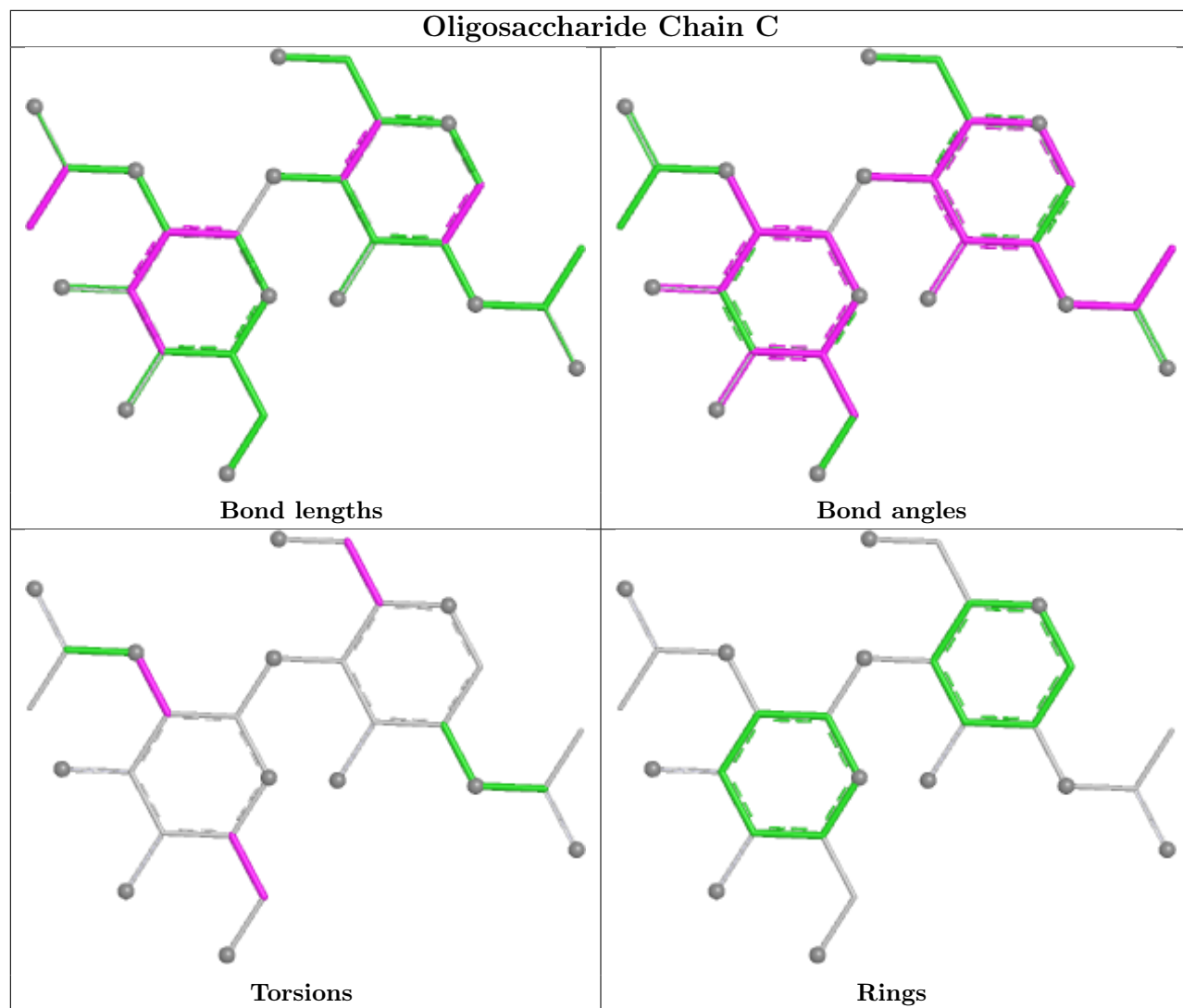
All (4) ring outliers are listed below:

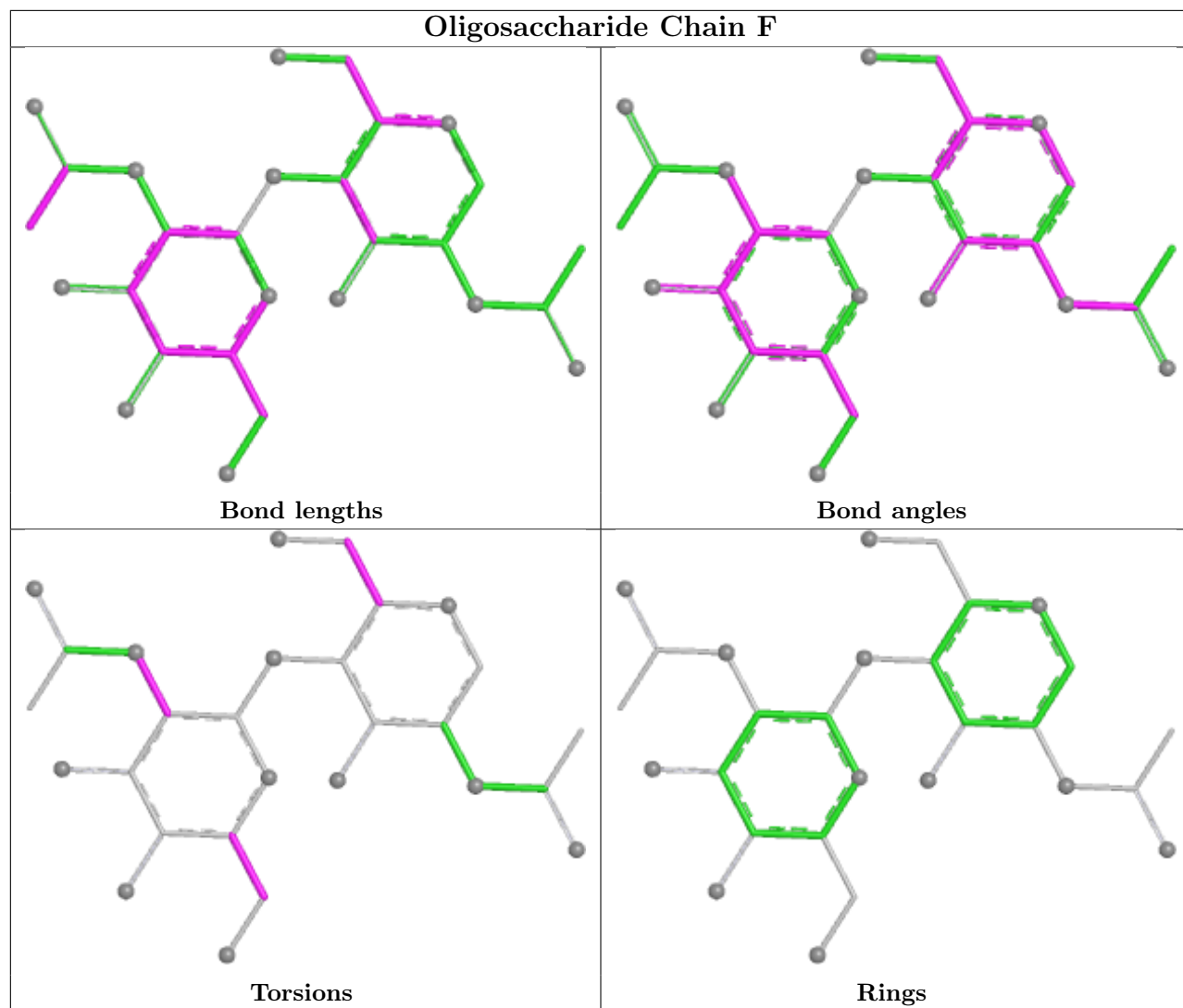
Mol	Chain	Res	Type	Atoms
4	E	4	MAN	C1-C2-C3-C4-C5-O5
6	I	4	MAN	C1-C2-C3-C4-C5-O5
4	E	3	BMA	C1-C2-C3-C4-C5-O5
6	I	3	BMA	C1-C2-C3-C4-C5-O5

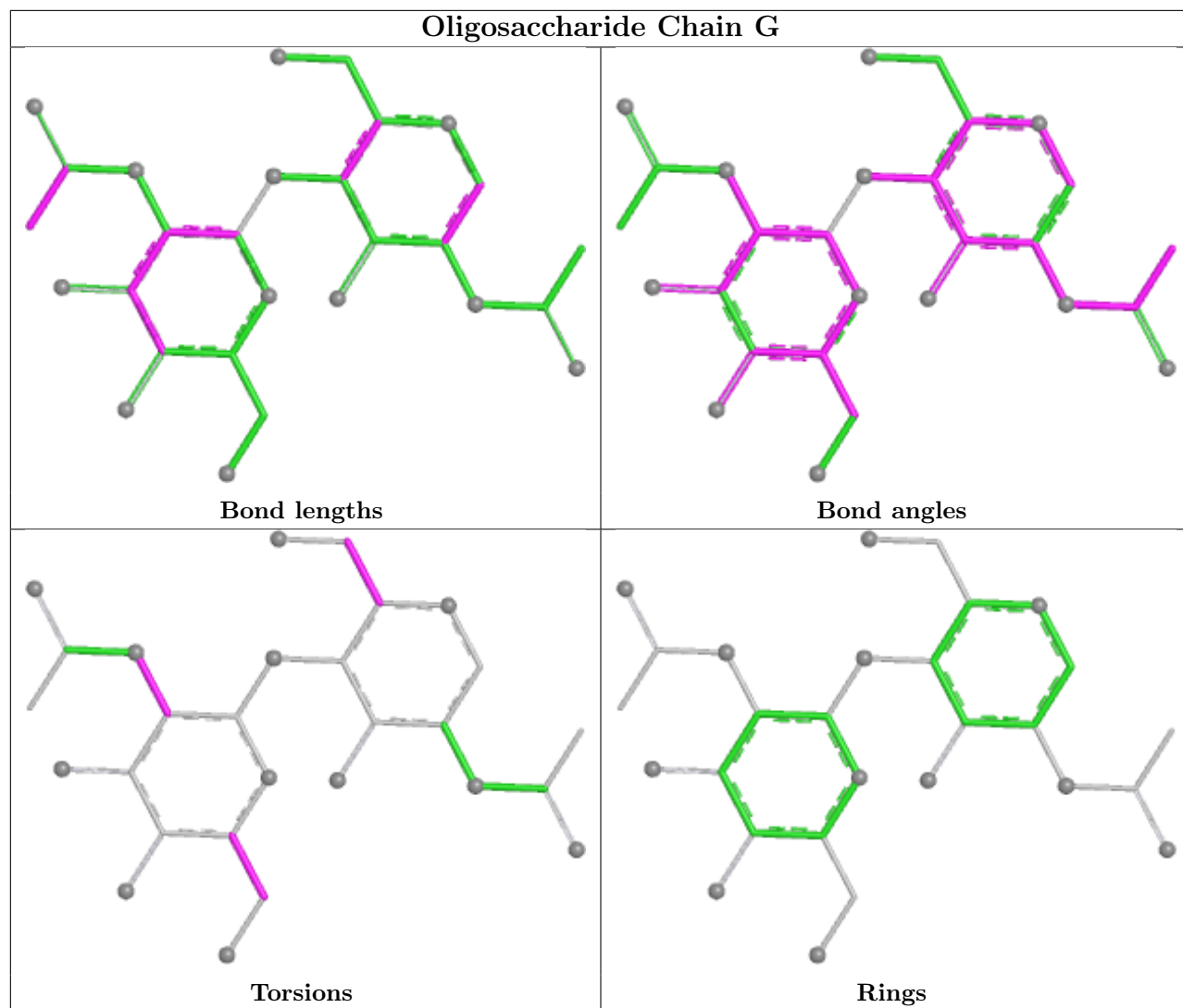
16 monomers are involved in 113 short contacts:

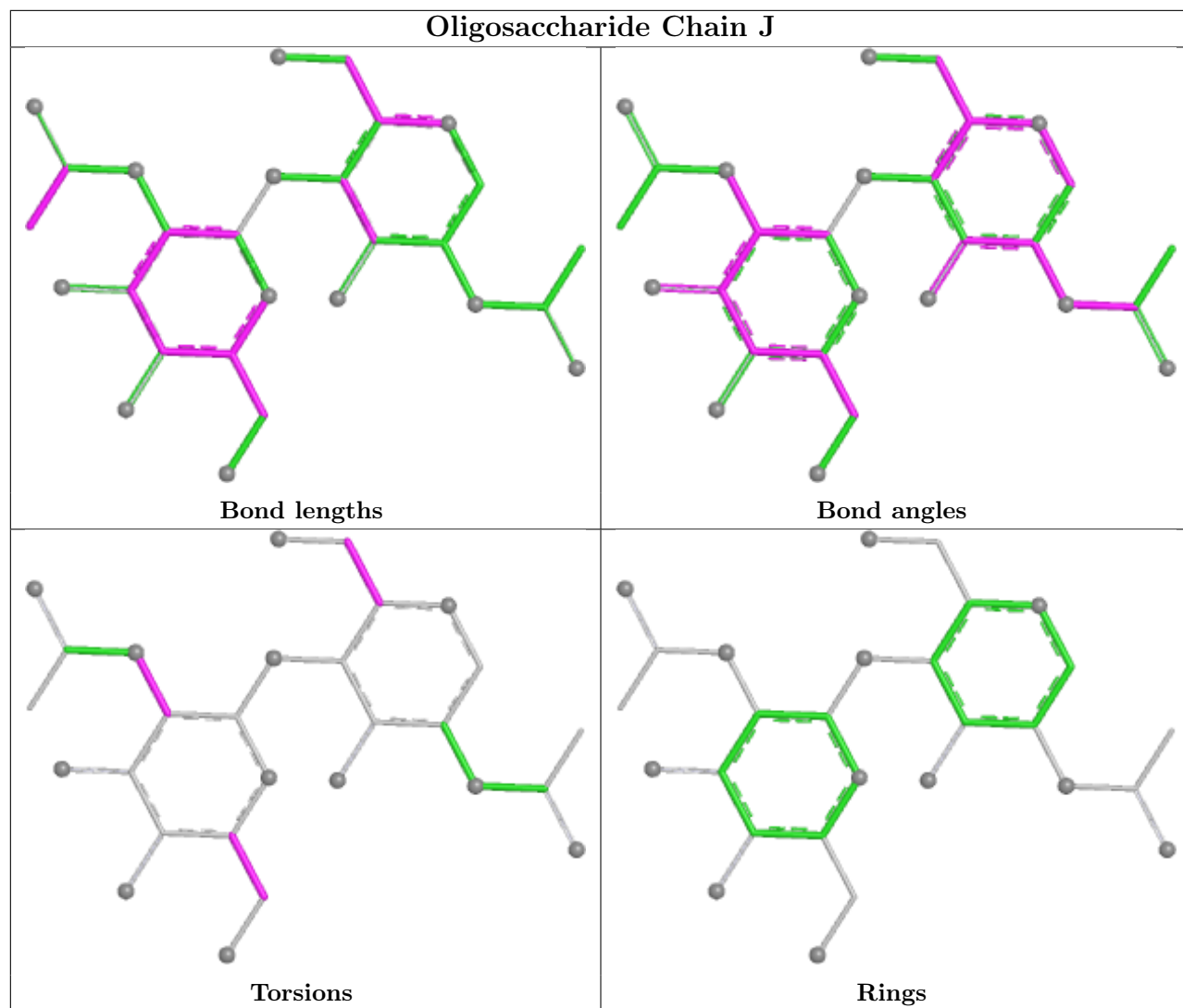
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	I	5	MAN	0	34
4	E	5	BMA	18	0
5	H	3	BMA	1	0
4	E	4	MAN	15	0
6	I	6	MAN	3	0
4	E	3	BMA	3	0
3	D	3	BMA	1	0
4	E	6	MAN	4	0
6	I	4	MAN	0	25
6	I	1	NAG	4	4
4	E	2	NAG	2	0
4	E	1	NAG	5	0
3	D	2	NAG	1	0
6	I	3	BMA	2	0
5	H	2	NAG	1	0
6	I	2	NAG	2	0

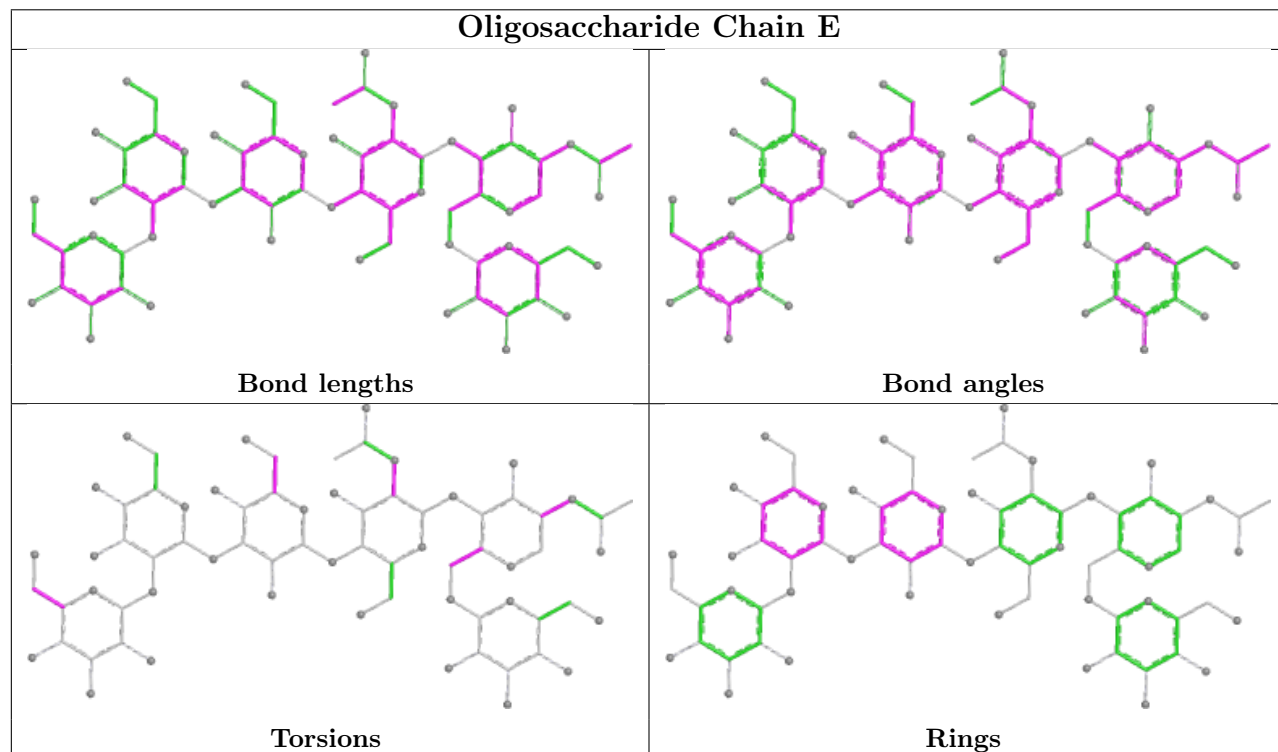
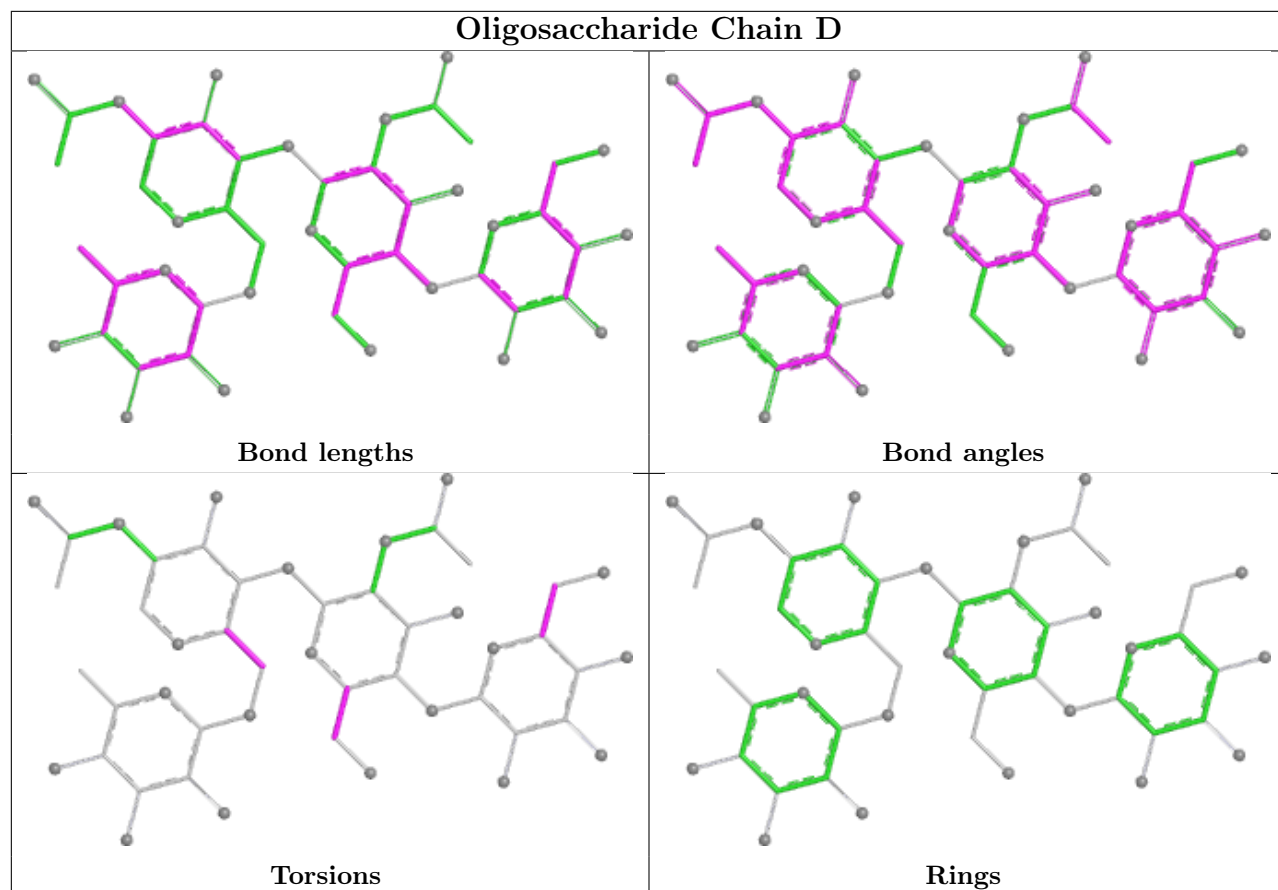
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

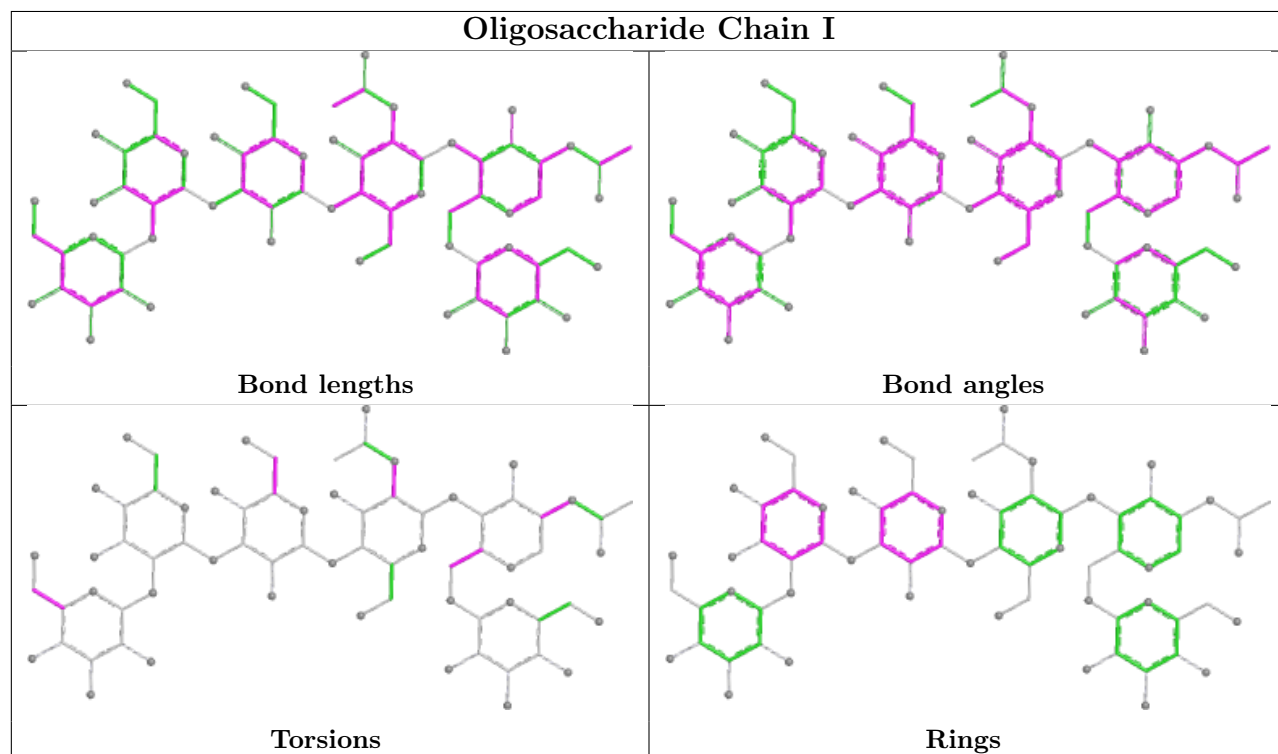
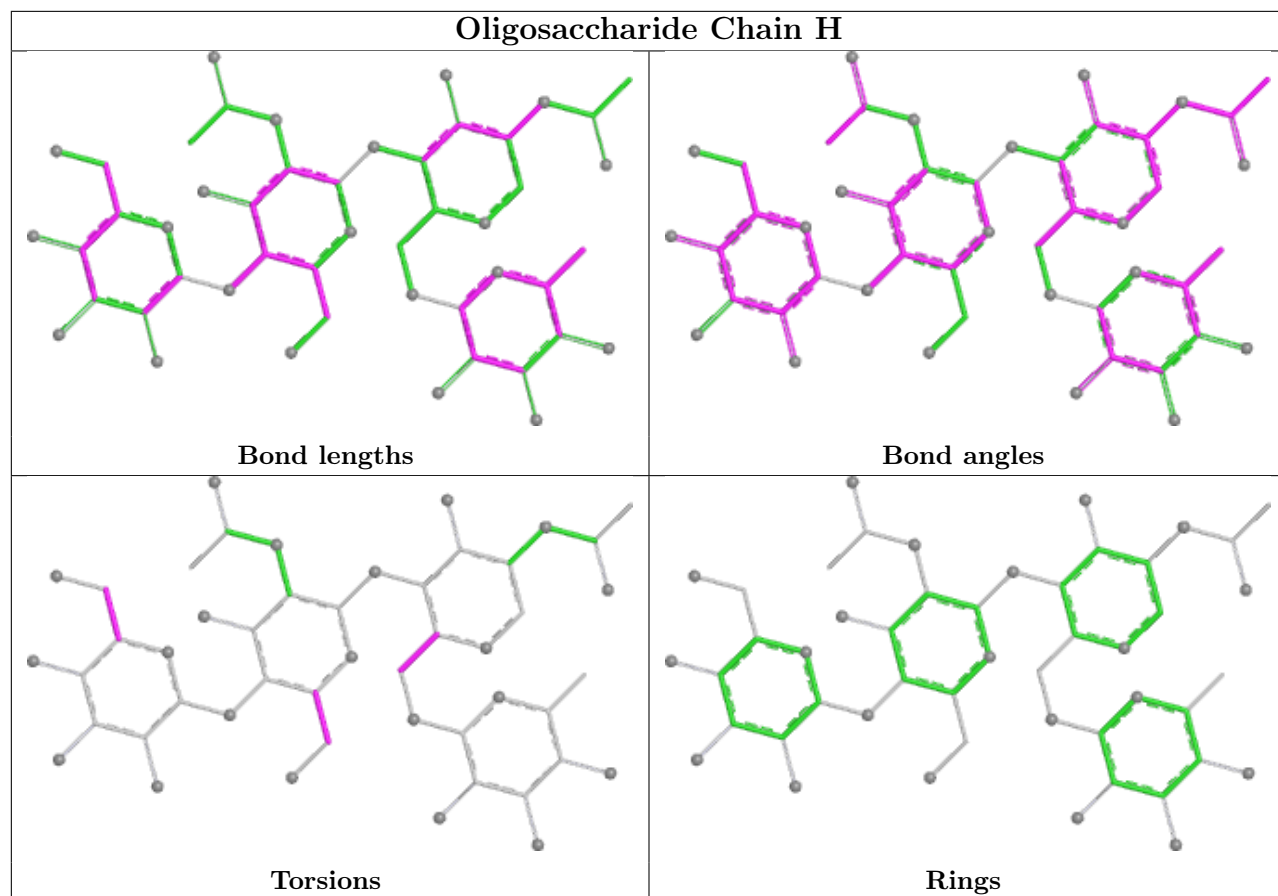












5.6 Ligand geometry

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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
8	ST6	B	489	-	17,18,18	1.74	2 (11%)	22,24,24	1.27	4 (18%)
8	ST6	A	471	-	17,18,18	1.74	2 (11%)	22,24,24	1.27	4 (18%)

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
8	ST6	B	489	-	-	8/14/14/14	0/1/1/1
8	ST6	A	471	-	-	8/14/14/14	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	471	ST6	C1-C'	-5.17	1.38	1.49
8	B	489	ST6	C1-C'	-5.17	1.38	1.49
8	A	471	ST6	C3-N3	-2.76	1.36	1.41
8	B	489	ST6	C3-N3	-2.76	1.36	1.41

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	471	ST6	C3-N3-C3'	-3.02	116.47	126.61
8	B	489	ST6	C3-N3-C3'	-3.02	116.47	126.61
8	A	471	ST6	CM4-C4'-N4	2.59	118.85	114.95
8	B	489	ST6	CM4-C4'-N4	2.59	118.85	114.95
8	A	471	ST6	C4-N4-C4'	-2.37	121.78	127.50
8	B	489	ST6	C4-N4-C4'	-2.37	121.78	127.50
8	A	471	ST6	CM3-C3'-N3	2.13	117.96	114.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	489	ST6	CM3-C3'-N3	2.13	117.96	114.32

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	471	ST6	O1'-C'-C1-C6
8	B	489	ST6	O1'-C'-C1-C6
8	A	471	ST6	O2'-C'-C1-C6
8	B	489	ST6	O2'-C'-C1-C6
8	A	471	ST6	O2'-C'-C1-C2
8	B	489	ST6	O2'-C'-C1-C2
8	A	471	ST6	O1'-C'-C1-C2
8	B	489	ST6	O1'-C'-C1-C2
8	A	471	ST6	C3-C4-N4-C4'
8	B	489	ST6	C3-C4-N4-C4'
8	A	471	ST6	C5-C4-N4-C4'
8	B	489	ST6	C5-C4-N4-C4'
8	A	471	ST6	C2-C3-N3-C3'
8	B	489	ST6	C2-C3-N3-C3'
8	A	471	ST6	C4-C3-N3-C3'
8	B	489	ST6	C4-C3-N3-C3'

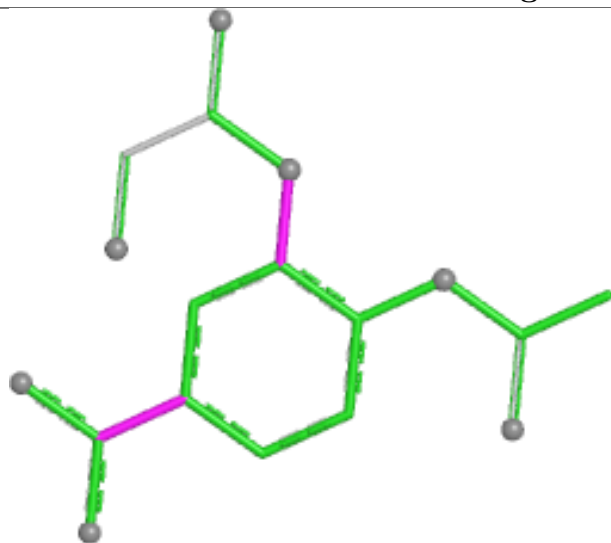
There are no ring outliers.

2 monomers are involved in 2 short contacts:

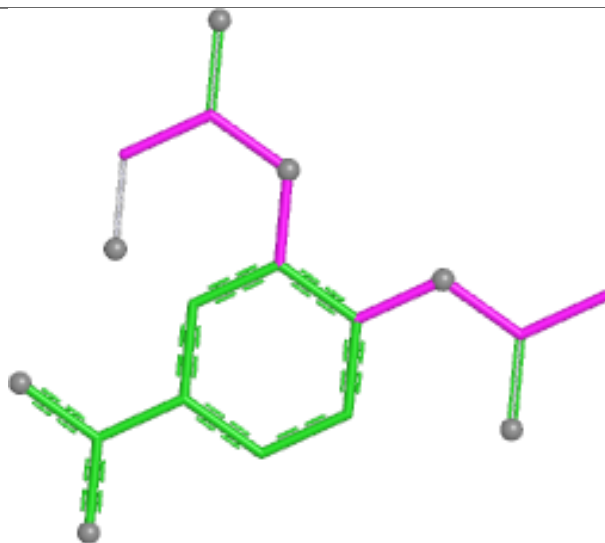
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	B	489	ST6	1	0
8	A	471	ST6	1	0

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.

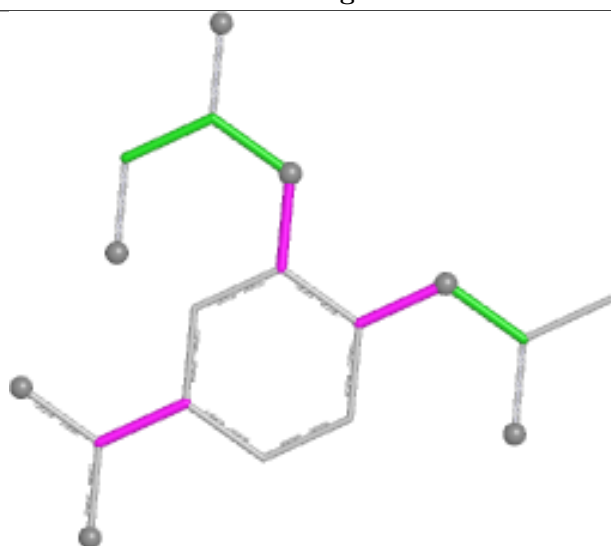
Ligand ST6 B 489



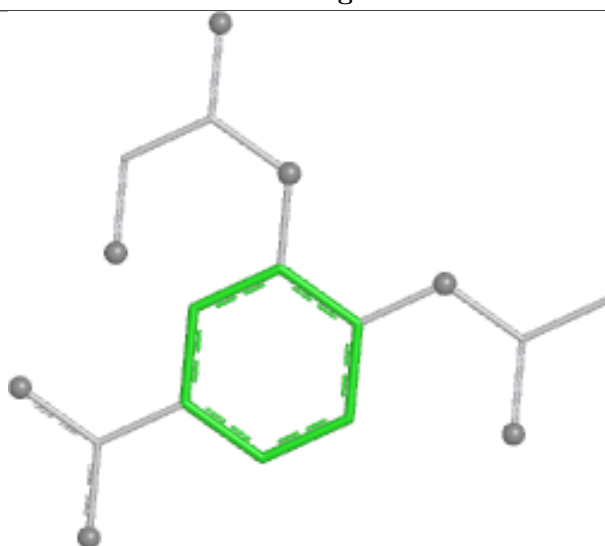
Bond lengths



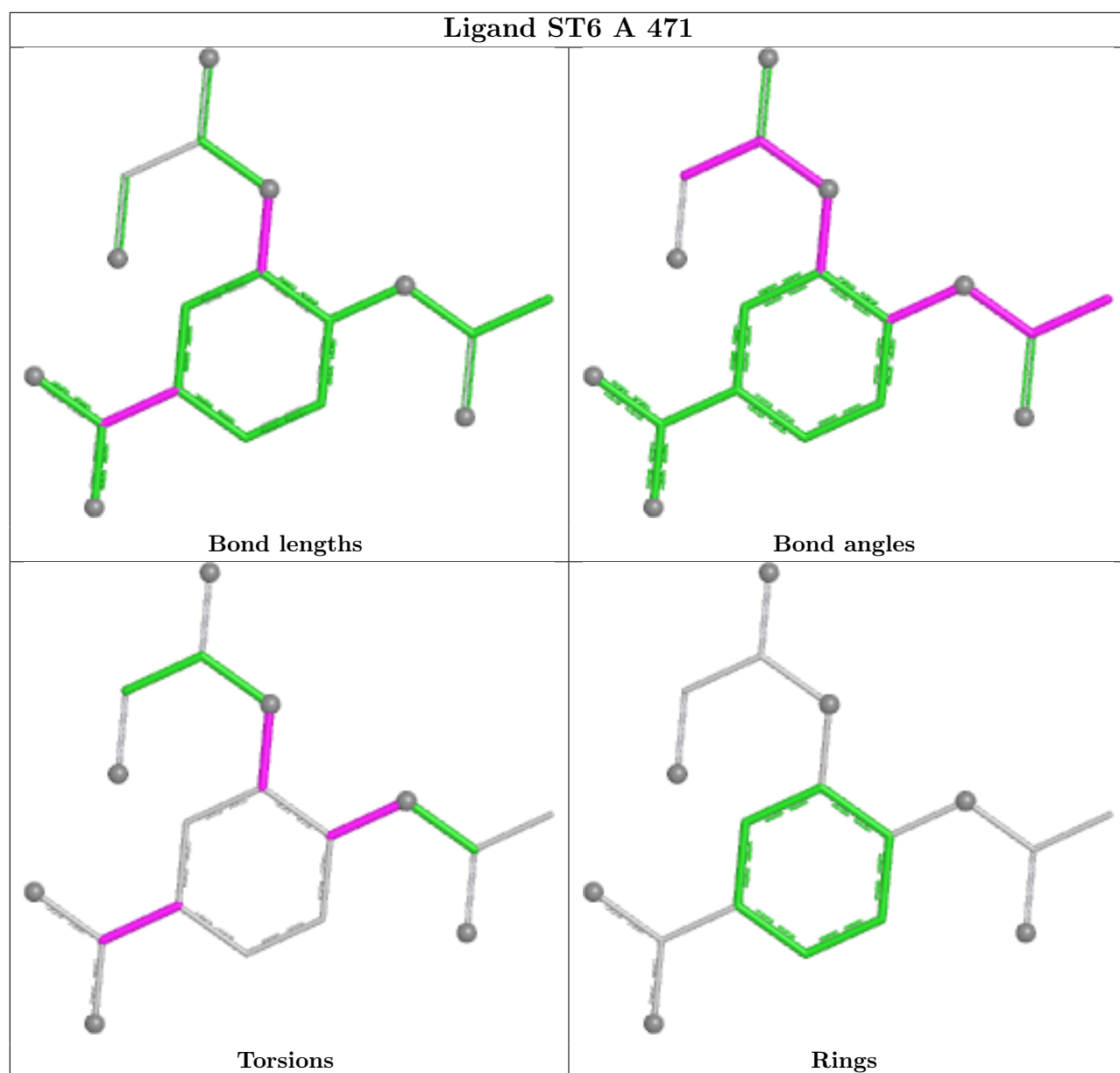
Bond angles



Torsions



Rings



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	388/388 (100%)	-0.56	1 (0%) 90 88	3, 9, 23, 32	0
1	B	388/388 (100%)	-0.54	0 100 100	3, 9, 23, 32	0
All	All	776/776 (100%)	-0.55	1 (0%) 92 90	3, 9, 23, 32	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	347	GLN	2.1

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

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

6.3 Carbohydrates [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	NAG	H	2	14/15	0.66	0.14	15,15,42,42	14
6	MAN	I	6	11/12	0.75	0.12	15,15,25,30	11
2	NAG	J	2	14/15	0.76	0.13	15,15,35,36	14
3	FUL	D	4	10/11	0.77	0.12	15,15,29,30	10
5	NAG	H	1	14/15	0.77	0.11	15,25,32,35	0
2	NAG	G	2	14/15	0.77	0.15	15,15,34,36	14
3	NAG	D	2	14/15	0.77	0.11	15,15,42,42	14
4	MAN	E	6	11/12	0.78	0.15	15,15,25,30	11

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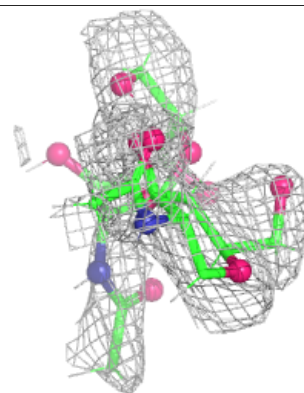
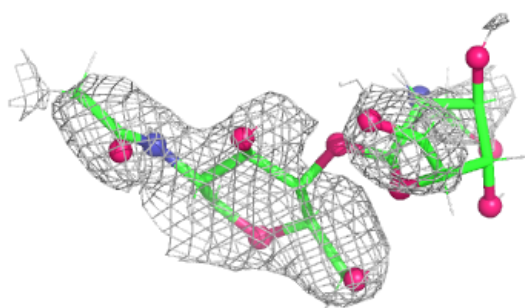
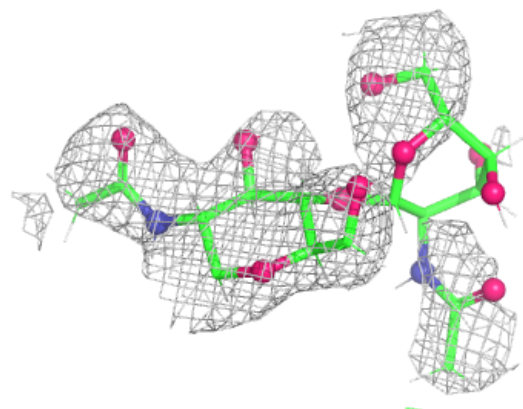
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NAG	F	2	14/15	0.78	0.13	15,15,35,36	14
5	FUC	H	4	10/11	0.80	0.13	15,15,29,30	10
5	BMA	H	3	11/12	0.81	0.17	15,15,45,46	11
2	NAG	C	2	14/15	0.83	0.14	15,15,34,36	14
2	NAG	F	1	14/15	0.84	0.12	15,15,34,36	0
2	NAG	J	1	14/15	0.85	0.12	15,15,34,36	0
6	BMA	I	3	11/12	0.85	0.14	4,15,19,21	0
4	BMA	E	3	11/12	0.85	0.13	4,15,19,21	0
2	NAG	G	1	14/15	0.86	0.11	15,15,20,21	14
4	NAG	E	1	14/15	0.86	0.10	13,15,22,26	0
6	NAG	I	1	14/15	0.87	0.08	13,15,22,26	0
3	BMA	D	3	11/12	0.88	0.10	15,15,45,46	11
3	NAG	D	1	14/15	0.88	0.07	15,25,32,35	0
4	NAG	E	2	14/15	0.90	0.13	2,15,23,25	0
2	NAG	C	1	14/15	0.93	0.07	15,15,20,21	14
6	NAG	I	2	14/15	0.93	0.11	2,15,23,25	0
4	MAN	E	4	11/12	0.96	0.12	2,11,15,15	0
6	MAN	I	5	11/12	0.97	0.08	2,13,15,15	0
4	BMA	E	5	11/12	0.97	0.08	2,13,15,15	0
6	MAN	I	4	11/12	0.99	0.07	2,11,15,15	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.

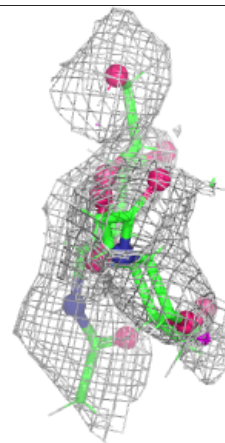
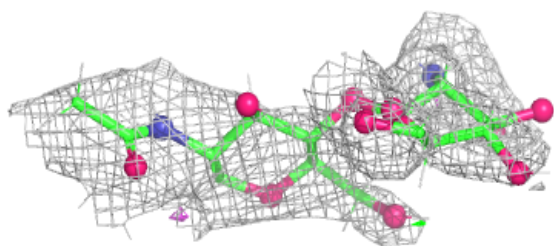
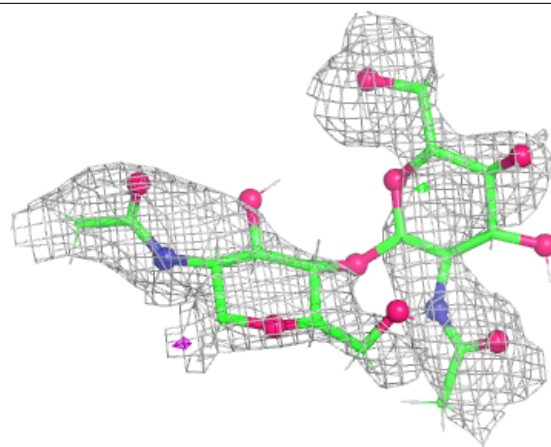
Electron density around Chain C:

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



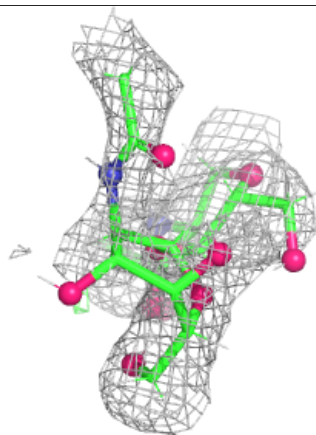
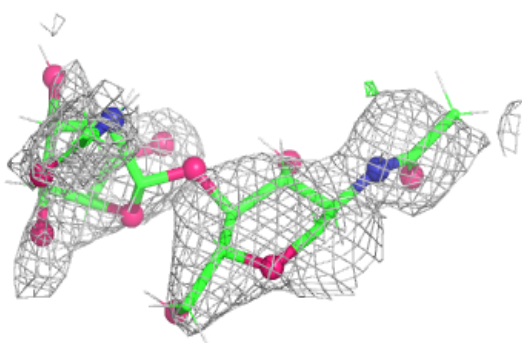
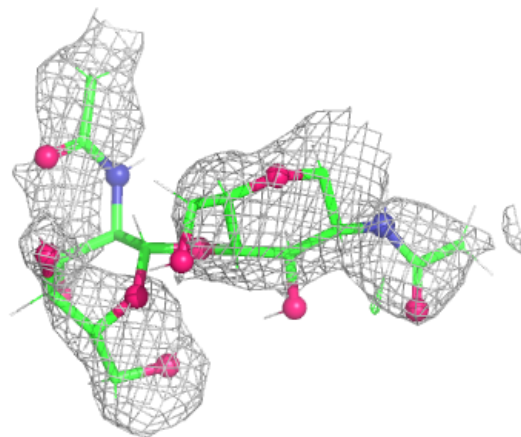
Electron density around Chain F:

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



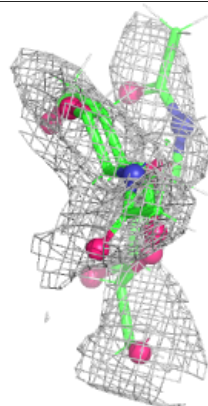
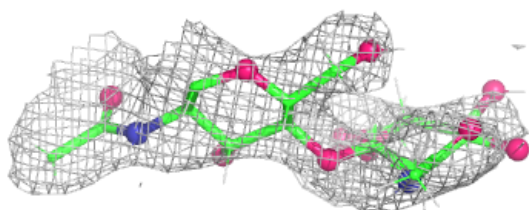
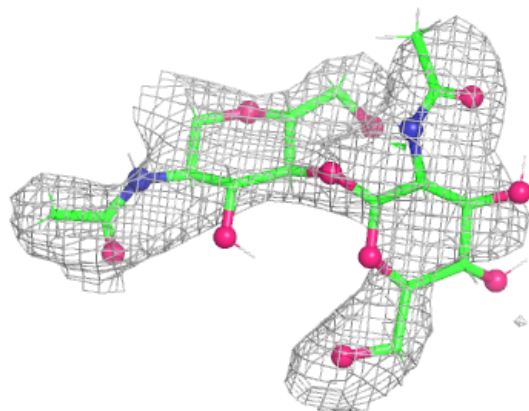
Electron density around Chain G:

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

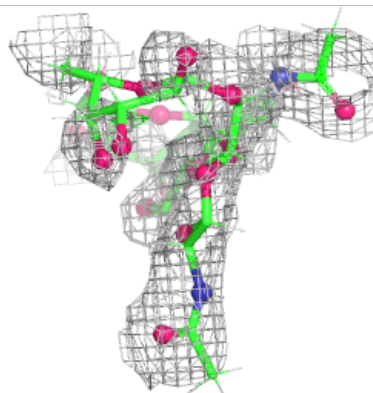
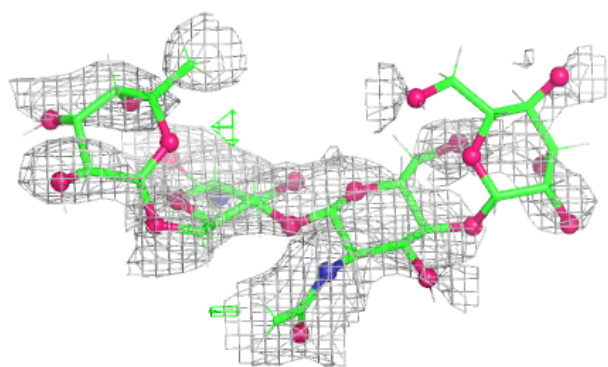
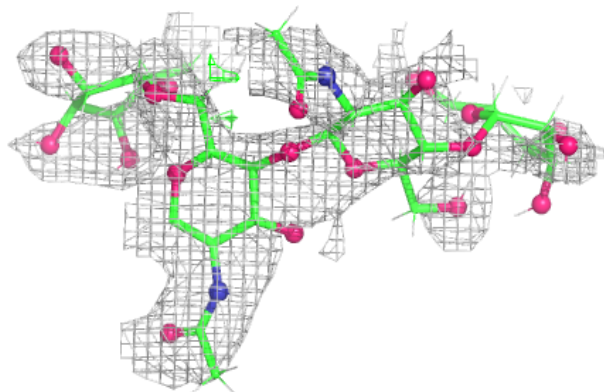


Electron density around Chain J:

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

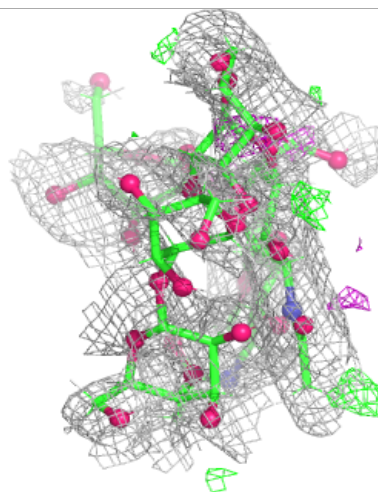
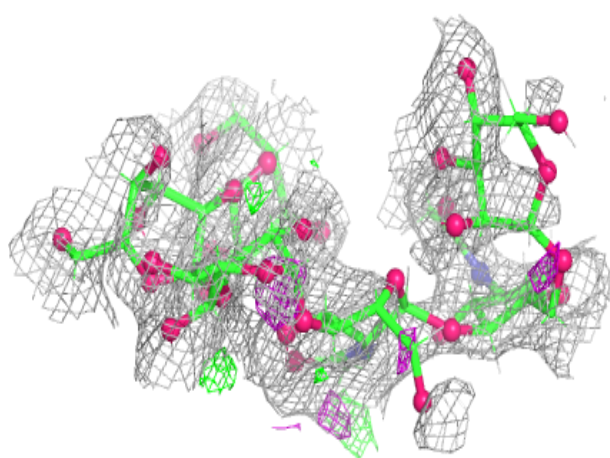
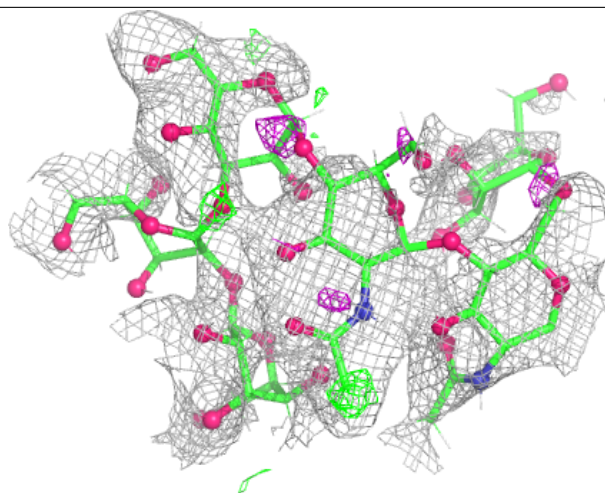
**Electron density around Chain D:**

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



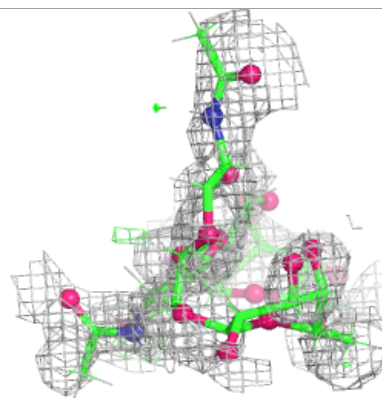
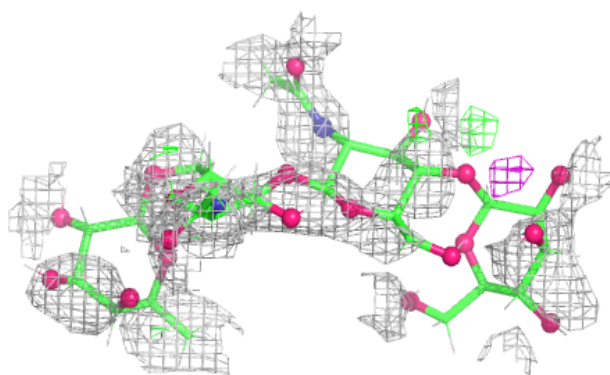
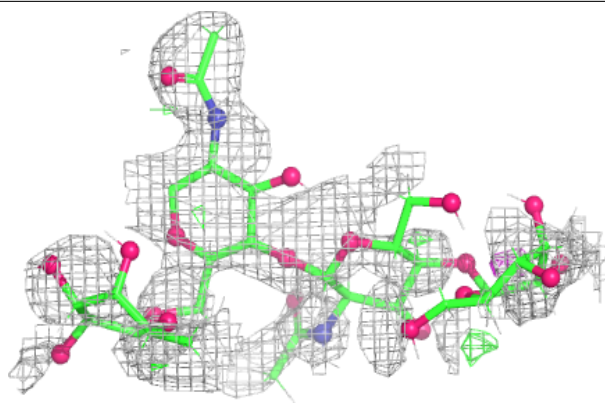
Electron density around Chain E:

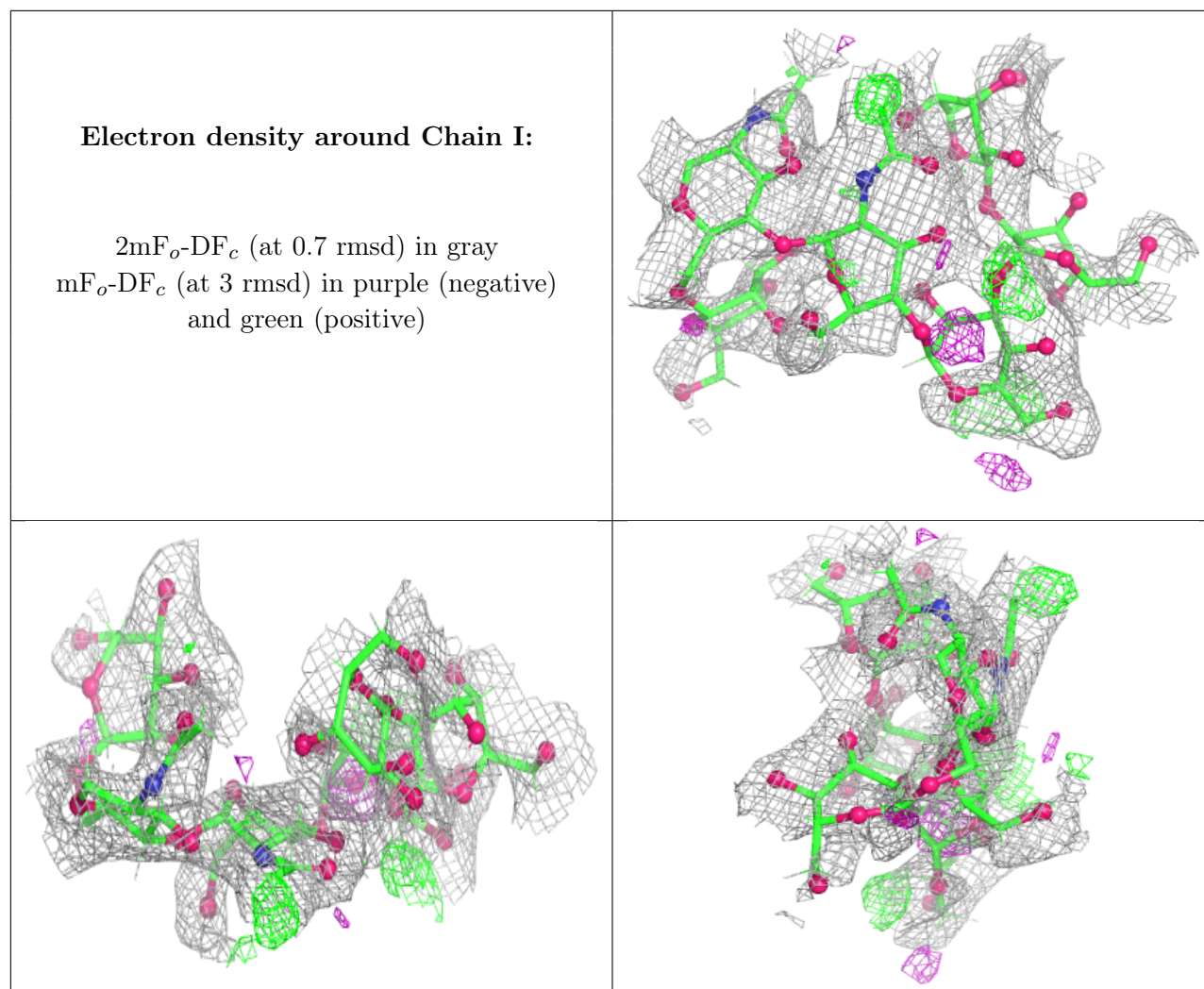
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain H:

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





6.4 Ligands ⓘ

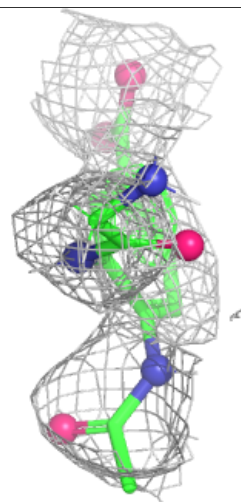
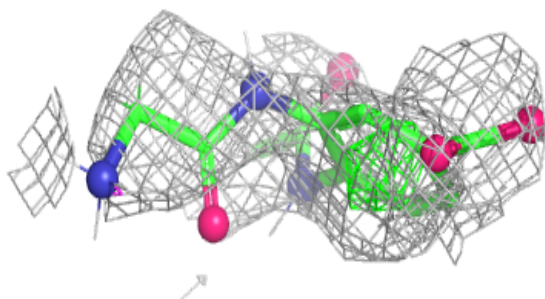
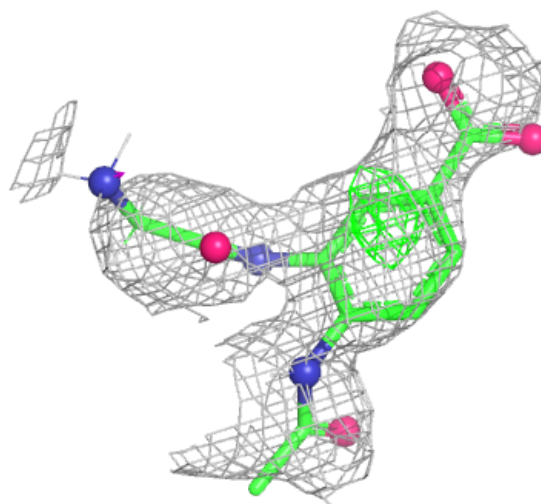
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	CA	B	488	1/1	0.61	0.04	24,24,24,24	0
8	ST6	B	489	18/18	0.67	0.20	0,61,64,65	18
7	CA	A	470	1/1	0.86	0.04	24,24,24,24	0
8	ST6	A	471	18/18	0.91	0.12	0,61,64,65	18

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.

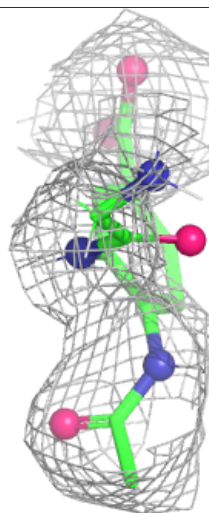
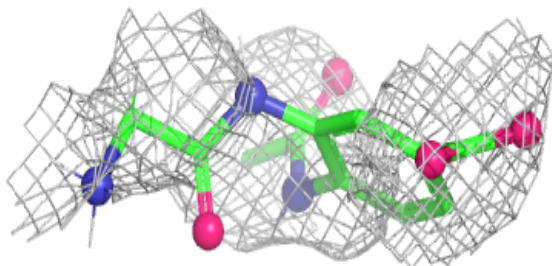
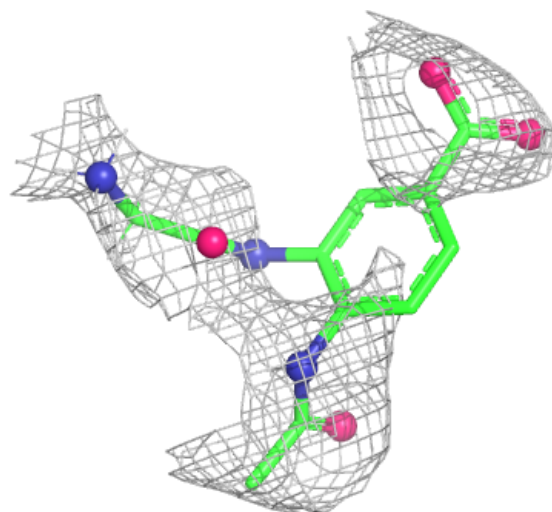
Electron density around ST6 B 489:

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



Electron density around ST6 A 471:

$2mF_o-DF_c$ (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.