Full wwPDB X-ray Structure Validation Report (i)

Aug 7, 2023 – 02:27 AM EDT

PDB ID	:	1LL4
Title	:	STRUCTURE OF C. IMMITIS CHITINASE 1 COMPLEXED WITH ALLOSAMIDIN
Authors	:	Bortone, K.; Monzingo, A.F.; Ernst, S.; Robertus, J.D.
Deposited on	:	2002-04-26
Resolution	:	2.80 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 (i) 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 (i)) were used in the production of this report:

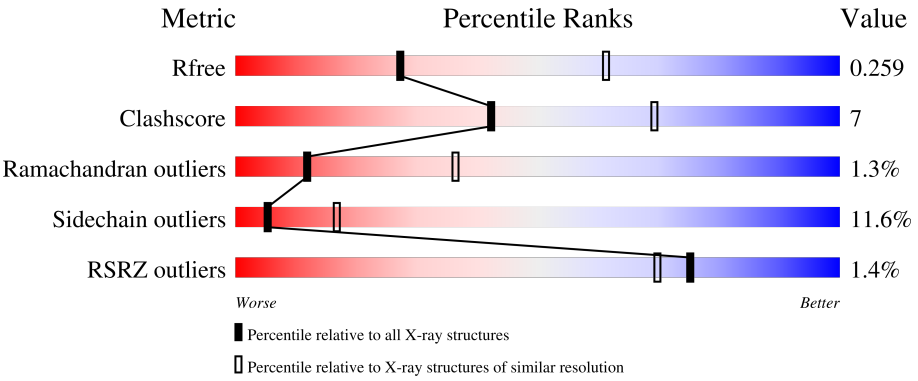
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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 <=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	392	72% 23% .
1	B	392	3% 72% 23% 5%
1	C	392	72% 24% .
1	D	392	70% 25% 5%
2	E	2	100%

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Mol	Chain	Length	Quality of chain
2	F	2	100%
2	G	2	100%
2	H	2	100%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 12604 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.

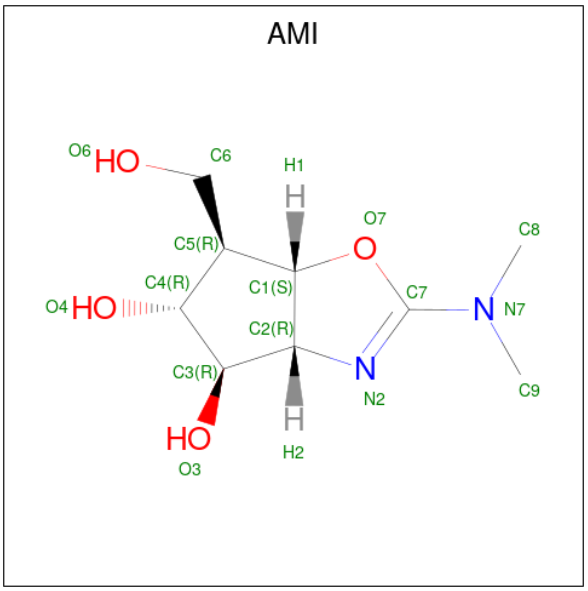
- Molecule 1 is a protein called CHITINASE 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	392	Total	C	N	O	S	0	0	0
			3083	1963	510	598	12			
1	B	392	Total	C	N	O	S	0	0	0
			3083	1963	510	598	12			
1	C	392	Total	C	N	O	S	0	0	0
			3083	1963	510	598	12			
1	D	392	Total	C	N	O	S	0	0	0
			3083	1963	510	598	12			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	F	2	Total	C	N	O	0	0	0
			28	16	2	10			
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			

- Molecule 3 is ALLOSAMIZOLINE (three-letter code: AMI) (formula: $C_9H_{16}N_2O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O 15 9 2 4	0	0
3	B	1	Total C N O 15 9 2 4	0	0
3	C	1	Total C N O 15 9 2 4	0	0
3	D	1	Total C N O 15 9 2 4	0	0

- Molecule 4 is water.

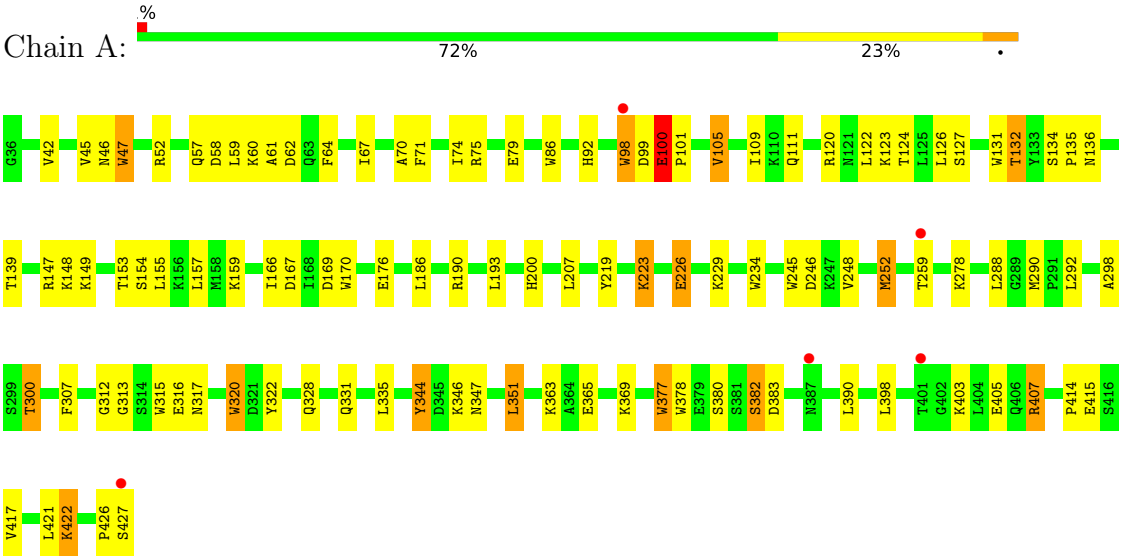
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	28	Total O 28 28	0	0
4	B	22	Total O 22 22	0	0
4	C	24	Total O 24 24	0	0
4	D	26	Total O 26 26	0	0

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.

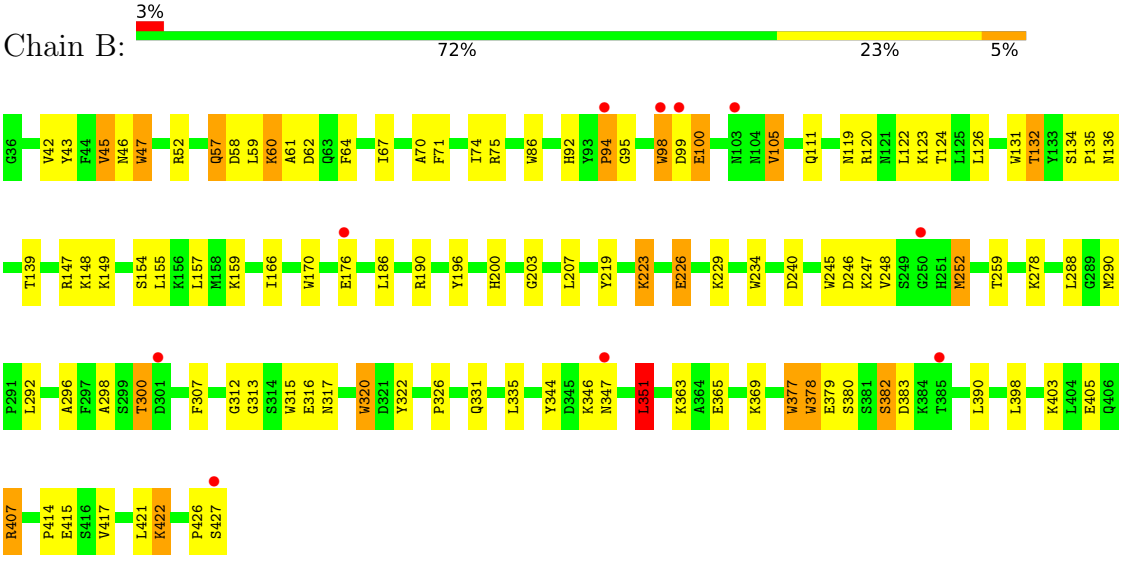
• Molecule 1: CHITINASE 1

Chain A:



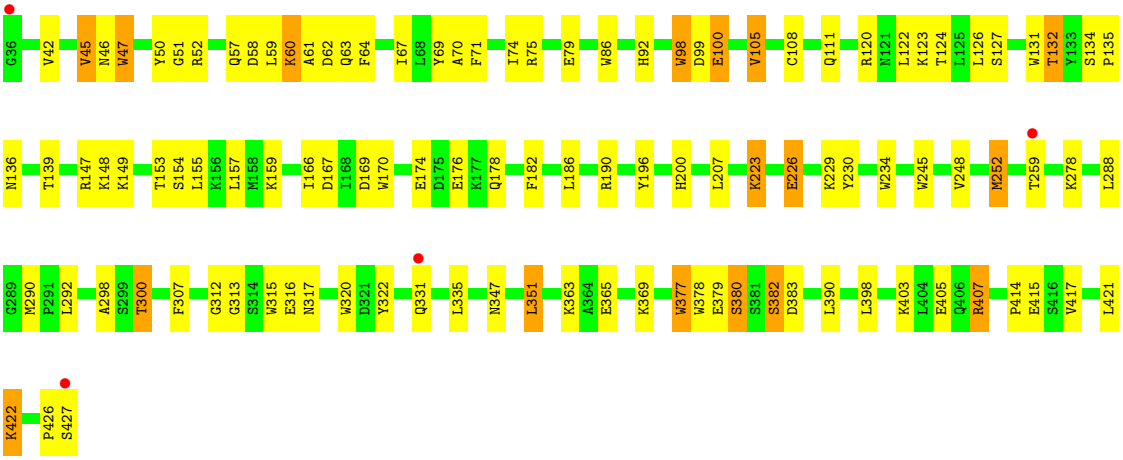
• Molecule 1: CHITINASE 1

Chain B:



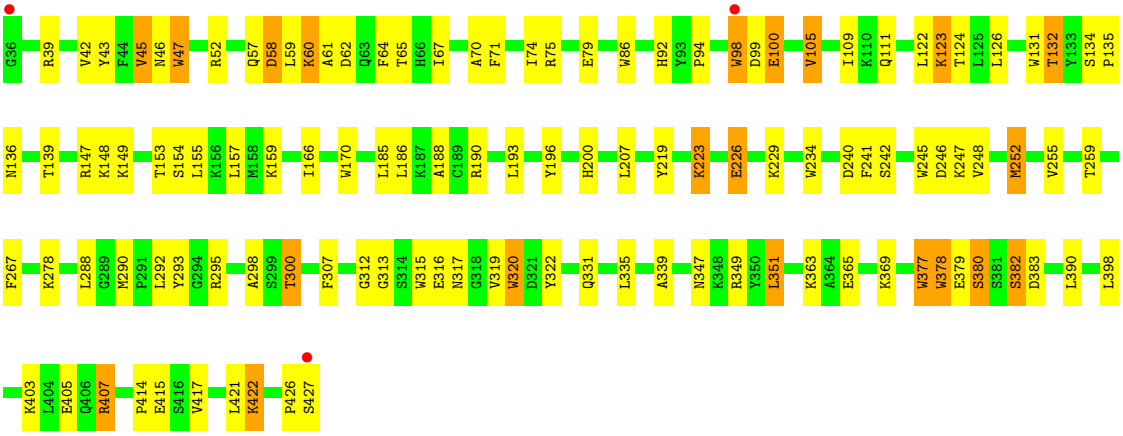
• Molecule 1: CHITINASE 1

Chain C:



• Molecule 1: CHITINASE 1

Chain D:



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

Chain E:

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

Chain F:

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

Chain G:

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

Chain H:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	61.05Å 78.19Å 88.46Å 80.61° 82.27° 66.72°	Depositor
Resolution (Å)	5.00 – 2.80 28.60 – 2.80	Depositor EDS
% Data completeness (in resolution range)	(Not available) (5.00-2.80) 91.0 (28.60-2.80)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.44 (at 2.80Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.197 , 0.258 0.209 , 0.259	Depositor DCC
R_{free} test set	1705 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å^2)	18.2	Xtriage
Anisotropy	0.585	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.40 , 62.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	12604	wwPDB-VP
Average B, all atoms (Å^2)	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.60% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: AMI, NAA

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	0.83	0/3165	1.53	54/4282 (1.3%)
1	B	0.84	0/3165	1.55	55/4282 (1.3%)
1	C	0.83	0/3165	1.54	59/4282 (1.4%)
1	D	0.84	0/3165	1.56	63/4282 (1.5%)
All	All	0.84	0/12660	1.54	231/17128 (1.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	C	0	1
All	All	0	2

There are no bond length outliers.

All (231) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	407	ARG	NE-CZ-NH2	-12.24	114.18	120.30
1	C	75	ARG	NE-CZ-NH2	11.78	126.19	120.30
1	C	407	ARG	NE-CZ-NH2	-11.23	114.68	120.30
1	B	190	ARG	NE-CZ-NH1	11.01	125.80	120.30
1	D	190	ARG	NE-CZ-NH1	10.06	125.33	120.30
1	B	407	ARG	NE-CZ-NH2	-9.84	115.38	120.30
1	D	75	ARG	NE-CZ-NH1	-9.81	115.40	120.30
1	C	75	ARG	NE-CZ-NH1	-9.78	115.41	120.30
1	A	407	ARG	NE-CZ-NH2	-9.55	115.53	120.30
1	C	190	ARG	NE-CZ-NH1	9.55	125.07	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	47	TRP	CD1-CG-CD2	9.26	113.71	106.30
1	C	377	TRP	CD1-CG-CD2	9.12	113.59	106.30
1	A	98	TRP	CD1-CG-CD2	9.03	113.53	106.30
1	D	315	TRP	CD1-CG-CD2	9.01	113.50	106.30
1	B	320	TRP	CD1-CG-CD2	9.00	113.50	106.30
1	B	47	TRP	CD1-CG-CD2	8.96	113.47	106.30
1	D	377	TRP	CD1-CG-CD2	8.86	113.39	106.30
1	D	98	TRP	CD1-CG-CD2	8.84	113.37	106.30
1	A	377	TRP	CD1-CG-CD2	8.83	113.36	106.30
1	B	377	TRP	CD1-CG-CD2	8.80	113.34	106.30
1	A	47	TRP	CD1-CG-CD2	8.76	113.31	106.30
1	A	75	ARG	NE-CZ-NH1	-8.50	116.05	120.30
1	A	315	TRP	CD1-CG-CD2	8.46	113.07	106.30
1	D	320	TRP	CD1-CG-CD2	8.45	113.06	106.30
1	B	47	TRP	CE2-CD2-CG	-8.42	100.56	107.30
1	D	234	TRP	CD1-CG-CD2	8.40	113.02	106.30
1	B	315	TRP	CD1-CG-CD2	8.39	113.01	106.30
1	C	131	TRP	CE2-CD2-CG	-8.39	100.59	107.30
1	D	252	MET	CG-SD-CE	-8.39	86.78	100.20
1	D	315	TRP	CE2-CD2-CG	-8.31	100.65	107.30
1	D	47	TRP	CE2-CD2-CG	-8.28	100.67	107.30
1	A	320	TRP	CD1-CG-CD2	8.23	112.88	106.30
1	A	47	TRP	CE2-CD2-CG	-8.22	100.73	107.30
1	C	131	TRP	CD1-CG-CD2	8.19	112.85	106.30
1	B	315	TRP	CE2-CD2-CG	-8.17	100.76	107.30
1	B	98	TRP	CD1-CG-CD2	8.15	112.82	106.30
1	C	86	TRP	CD1-CG-CD2	8.12	112.79	106.30
1	C	47	TRP	CD1-CG-CD2	8.09	112.77	106.30
1	B	234	TRP	CD1-CG-CD2	8.07	112.76	106.30
1	B	320	TRP	CE2-CD2-CG	-8.06	100.85	107.30
1	C	98	TRP	CD1-CG-CD2	8.04	112.73	106.30
1	A	234	TRP	CD1-CG-CD2	7.99	112.69	106.30
1	B	75	ARG	NE-CZ-NH2	7.98	124.29	120.30
1	B	86	TRP	CD1-CG-CD2	7.96	112.67	106.30
1	C	234	TRP	CD1-CG-CD2	7.96	112.67	106.30
1	A	315	TRP	CE2-CD2-CG	-7.96	100.94	107.30
1	A	86	TRP	CD1-CG-CD2	7.95	112.66	106.30
1	A	131	TRP	CD1-CG-CD2	7.94	112.66	106.30
1	B	147	ARG	NE-CZ-NH2	-7.94	116.33	120.30
1	C	245	TRP	CD1-CG-CD2	7.92	112.64	106.30
1	B	98	TRP	CE2-CD2-CG	-7.88	101.00	107.30
1	D	377	TRP	CE2-CD2-CG	-7.87	101.00	107.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	377	TRP	CE2-CD2-CG	-7.85	101.02	107.30
1	D	86	TRP	CE2-CD2-CG	-7.85	101.02	107.30
1	A	147	ARG	NE-CZ-NH2	-7.84	116.38	120.30
1	B	86	TRP	CE2-CD2-CG	-7.82	101.04	107.30
1	A	131	TRP	CE2-CD2-CG	-7.82	101.05	107.30
1	A	234	TRP	CE2-CD2-CG	-7.80	101.06	107.30
1	A	98	TRP	CE2-CD2-CG	-7.77	101.09	107.30
1	C	190	ARG	NE-CZ-NH2	-7.72	116.44	120.30
1	D	147	ARG	NE-CZ-NH2	-7.66	116.47	120.30
1	D	98	TRP	CE2-CD2-CG	-7.64	101.19	107.30
1	C	47	TRP	CE2-CD2-CG	-7.63	101.20	107.30
1	C	245	TRP	CE2-CD2-CG	-7.63	101.20	107.30
1	D	245	TRP	CD1-CG-CD2	7.63	112.40	106.30
1	A	245	TRP	CE2-CD2-CG	-7.62	101.20	107.30
1	A	245	TRP	CD1-CG-CD2	7.62	112.39	106.30
1	A	377	TRP	CE2-CD2-CG	-7.59	101.23	107.30
1	D	86	TRP	CD1-CG-CD2	7.59	112.37	106.30
1	A	75	ARG	NE-CZ-NH2	7.59	124.09	120.30
1	B	52	ARG	NE-CZ-NH1	7.57	124.08	120.30
1	D	131	TRP	CD1-CG-CD2	7.57	112.35	106.30
1	C	377	TRP	CE2-CD2-CG	-7.56	101.25	107.30
1	C	86	TRP	CE2-CD2-CG	-7.55	101.26	107.30
1	B	234	TRP	CE2-CD2-CG	-7.54	101.27	107.30
1	D	131	TRP	CE2-CD2-CG	-7.52	101.28	107.30
1	B	245	TRP	CD1-CG-CD2	7.49	112.29	106.30
1	C	315	TRP	CD1-CG-CD2	7.48	112.28	106.30
1	D	75	ARG	NE-CZ-NH2	7.41	124.00	120.30
1	A	378	TRP	CE2-CD2-CG	-7.41	101.38	107.30
1	D	245	TRP	CE2-CD2-CG	-7.35	101.42	107.30
1	D	234	TRP	CE2-CD2-CG	-7.33	101.44	107.30
1	C	147	ARG	NE-CZ-NH2	-7.28	116.66	120.30
1	C	320	TRP	CD1-CG-CD2	7.27	112.11	106.30
1	A	86	TRP	CE2-CD2-CG	-7.26	101.49	107.30
1	A	190	ARG	NE-CZ-NH1	7.25	123.92	120.30
1	B	170	TRP	CE2-CD2-CG	-7.25	101.50	107.30
1	D	320	TRP	CE2-CD2-CG	-7.23	101.52	107.30
1	C	98	TRP	CE2-CD2-CG	-7.19	101.55	107.30
1	D	170	TRP	CE2-CD2-CG	-7.17	101.56	107.30
1	B	75	ARG	NE-CZ-NH1	-7.14	116.73	120.30
1	A	252	MET	CG-SD-CE	-7.13	88.80	100.20
1	B	252	MET	CG-SD-CE	-7.12	88.80	100.20
1	A	320	TRP	CE2-CD2-CG	-7.11	101.61	107.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	320	TRP	CE2-CD2-CG	-7.08	101.64	107.30
1	C	252	MET	CG-SD-CE	-7.07	88.88	100.20
1	D	378	TRP	CE2-CD2-CG	-6.99	101.71	107.30
1	B	245	TRP	CE2-CD2-CG	-6.95	101.74	107.30
1	C	234	TRP	CE2-CD2-CG	-6.93	101.75	107.30
1	B	131	TRP	CE2-CD2-CG	-6.83	101.84	107.30
1	B	170	TRP	CD1-CG-CD2	6.80	111.74	106.30
1	C	105	VAL	CB-CA-C	-6.74	98.59	111.40
1	C	315	TRP	CE2-CD2-CG	-6.73	101.91	107.30
1	A	170	TRP	CE2-CD2-CG	-6.72	101.92	107.30
1	A	105	VAL	CB-CA-C	-6.68	98.71	111.40
1	D	190	ARG	NE-CZ-NH2	-6.68	116.96	120.30
1	B	131	TRP	CD1-CG-CD2	6.61	111.59	106.30
1	C	378	TRP	CE2-CD2-CG	-6.59	102.03	107.30
1	D	378	TRP	CD1-CG-CD2	6.59	111.57	106.30
1	D	407	ARG	NE-CZ-NH1	6.53	123.56	120.30
1	B	378	TRP	CE2-CD2-CG	-6.47	102.13	107.30
1	A	147	ARG	NE-CZ-NH1	6.45	123.52	120.30
1	A	219	TYR	CB-CG-CD1	-6.44	117.14	121.00
1	D	246	ASP	CB-CG-OD2	6.42	124.08	118.30
1	D	105	VAL	CB-CA-C	-6.40	99.23	111.40
1	D	170	TRP	CD1-CG-CD2	6.39	111.42	106.30
1	A	170	TRP	CD1-CG-CD2	6.39	111.41	106.30
1	C	170	TRP	CE2-CD2-CG	-6.32	102.25	107.30
1	B	190	ARG	NE-CZ-NH2	-6.27	117.16	120.30
1	B	427	SER	N-CA-C	-6.24	94.16	111.00
1	B	407	ARG	NE-CZ-NH1	6.21	123.41	120.30
1	B	105	VAL	CB-CA-C	-6.18	99.66	111.40
1	A	378	TRP	CD1-CG-CD2	6.12	111.19	106.30
1	B	378	TRP	CD1-CG-CD2	6.07	111.16	106.30
1	D	98	TRP	CG-CD1-NE1	-6.00	104.11	110.10
1	C	377	TRP	CG-CD1-NE1	-5.98	104.12	110.10
1	B	47	TRP	CG-CD2-CE3	5.96	139.27	133.90
1	D	47	TRP	CG-CD2-CE3	5.95	139.25	133.90
1	D	60	LYS	CA-CB-CG	5.92	126.43	113.40
1	D	315	TRP	CG-CD1-NE1	-5.90	104.20	110.10
1	D	377	TRP	CG-CD1-NE1	-5.90	104.20	110.10
1	C	132	THR	N-CA-CB	-5.87	99.14	110.30
1	D	47	TRP	CB-CG-CD1	-5.87	119.37	127.00
1	D	427	SER	N-CA-C	-5.87	95.15	111.00
1	D	47	TRP	CG-CD1-NE1	-5.87	104.23	110.10
1	A	98	TRP	O-C-N	5.86	132.08	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	170	TRP	CD1-CG-CD2	5.85	110.98	106.30
1	C	378	TRP	CD1-CG-CD2	5.85	110.98	106.30
1	A	351	LEU	CA-CB-CG	5.80	128.64	115.30
1	B	320	TRP	CG-CD1-NE1	-5.79	104.31	110.10
1	B	288	LEU	CA-CB-CG	5.78	128.60	115.30
1	B	132	THR	N-CA-CB	-5.78	99.33	110.30
1	D	45	VAL	CA-CB-CG2	-5.76	102.26	110.90
1	C	245	TRP	CG-CD2-CE3	5.76	139.08	133.90
1	D	320	TRP	CG-CD1-NE1	-5.76	104.34	110.10
1	C	60	LYS	CA-CB-CG	5.73	126.00	113.40
1	D	132	THR	N-CA-CB	-5.72	99.42	110.30
1	C	427	SER	N-CA-C	-5.72	95.56	111.00
1	A	47	TRP	CG-CD1-NE1	-5.69	104.41	110.10
1	D	223	LYS	CG-CD-CE	-5.68	94.87	111.90
1	C	47	TRP	CG-CD2-CE3	5.67	139.01	133.90
1	B	377	TRP	CG-CD1-NE1	-5.65	104.45	110.10
1	D	351	LEU	CA-CB-CG	5.64	128.28	115.30
1	A	132	THR	N-CA-CB	-5.61	99.64	110.30
1	A	377	TRP	CG-CD1-NE1	-5.59	104.51	110.10
1	C	120	ARG	NE-CZ-NH1	5.58	123.09	120.30
1	A	98	TRP	CG-CD1-NE1	-5.56	104.54	110.10
1	C	245	TRP	CB-CG-CD1	-5.56	119.78	127.00
1	A	47	TRP	CG-CD2-CE3	5.55	138.90	133.90
1	C	45	VAL	CA-CB-CG2	-5.55	102.57	110.90
1	D	98	TRP	O-C-N	5.55	131.58	122.70
1	A	427	SER	N-CA-C	-5.54	96.05	111.00
1	A	245	TRP	CG-CD2-CE3	5.52	138.87	133.90
1	A	190	ARG	NE-CZ-NH2	-5.50	117.55	120.30
1	C	100	GLU	N-CA-C	5.50	125.85	111.00
1	A	288	LEU	CA-CB-CG	5.49	127.94	115.30
1	B	245	TRP	CB-CG-CD1	-5.49	119.87	127.00
1	A	120	ARG	NE-CZ-NH2	-5.49	117.56	120.30
1	D	219	TYR	CB-CG-CD1	-5.44	117.73	121.00
1	B	234	TRP	CG-CD2-CE3	5.44	138.80	133.90
1	B	100	GLU	N-CA-C	5.43	125.68	111.00
1	D	52	ARG	NE-CZ-NH1	5.43	123.02	120.30
1	A	52	ARG	NE-CZ-NH2	-5.42	117.59	120.30
1	D	147	ARG	NE-CZ-NH1	5.41	123.01	120.30
1	C	351	LEU	CA-CB-CG	5.39	127.70	115.30
1	D	100	GLU	N-CA-C	5.39	125.54	111.00
1	B	47	TRP	CB-CG-CD1	-5.38	120.00	127.00
1	C	98	TRP	O-C-N	5.38	131.30	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	288	LEU	CA-CB-CG	5.37	127.66	115.30
1	D	349	ARG	NE-CZ-NH1	5.37	122.98	120.30
1	B	120	ARG	NE-CZ-NH2	-5.37	117.62	120.30
1	D	234	TRP	CG-CD2-CE3	5.36	138.72	133.90
1	B	98	TRP	O-C-N	5.34	131.25	122.70
1	C	288	LEU	CA-CB-CG	5.33	127.56	115.30
1	B	45	VAL	CA-CB-CG2	-5.32	102.92	110.90
1	B	351	LEU	CA-CB-CG	5.31	127.51	115.30
1	C	379	GLU	CA-CB-CG	5.31	125.08	113.40
1	D	245	TRP	CG-CD2-CE3	5.31	138.68	133.90
1	B	246	ASP	CB-CG-OD2	5.30	123.07	118.30
1	B	219	TYR	CB-CG-CD1	-5.29	117.82	121.00
1	B	60	LYS	CA-CB-CG	5.29	125.04	113.40
1	D	245	TRP	CB-CG-CD1	-5.28	120.14	127.00
1	D	319	VAL	CG1-CB-CG2	-5.28	102.46	110.90
1	C	234	TRP	CG-CD1-NE1	-5.27	104.83	110.10
1	B	170	TRP	CG-CD1-NE1	-5.26	104.84	110.10
1	A	100	GLU	N-CA-C	5.24	125.14	111.00
1	B	315	TRP	CG-CD1-NE1	-5.24	104.86	110.10
1	C	98	TRP	CG-CD2-CE3	5.24	138.61	133.90
1	C	47	TRP	CB-CG-CD1	-5.23	120.20	127.00
1	A	246	ASP	CB-CG-OD1	-5.23	113.59	118.30
1	C	131	TRP	CG-CD2-CE3	5.22	138.60	133.90
1	C	147	ARG	NE-CZ-NH1	5.22	122.91	120.30
1	A	86	TRP	CG-CD1-NE1	-5.21	104.89	110.10
1	B	245	TRP	CG-CD2-CE3	5.20	138.58	133.90
1	B	147	ARG	NE-CZ-NH1	5.20	122.90	120.30
1	A	320	TRP	CG-CD1-NE1	-5.19	104.91	110.10
1	D	315	TRP	CG-CD2-CE3	5.19	138.57	133.90
1	D	407	ARG	CA-CB-CG	-5.17	102.03	113.40
1	C	380	SER	N-CA-C	5.16	124.92	111.00
1	A	98	TRP	CG-CD2-CE3	5.16	138.54	133.90
1	D	234	TRP	CB-CG-CD1	-5.15	120.31	127.00
1	A	320	TRP	CB-CG-CD1	-5.14	120.31	127.00
1	D	131	TRP	CG-CD2-CE3	5.14	138.53	133.90
1	D	380	SER	N-CA-C	5.13	124.85	111.00
1	A	131	TRP	CB-CG-CD1	-5.13	120.34	127.00
1	C	407	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	C	234	TRP	CG-CD2-CE3	5.11	138.50	133.90
1	C	86	TRP	CG-CD1-NE1	-5.09	105.01	110.10
1	A	234	TRP	CG-CD2-CE3	5.08	138.47	133.90
1	C	63	GLN	CA-CB-CG	5.07	124.55	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	98	TRP	CG-CD1-NE1	-5.06	105.04	110.10
1	B	47	TRP	CG-CD1-NE1	-5.06	105.04	110.10
1	A	245	TRP	CB-CG-CD1	-5.03	120.47	127.00
1	C	86	TRP	CG-CD2-CE3	5.03	138.42	133.90
1	D	234	TRP	CG-CD1-NE1	-5.02	105.08	110.10
1	D	293	TYR	CB-CG-CD1	-5.02	117.99	121.00
1	C	52	ARG	NE-CZ-NH2	-5.02	117.79	120.30
1	C	131	TRP	CG-CD1-NE1	-5.02	105.08	110.10
1	A	131	TRP	CG-CD2-CE3	5.01	138.41	133.90
1	C	45	VAL	N-CA-CB	-5.01	100.47	111.50
1	B	245	TRP	CG-CD1-NE1	-5.00	105.09	110.10

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	344	TYR	Sidechain
1	C	230	TYR	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3083	0	2961	40	0
1	B	3083	0	2961	47	0
1	C	3083	0	2961	47	0
1	D	3083	0	2961	44	0
2	E	28	0	25	5	0
2	F	28	0	25	5	0
2	G	28	0	25	6	0
2	H	28	0	25	4	0
3	A	15	0	15	3	0
3	B	15	0	15	3	0
3	C	15	0	15	3	0
3	D	15	0	15	5	0
4	A	28	0	0	3	0
4	B	22	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	24	0	0	1	0
4	D	26	0	0	0	0
All	All	12604	0	12004	168	0

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

All (168) 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:132:THR:HG21	2:F:2:NAA:H81	1.26	1.18
1:A:132:THR:HG21	2:E:2:NAA:H81	1.41	1.02
1:B:132:THR:HG21	2:F:2:NAA:C8	1.91	1.00
1:C:132:THR:HG21	2:G:2:NAA:H81	1.43	0.99
1:C:132:THR:HG21	2:G:2:NAA:C8	1.99	0.92
1:D:132:THR:HG21	2:H:2:NAA:H81	1.51	0.92
1:A:132:THR:HG21	2:E:2:NAA:C8	2.06	0.85
1:A:71:PHE:HZ	3:A:503:AMI:H82	1.46	0.80
1:B:95:GLY:H	1:C:51:GLY:HA2	1.47	0.80
1:B:47:TRP:CZ2	2:F:1:NAA:H4	2.22	0.74
1:C:47:TRP:CZ2	2:G:1:NAA:H4	2.23	0.73
1:B:132:THR:CG2	2:F:2:NAA:H81	2.14	0.73
1:D:132:THR:HG21	2:H:2:NAA:C8	2.22	0.70
1:A:71:PHE:CZ	3:A:503:AMI:H82	2.27	0.69
1:C:71:PHE:HZ	3:C:503:AMI:H82	1.59	0.68
1:A:98:TRP:HB2	4:A:1086:HOH:O	1.92	0.68
4:A:1029:HOH:O	2:E:1:NAA:H81	1.95	0.67
1:D:47:TRP:CZ2	2:H:1:NAA:H4	2.31	0.65
1:B:154:SER:HB3	1:B:166:ILE:HD13	1.79	0.65
1:B:92:HIS:NE2	1:B:98:TRP:HA	2.11	0.64
1:A:47:TRP:CZ2	2:E:1:NAA:H4	2.34	0.63
1:A:132:THR:CG2	2:E:2:NAA:H81	2.24	0.63
1:C:154:SER:HB3	1:C:166:ILE:HD13	1.81	0.63
1:D:92:HIS:NE2	1:D:98:TRP:HA	2.14	0.62
1:A:92:HIS:NE2	1:A:98:TRP:HA	2.14	0.61
1:A:154:SER:HB3	1:A:166:ILE:HD13	1.83	0.60
1:C:92:HIS:NE2	1:C:98:TRP:HA	2.16	0.60
1:B:292:LEU:O	1:B:382:SER:HB2	2.02	0.60
1:D:154:SER:HB3	1:D:166:ILE:HD13	1.85	0.59
1:C:42:VAL:HB	1:C:64:PHE:CE2	2.38	0.59
1:C:71:PHE:CZ	3:C:503:AMI:H82	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:169:ASP:OD1	3:A:503:AMI:H83	2.04	0.58
1:B:94:PRO:HB3	1:C:50:TYR:HA	1.86	0.57
1:D:292:LEU:HD13	1:D:383:ASP:HB2	1.87	0.57
1:A:300:THR:HG23	1:A:307:PHE:HB3	1.87	0.56
1:C:132:THR:CG2	2:G:2:NAA:H81	2.27	0.56
1:B:292:LEU:HD13	1:B:383:ASP:HB2	1.89	0.55
1:B:312:GLY:HA2	1:B:317:ASN:HD22	1.72	0.55
1:A:42:VAL:HB	1:A:64:PHE:CE2	2.42	0.55
1:C:292:LEU:O	1:C:382:SER:HB2	2.07	0.55
1:D:42:VAL:HB	1:D:64:PHE:CE2	2.42	0.54
1:B:95:GLY:H	1:C:51:GLY:CA	2.19	0.54
1:C:47:TRP:CH2	2:G:1:NAA:H4	2.43	0.54
1:A:292:LEU:HD13	1:A:383:ASP:HB2	1.89	0.54
1:B:95:GLY:CA	1:C:51:GLY:O	2.56	0.54
1:D:61:ALA:HB1	1:D:122:LEU:HD22	1.89	0.54
1:A:61:ALA:HB1	1:A:122:LEU:HD22	1.89	0.53
1:B:95:GLY:HA2	1:C:51:GLY:O	2.08	0.53
1:C:300:THR:HG23	1:C:307:PHE:HB3	1.90	0.53
1:A:226:GLU:HA	1:A:229:LYS:HZ3	1.73	0.53
1:C:369:LYS:HE3	4:C:1092:HOH:O	2.09	0.53
1:D:312:GLY:HA2	1:D:317:ASN:HD22	1.73	0.53
1:B:61:ALA:HB1	1:B:122:LEU:HD22	1.90	0.53
1:B:42:VAL:HB	1:B:64:PHE:CE2	2.43	0.53
1:D:71:PHE:HZ	3:D:503:AMI:H82	1.71	0.53
1:C:414:PRO:O	1:C:422:LYS:HE2	2.09	0.52
1:B:92:HIS:CD2	1:B:98:TRP:HA	2.44	0.52
1:A:312:GLY:HA2	1:A:317:ASN:HD22	1.74	0.52
1:A:328:GLN:HB3	1:D:58:ASP:HB2	1.91	0.52
1:B:313:GLY:HA3	1:B:316:GLU:O	2.09	0.52
1:C:313:GLY:HA3	1:C:316:GLU:O	2.08	0.52
1:A:292:LEU:O	1:A:382:SER:HB2	2.10	0.52
1:C:312:GLY:HA2	1:C:317:ASN:HD22	1.74	0.52
1:B:119:ASN:HB3	4:B:1088:HOH:O	2.11	0.51
1:B:300:THR:HG23	1:B:307:PHE:HB3	1.92	0.51
1:C:292:LEU:HD13	1:C:383:ASP:HB2	1.92	0.51
1:A:79:GLU:OE1	1:B:247:LYS:HD3	2.11	0.51
1:D:313:GLY:HA3	1:D:316:GLU:O	2.11	0.50
1:D:365:GLU:O	1:D:369:LYS:HB2	2.10	0.50
1:C:61:ALA:HB1	1:C:122:LEU:HD22	1.93	0.50
1:D:42:VAL:HG23	1:D:377:TRP:HB2	1.94	0.49
1:B:43:TYR:CE2	3:B:503:AMI:H81	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:226:GLU:HA	1:C:229:LYS:HZ3	1.78	0.49
1:B:47:TRP:CH2	2:F:1:NAA:H4	2.47	0.49
1:C:79:GLU:HG3	1:C:153:THR:HG21	1.95	0.49
1:D:292:LEU:O	1:D:382:SER:HB2	2.12	0.49
1:A:79:GLU:HG3	1:A:153:THR:HG21	1.95	0.49
1:A:313:GLY:HA3	1:A:316:GLU:O	2.12	0.49
1:A:365:GLU:O	1:A:369:LYS:HB2	2.13	0.49
1:B:42:VAL:HG23	1:B:377:TRP:HB2	1.95	0.49
1:C:176:GLU:CD	1:C:223:LYS:HZ1	2.16	0.48
1:D:300:THR:HG23	1:D:307:PHE:HB3	1.95	0.48
1:D:92:HIS:CD2	1:D:98:TRP:HA	2.48	0.48
1:B:344:TYR:HE2	1:B:346:LYS:HD3	1.78	0.48
1:A:42:VAL:HG23	1:A:377:TRP:HB2	1.96	0.48
1:A:92:HIS:CD2	1:A:98:TRP:HA	2.49	0.47
1:C:42:VAL:HG23	1:C:377:TRP:HB2	1.96	0.47
1:C:169:ASP:OD1	3:C:503:AMI:H83	2.14	0.47
1:D:43:TYR:CE2	3:D:503:AMI:H81	2.49	0.47
1:D:240:ASP:OD1	3:D:503:AMI:H62	2.14	0.47
1:D:378:TRP:HE1	2:H:1:NAA:H83	1.79	0.47
1:D:134:SER:N	1:D:135:PRO:HD2	2.29	0.47
1:C:134:SER:N	1:C:135:PRO:HD2	2.30	0.47
1:A:200:HIS:HE1	1:A:415:GLU:OE1	1.98	0.47
1:D:155:LEU:HD21	1:D:196:TYR:HB2	1.97	0.47
1:A:313:GLY:HA2	1:A:320:TRP:CE2	2.51	0.46
1:B:365:GLU:O	1:B:369:LYS:HB2	2.14	0.46
1:B:200:HIS:HE1	1:B:415:GLU:OE1	1.98	0.46
1:C:365:GLU:O	1:C:369:LYS:HB2	2.15	0.46
1:B:176:GLU:CD	1:B:223:LYS:HZ1	2.19	0.46
1:D:71:PHE:CZ	3:D:503:AMI:H82	2.49	0.46
1:D:200:HIS:HE1	1:D:415:GLU:OE1	1.99	0.46
1:C:92:HIS:CD2	1:C:98:TRP:HA	2.51	0.46
1:A:155:LEU:HD13	1:A:193:LEU:HD12	1.98	0.45
1:D:298:ALA:O	1:D:307:PHE:HB2	2.17	0.45
1:A:290:MET:HG2	1:A:363:LYS:HD3	1.98	0.45
1:C:290:MET:HG2	1:C:363:LYS:HD3	1.98	0.45
1:A:57:GLN:HG3	1:A:111:GLN:HE21	1.82	0.45
1:C:132:THR:HG21	2:G:2:NAA:H83	1.93	0.45
1:C:322:TYR:CE2	1:C:390:LEU:HG	2.52	0.45
1:A:134:SER:N	1:A:135:PRO:HD2	2.32	0.45
1:A:176:GLU:CD	1:A:223:LYS:HZ2	2.20	0.45
1:B:134:SER:N	1:B:135:PRO:HD2	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:414:PRO:O	1:B:422:LYS:HE2	2.17	0.45
1:C:155:LEU:HD21	1:C:196:TYR:HB2	1.98	0.44
1:D:414:PRO:O	1:D:422:LYS:HE2	2.17	0.44
1:A:322:TYR:CE2	1:A:390:LEU:HG	2.52	0.44
1:A:414:PRO:O	1:A:422:LYS:HE2	2.17	0.44
1:C:69:TYR:OH	1:C:108:CYS:HB2	2.18	0.44
1:B:43:TYR:CE1	3:B:503:AMI:H91	2.53	0.44
1:B:67:ILE:O	1:B:124:THR:HA	2.18	0.44
1:A:344:TYR:HE2	1:A:346:LYS:HD3	1.83	0.43
1:C:57:GLN:HG3	1:C:111:GLN:HE21	1.83	0.43
1:B:203:GLY:HA3	4:B:1065:HOH:O	2.18	0.43
1:C:79:GLU:OE1	1:D:247:LYS:HD3	2.19	0.43
1:B:298:ALA:O	1:B:307:PHE:HB2	2.19	0.43
1:D:65:THR:O	1:D:123:LYS:HE3	2.19	0.43
1:D:79:GLU:HG3	1:D:153:THR:HG21	1.99	0.43
1:A:67:ILE:O	1:A:124:THR:HA	2.18	0.43
1:A:298:ALA:O	1:A:307:PHE:HB2	2.19	0.43
1:D:70:ALA:HA	1:D:71:PHE:HA	1.65	0.43
1:D:322:TYR:CE2	1:D:390:LEU:HG	2.53	0.43
1:D:242:SER:O	1:D:295:ARG:HD2	2.19	0.43
1:C:200:HIS:HE1	1:C:415:GLU:OE1	2.01	0.43
1:C:67:ILE:O	1:C:124:THR:HA	2.19	0.43
1:D:67:ILE:O	1:D:124:THR:HA	2.19	0.43
1:B:70:ALA:HA	1:B:71:PHE:HA	1.66	0.42
1:B:378:TRP:HA	1:B:379:GLU:HA	1.83	0.42
1:C:127:SER:HA	1:C:167:ASP:O	2.19	0.42
1:B:226:GLU:HA	1:B:229:LYS:HZ3	1.84	0.42
1:C:70:ALA:HA	1:C:71:PHE:HA	1.66	0.42
1:D:57:GLN:HG3	1:D:111:GLN:HE21	1.84	0.42
1:A:70:ALA:HA	1:A:71:PHE:HA	1.66	0.42
1:B:57:GLN:HG3	1:B:111:GLN:HE21	1.84	0.42
1:C:298:ALA:O	1:C:307:PHE:HB2	2.20	0.42
1:C:174:GLU:HG2	1:C:178:GLN:NE2	2.35	0.41
1:D:290:MET:HG2	1:D:363:LYS:HD3	2.02	0.41
1:B:313:GLY:HA2	1:B:320:TRP:CE2	2.55	0.41
1:D:313:GLY:HA2	1:D:320:TRP:CE2	2.55	0.41
1:A:127:SER:HA	1:A:167:ASP:O	2.20	0.41
1:D:39:ARG:HH11	1:D:39:ARG:HD3	1.69	0.41
1:D:378:TRP:HA	1:D:379:GLU:HA	1.84	0.41
1:A:223:LYS:HE3	4:A:1040:HOH:O	2.21	0.41
1:D:240:ASP:OD1	3:D:503:AMI:C6	2.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:226:GLU:HA	1:D:229:LYS:HZ3	1.85	0.41
1:D:241:PHE:CG	1:D:267:PHE:HB2	2.55	0.41
1:B:155:LEU:HD21	1:B:196:TYR:HB2	2.02	0.41
1:B:94:PRO:HB3	1:C:50:TYR:CA	2.51	0.41
1:B:95:GLY:N	1:C:51:GLY:HA2	2.27	0.41
1:D:255:VAL:CG2	1:D:339:ALA:HB3	2.51	0.41
1:B:322:TYR:CE2	1:B:390:LEU:HG	2.55	0.41
1:B:296:ALA:HA	1:B:351:LEU:O	2.20	0.40
1:D:185:LEU:O	1:D:188:ALA:HB3	2.21	0.40
1:B:240:ASP:OD1	3:B:503:AMI:H62	2.21	0.40
1:B:94:PRO:HB3	1:C:50:TYR:C	2.41	0.40
1:B:290:MET:HG2	1:B:363:LYS:HD3	2.04	0.40
1:D:155:LEU:HD13	1:D:193:LEU:HD12	2.03	0.40
1:A:100:GLU:HG3	1:A:101:PRO:HD2	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	390/392 (100%)	369 (95%)	16 (4%)	5 (1%)	12	36
1	B	390/392 (100%)	368 (94%)	17 (4%)	5 (1%)	12	36
1	C	390/392 (100%)	370 (95%)	15 (4%)	5 (1%)	12	36
1	D	390/392 (100%)	369 (95%)	16 (4%)	5 (1%)	12	36
All	All	1560/1568 (100%)	1476 (95%)	64 (4%)	20 (1%)	12	36

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	99	ASP

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Mol	Chain	Res	Type
1	A	100	GLU
1	B	99	ASP
1	B	100	GLU
1	C	99	ASP
1	C	100	GLU
1	D	99	ASP
1	D	100	GLU
1	A	46	ASN
1	B	46	ASN
1	C	46	ASN
1	C	380	SER
1	D	46	ASN
1	D	380	SER
1	A	426	PRO
1	B	380	SER
1	B	426	PRO
1	D	426	PRO
1	A	380	SER
1	C	426	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	326/326 (100%)	289 (89%)	37 (11%)	6	18
1	B	326/326 (100%)	287 (88%)	39 (12%)	5	15
1	C	326/326 (100%)	289 (89%)	37 (11%)	6	18
1	D	326/326 (100%)	288 (88%)	38 (12%)	5	16
All	All	1304/1304 (100%)	1153 (88%)	151 (12%)	5	17

All (151) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	VAL
1	A	58	ASP

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Mol	Chain	Res	Type
1	A	59	LEU
1	A	60	LYS
1	A	62	ASP
1	A	74	ILE
1	A	105	VAL
1	A	109	ILE
1	A	123	LYS
1	A	126	LEU
1	A	136	ASN
1	A	139	THR
1	A	148	LYS
1	A	149	LYS
1	A	157	LEU
1	A	159	LYS
1	A	186	LEU
1	A	207	LEU
1	A	223	LYS
1	A	226	GLU
1	A	248	VAL
1	A	252	MET
1	A	259	THR
1	A	278	LYS
1	A	300	THR
1	A	331	GLN
1	A	335	LEU
1	A	347	ASN
1	A	351	LEU
1	A	382	SER
1	A	398	LEU
1	A	403	LYS
1	A	405	GLU
1	A	407	ARG
1	A	417	VAL
1	A	421	LEU
1	A	422	LYS
1	B	45	VAL
1	B	57	GLN
1	B	58	ASP
1	B	59	LEU
1	B	60	LYS
1	B	62	ASP
1	B	74	ILE

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Mol	Chain	Res	Type
1	B	94	PRO
1	B	105	VAL
1	B	123	LYS
1	B	126	LEU
1	B	136	ASN
1	B	139	THR
1	B	148	LYS
1	B	149	LYS
1	B	157	LEU
1	B	159	LYS
1	B	186	LEU
1	B	207	LEU
1	B	223	LYS
1	B	226	GLU
1	B	248	VAL
1	B	252	MET
1	B	259	THR
1	B	278	LYS
1	B	300	THR
1	B	326	PRO
1	B	331	GLN
1	B	335	LEU
1	B	347	ASN
1	B	351	LEU
1	B	382	SER
1	B	398	LEU
1	B	403	LYS
1	B	405	GLU
1	B	407	ARG
1	B	417	VAL
1	B	421	LEU
1	B	422	LYS
1	C	45	VAL
1	C	58	ASP
1	C	59	LEU
1	C	60	LYS
1	C	62	ASP
1	C	74	ILE
1	C	105	VAL
1	C	123	LYS
1	C	126	LEU
1	C	136	ASN

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Mol	Chain	Res	Type
1	C	139	THR
1	C	148	LYS
1	C	149	LYS
1	C	157	LEU
1	C	159	LYS
1	C	182	PHE
1	C	186	LEU
1	C	207	LEU
1	C	223	LYS
1	C	226	GLU
1	C	248	VAL
1	C	252	MET
1	C	259	THR
1	C	278	LYS
1	C	300	THR
1	C	331	GLN
1	C	335	LEU
1	C	347	ASN
1	C	351	LEU
1	C	382	SER
1	C	398	LEU
1	C	403	LYS
1	C	405	GLU
1	C	407	ARG
1	C	417	VAL
1	C	421	LEU
1	C	422	LYS
1	D	45	VAL
1	D	58	ASP
1	D	59	LEU
1	D	60	LYS
1	D	62	ASP
1	D	74	ILE
1	D	94	PRO
1	D	105	VAL
1	D	109	ILE
1	D	123	LYS
1	D	126	LEU
1	D	136	ASN
1	D	139	THR
1	D	148	LYS
1	D	149	LYS

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Mol	Chain	Res	Type
1	D	157	LEU
1	D	159	LYS
1	D	186	LEU
1	D	207	LEU
1	D	223	LYS
1	D	226	GLU
1	D	248	VAL
1	D	252	MET
1	D	259	THR
1	D	278	LYS
1	D	300	THR
1	D	331	GLN
1	D	335	LEU
1	D	347	ASN
1	D	351	LEU
1	D	382	SER
1	D	398	LEU
1	D	403	LYS
1	D	405	GLU
1	D	407	ARG
1	D	417	VAL
1	D	421	LEU
1	D	422	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	55	ASN
1	A	66	HIS
1	A	111	GLN
1	A	200	HIS
1	A	317	ASN
1	B	66	HIS
1	B	111	GLN
1	B	200	HIS
1	B	317	ASN
1	C	66	HIS
1	C	103	ASN
1	C	111	GLN
1	C	200	HIS
1	C	317	ASN
1	D	55	ASN

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Mol	Chain	Res	Type
1	D	66	HIS
1	D	111	GLN
1	D	200	HIS
1	D	317	ASN
1	D	347	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

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	NAA	E	1	3,2	14,14,15	1.22	2 (14%)	17,19,21	1.52	5 (29%)
2	NAA	E	2	2	14,14,15	0.84	0	17,19,21	1.56	4 (23%)
2	NAA	F	1	3,2	14,14,15	0.98	0	17,19,21	1.61	4 (23%)
2	NAA	F	2	2	14,14,15	0.97	1 (7%)	17,19,21	1.88	4 (23%)
2	NAA	G	1	3,2	14,14,15	0.95	0	17,19,21	1.49	4 (23%)
2	NAA	G	2	2	14,14,15	0.93	0	17,19,21	1.67	4 (23%)
2	NAA	H	1	3,2	14,14,15	1.12	0	17,19,21	1.52	4 (23%)
2	NAA	H	2	2	14,14,15	1.04	1 (7%)	17,19,21	1.63	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	NAA	E	1	3,2	-	2/6/23/26	0/1/1/1
2	NAA	E	2	2	-	2/6/23/26	0/1/1/1
2	NAA	F	1	3,2	-	2/6/23/26	0/1/1/1
2	NAA	F	2	2	-	2/6/23/26	0/1/1/1
2	NAA	G	1	3,2	-	2/6/23/26	0/1/1/1
2	NAA	G	2	2	-	2/6/23/26	0/1/1/1
2	NAA	H	1	3,2	-	2/6/23/26	0/1/1/1
2	NAA	H	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	E	1	NAA	O5-C1	-2.62	1.39	1.43
2	E	1	NAA	C4-C3	2.08	1.57	1.52
2	H	2	NAA	C2-N2	-2.03	1.42	1.46
2	F	2	NAA	C2-N2	-2.02	1.42	1.46

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	1	NAA	C1-C2-N2	-3.64	104.28	110.49
2	F	2	NAA	C2-N2-C7	-3.61	117.76	122.90
2	F	2	NAA	C8-C7-N2	3.50	122.02	116.10
2	E	2	NAA	C6-C5-C4	3.43	121.03	113.00
2	H	1	NAA	C1-C2-N2	-3.42	104.65	110.49
2	G	1	NAA	O3-C3-C2	3.13	115.94	109.47
2	E	1	NAA	O3-C3-C2	3.13	115.94	109.47
2	G	2	NAA	C2-N2-C7	-3.10	118.49	122.90
2	G	2	NAA	O4-C4-C3	-3.04	103.32	110.35
2	G	1	NAA	C1-C2-N2	-3.04	105.30	110.49
2	H	2	NAA	C2-N2-C7	-3.03	118.58	122.90
2	H	2	NAA	C6-C5-C4	3.02	120.08	113.00
2	F	2	NAA	C6-C5-C4	3.00	120.03	113.00
2	G	2	NAA	C6-C5-C4	2.95	119.91	113.00
2	F	2	NAA	O4-C4-C3	-2.92	103.61	110.35
2	F	1	NAA	O3-C3-C2	2.89	115.44	109.47
2	G	1	NAA	O5-C5-C6	-2.87	102.70	107.20
2	F	1	NAA	C6-C5-C4	2.86	119.69	113.00
2	E	1	NAA	C1-C2-N2	-2.77	105.75	110.49
2	G	2	NAA	C8-C7-N2	2.70	120.68	116.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	1	NAA	C6-C5-C4	2.70	119.32	113.00
2	G	1	NAA	C6-C5-C4	2.66	119.23	113.00
2	H	1	NAA	O3-C3-C2	2.66	114.96	109.47
2	F	1	NAA	O5-C5-C6	-2.65	103.04	107.20
2	E	1	NAA	O5-C5-C6	-2.57	103.18	107.20
2	H	2	NAA	C8-C7-N2	2.52	120.36	116.10
2	E	2	NAA	C2-N2-C7	-2.51	119.33	122.90
2	H	2	NAA	O4-C4-C3	-2.51	104.54	110.35
2	H	1	NAA	O5-C5-C6	-2.51	103.28	107.20
2	E	2	NAA	C1-O5-C5	-2.41	108.93	112.19
2	E	1	NAA	C6-C5-C4	2.36	118.54	113.00
2	E	2	NAA	O4-C4-C3	-2.35	104.91	110.35
2	E	1	NAA	C4-C3-C2	-2.27	107.69	111.02

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	1	NAA	C8-C7-N2-C2
2	E	1	NAA	O7-C7-N2-C2
2	F	1	NAA	C8-C7-N2-C2
2	F	1	NAA	O7-C7-N2-C2
2	G	1	NAA	C8-C7-N2-C2
2	G	1	NAA	O7-C7-N2-C2
2	H	1	NAA	C8-C7-N2-C2
2	H	1	NAA	O7-C7-N2-C2
2	E	2	NAA	C8-C7-N2-C2
2	E	2	NAA	O7-C7-N2-C2
2	F	2	NAA	C8-C7-N2-C2
2	F	2	NAA	O7-C7-N2-C2
2	G	2	NAA	C8-C7-N2-C2
2	G	2	NAA	O7-C7-N2-C2
2	H	2	NAA	C8-C7-N2-C2
2	H	2	NAA	O7-C7-N2-C2

There are no ring outliers.

8 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	2	NAA	2	0
2	F	2	NAA	3	0

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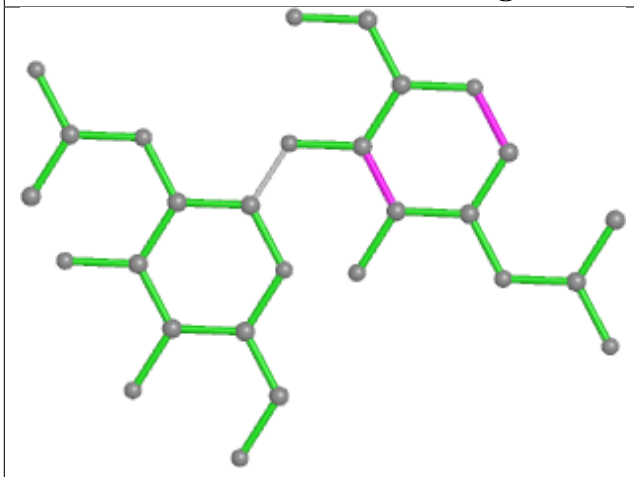
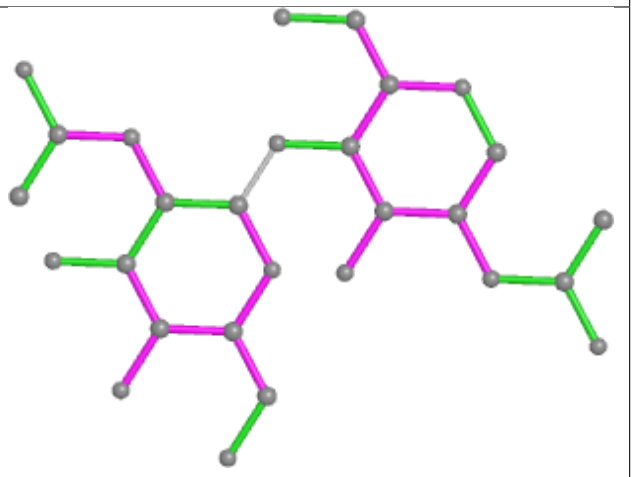
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	1	NAA	2	0
2	G	2	NAA	4	0
2	F	1	NAA	2	0
2	G	1	NAA	2	0
2	H	1	NAA	2	0
2	E	2	NAA	3	0

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

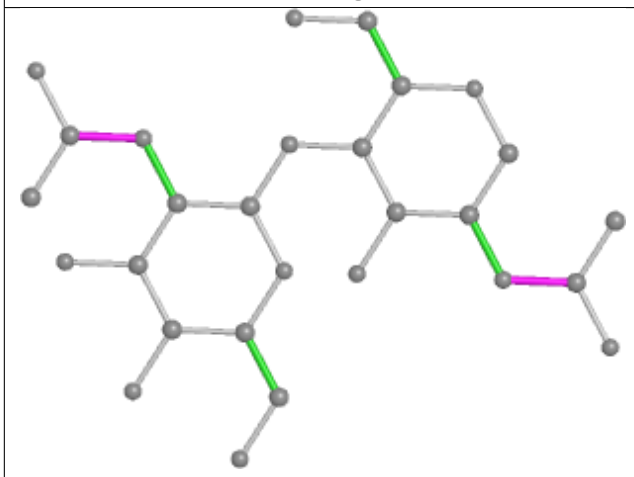
Oligosaccharide Chain E



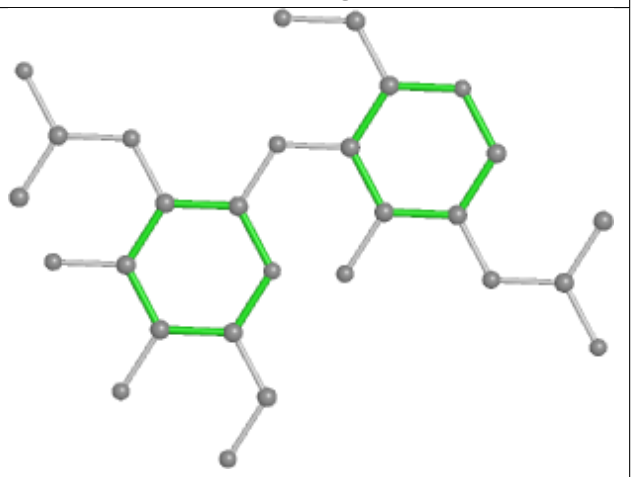
Bond lengths



Bond angles

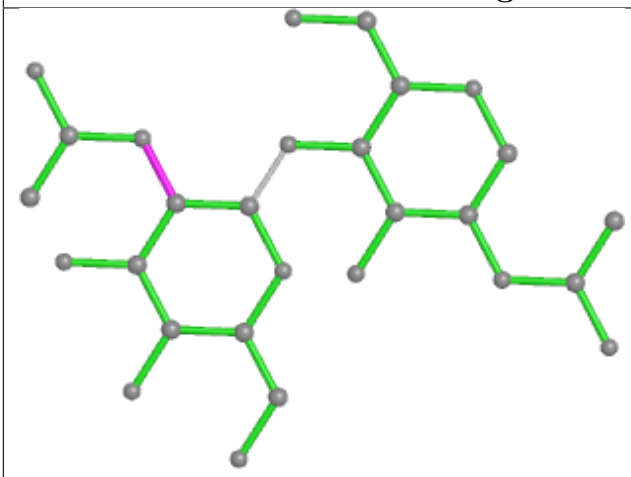


Torsions

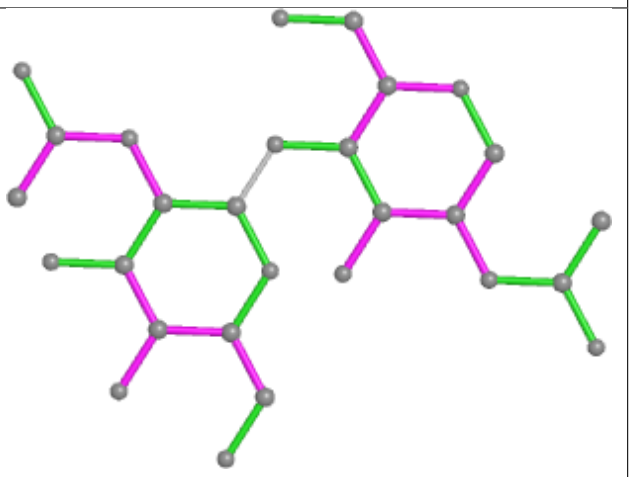


Rings

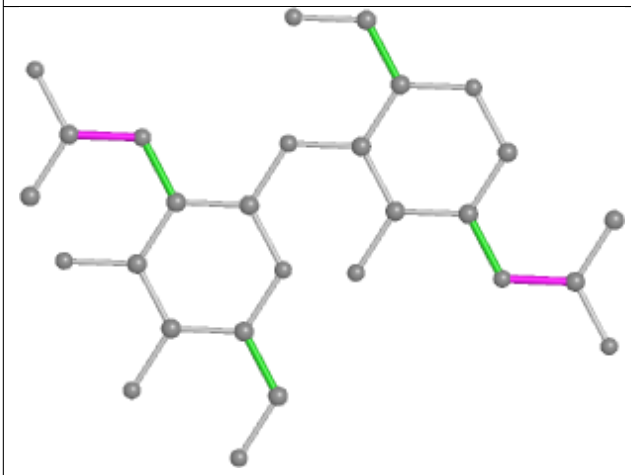
Oligosaccharide Chain F



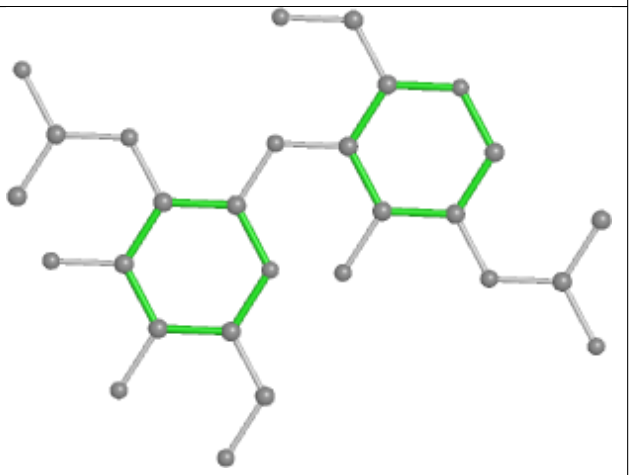
Bond lengths



Bond angles

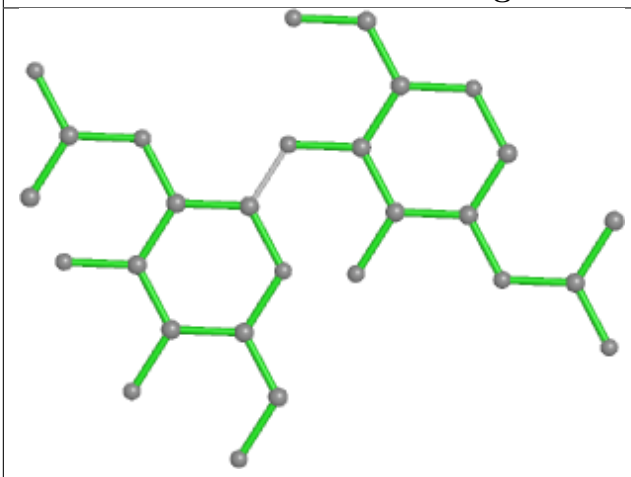


Torsions

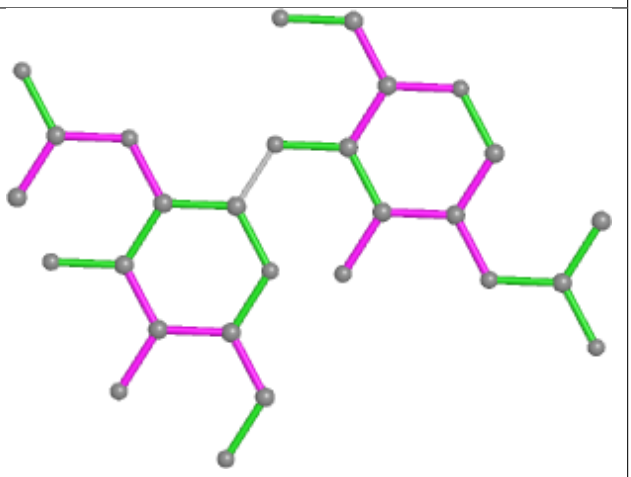


Rings

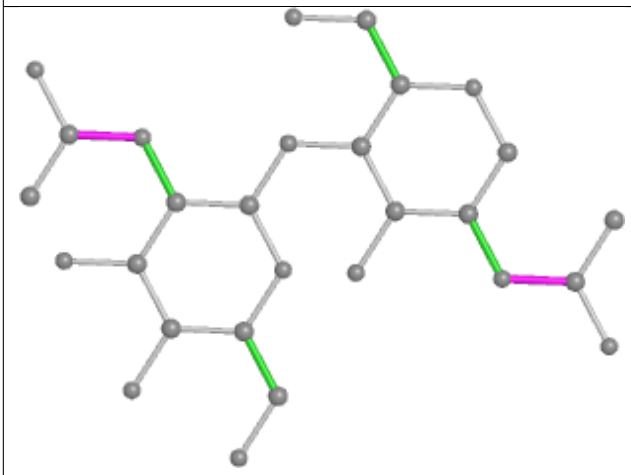
Oligosaccharide Chain G



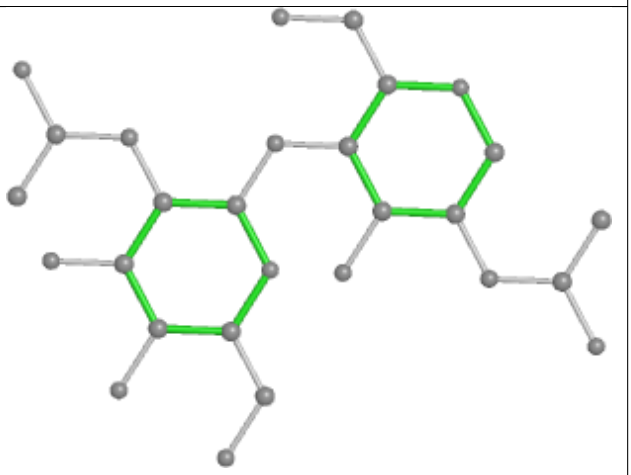
Bond lengths



Bond angles

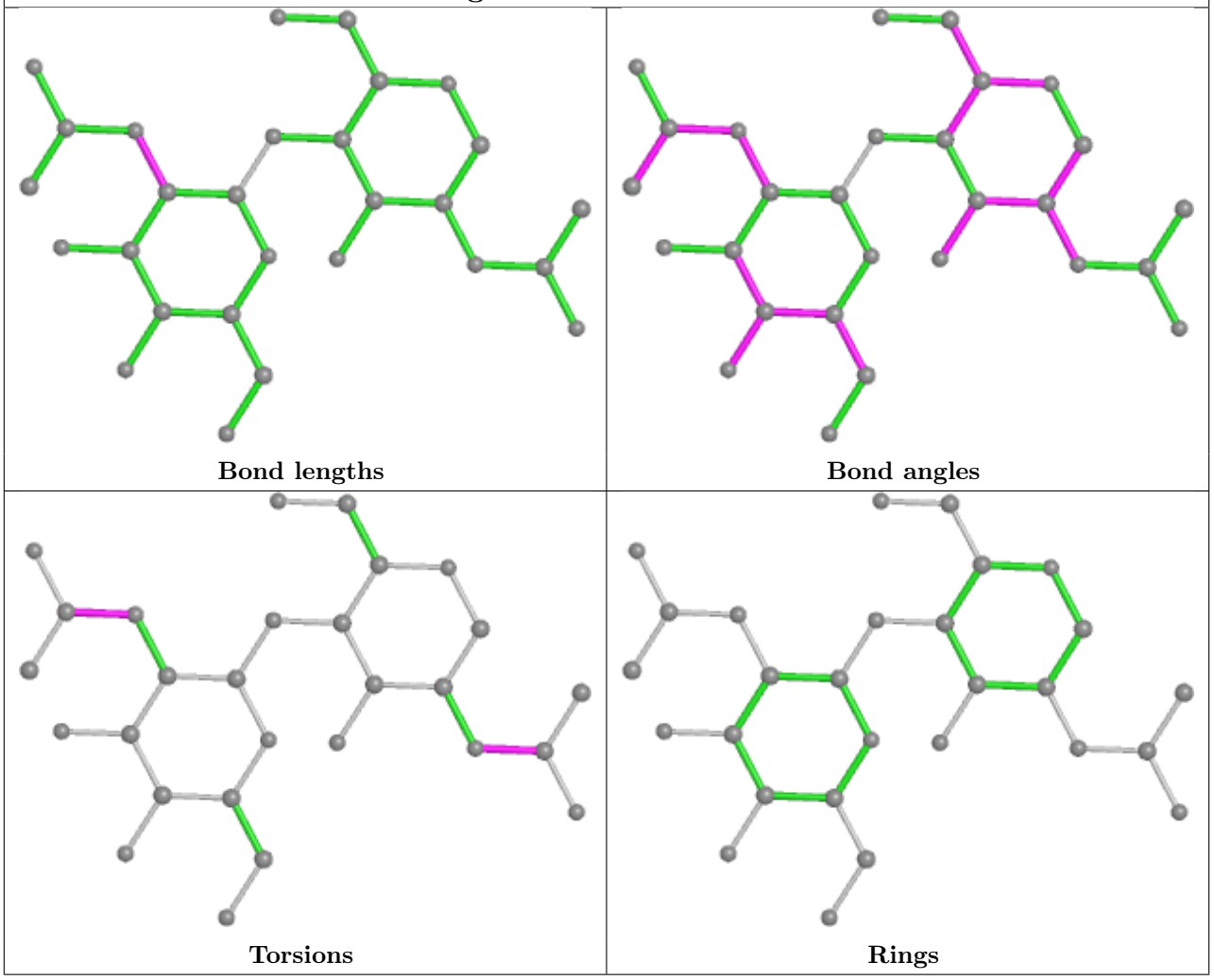


Torsions



Rings

Oligosaccharide Chain H



5.6 Ligand geometry (i)

4 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	AMI	C	503	2	13,16,16	1.42	2 (15%)	16,24,24	3.27	6 (37%)
3	AMI	D	503	2	13,16,16	1.18	1 (7%)	16,24,24	3.57	6 (37%)
3	AMI	B	503	2	13,16,16	1.63	4 (30%)	16,24,24	2.83	6 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	AMI	A	503	2	13,16,16	1.52	2 (15%)	16,24,24	2.91	5 (31%)

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	AMI	C	503	2	-	4/6/34/34	0/2/2/2
3	AMI	D	503	2	-	4/6/34/34	0/2/2/2
3	AMI	B	503	2	-	4/6/34/34	0/2/2/2
3	AMI	A	503	2	-	4/6/34/34	0/2/2/2

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	503	AMI	C2-N2	-3.79	1.43	1.47
3	B	503	AMI	C2-N2	-3.76	1.43	1.47
3	A	503	AMI	C2-N2	-3.66	1.43	1.47
3	D	503	AMI	C2-N2	-2.47	1.45	1.47
3	B	503	AMI	O7-C7	2.25	1.37	1.34
3	B	503	AMI	C4-C3	-2.20	1.47	1.53
3	A	503	AMI	C4-C3	-2.10	1.47	1.53
3	C	503	AMI	C4-C3	-2.08	1.47	1.53
3	B	503	AMI	C7-N7	2.00	1.36	1.33

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	503	AMI	O7-C7-N2	-11.74	111.57	117.80
3	C	503	AMI	O7-C7-N2	-10.88	112.03	117.80
3	A	503	AMI	O7-C7-N2	-9.07	112.99	117.80
3	B	503	AMI	O7-C7-N2	-8.38	113.36	117.80
3	D	503	AMI	O7-C1-C2	-4.84	98.30	104.40
3	B	503	AMI	C1-C2-N2	4.59	108.62	104.44
3	C	503	AMI	O7-C1-C2	-3.98	99.38	104.40
3	D	503	AMI	C1-C2-N2	3.88	107.98	104.44
3	A	503	AMI	C1-C2-N2	3.82	107.92	104.44
3	A	503	AMI	O3-C3-C2	-3.66	102.18	111.51
3	C	503	AMI	O3-C3-C2	-3.53	102.52	111.51
3	B	503	AMI	O3-C3-C2	-3.47	102.66	111.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	503	AMI	O7-C1-C2	-3.42	100.08	104.40
3	B	503	AMI	O7-C1-C2	-3.31	100.22	104.40
3	D	503	AMI	O3-C3-C2	-3.18	103.41	111.51
3	C	503	AMI	C1-C2-N2	2.87	107.05	104.44
3	D	503	AMI	C1-O7-C7	2.75	112.05	108.67
3	C	503	AMI	O3-C3-C4	2.61	120.28	111.82
3	A	503	AMI	O3-C3-C4	2.58	120.17	111.82
3	D	503	AMI	O3-C3-C4	2.40	119.60	111.82
3	B	503	AMI	O3-C3-C4	2.30	119.27	111.82
3	B	503	AMI	C4-C3-C2	-2.13	99.97	102.82
3	C	503	AMI	C4-C3-C2	-2.01	100.13	102.82

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	503	AMI	N2-C7-N7-C8
3	A	503	AMI	N2-C7-N7-C9
3	A	503	AMI	O7-C7-N7-C8
3	B	503	AMI	N2-C7-N7-C8
3	B	503	AMI	N2-C7-N7-C9
3	C	503	AMI	N2-C7-N7-C8
3	C	503	AMI	N2-C7-N7-C9
3	C	503	AMI	O7-C7-N7-C8
3	D	503	AMI	N2-C7-N7-C8
3	D	503	AMI	N2-C7-N7-C9
3	D	503	AMI	O7-C7-N7-C8
3	A	503	AMI	O7-C7-N7-C9
3	C	503	AMI	O7-C7-N7-C9
3	D	503	AMI	O7-C7-N7-C9
3	B	503	AMI	O7-C7-N7-C8
3	B	503	AMI	O7-C7-N7-C9

There are no ring outliers.

4 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	503	AMI	3	0
3	D	503	AMI	5	0
3	B	503	AMI	3	0
3	A	503	AMI	3	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, 95^{th} 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	392/392 (100%)	0.01	5 (1%) 77 72	4, 16, 25, 30	0
1	B	392/392 (100%)	0.09	10 (2%) 56 46	5, 18, 29, 40	0
1	C	392/392 (100%)	-0.04	4 (1%) 82 77	4, 16, 24, 37	0
1	D	392/392 (100%)	0.04	3 (0%) 86 81	4, 17, 25, 36	0
All	All	1568/1568 (100%)	0.03	22 (1%) 75 70	4, 17, 26, 40	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	98	TRP	6.4
1	C	427	SER	6.3
1	D	98	TRP	5.2
1	A	427	SER	4.7
1	A	98	TRP	4.3
1	B	94	PRO	3.7
1	B	301	ASP	3.1
1	C	331	GLN	2.8
1	D	427	SER	2.8
1	B	347	ASN	2.6
1	B	176	GLU	2.6
1	A	401	THR	2.5
1	A	387	ASN	2.5
1	B	250	GLY	2.4
1	B	99	ASP	2.3
1	C	36	GLY	2.3
1	C	259	THR	2.2
1	D	36	GLY	2.1
1	B	103	ASN	2.1
1	A	259	THR	2.1
1	B	427	SER	2.0
1	B	385	THR	2.0

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

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

6.3 Carbohydrates (i)

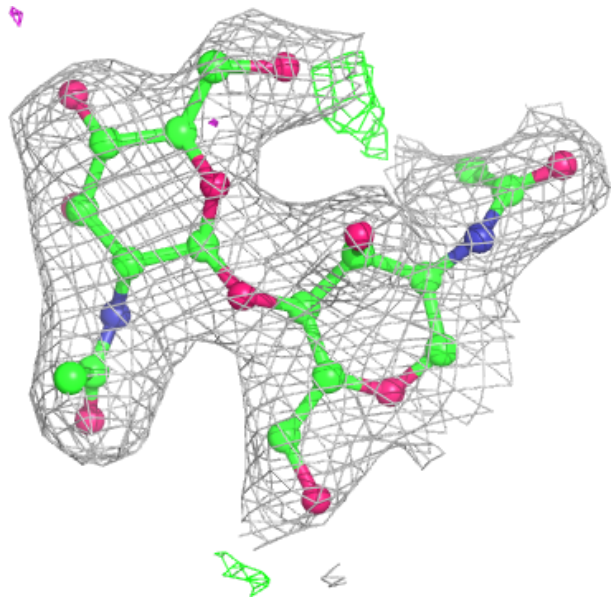
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

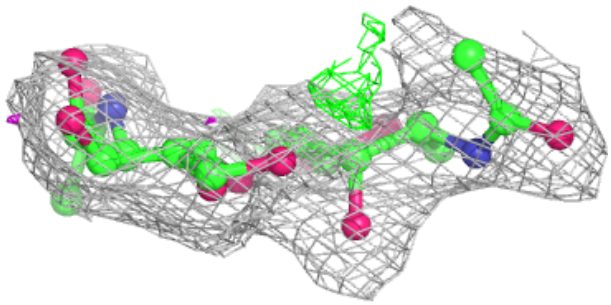
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	NAA	F	2	14/15	0.88	0.29	11,23,29,30	0
2	NAA	F	1	14/15	0.89	0.19	15,17,19,21	0
2	NAA	G	2	14/15	0.89	0.24	10,19,24,29	0
2	NAA	G	1	14/15	0.90	0.18	10,19,23,24	0
2	NAA	E	2	14/15	0.90	0.20	12,15,19,19	0
2	NAA	E	1	14/15	0.92	0.18	5,9,12,18	0
2	NAA	H	1	14/15	0.92	0.18	20,24,27,27	0
2	NAA	H	2	14/15	0.95	0.17	4,15,20,24	0

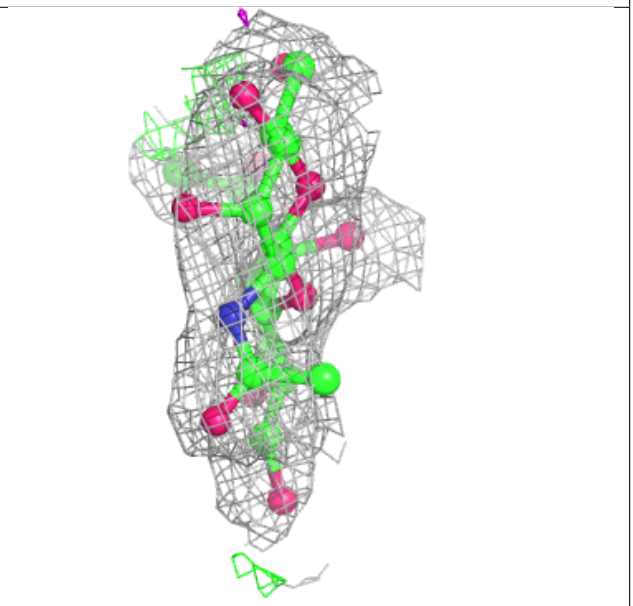
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain E:

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

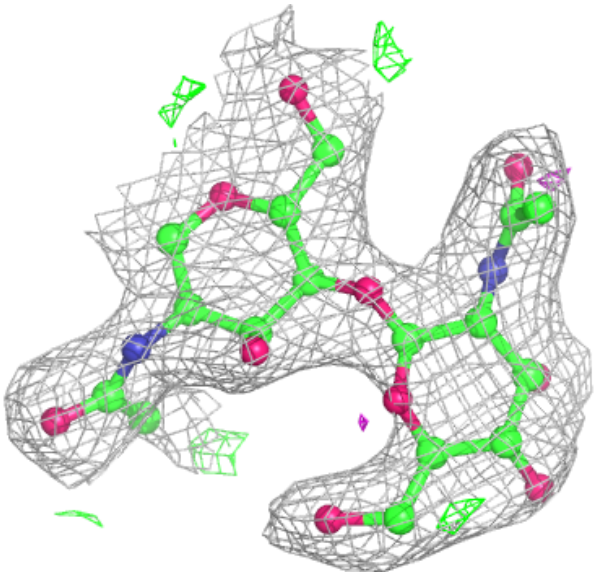


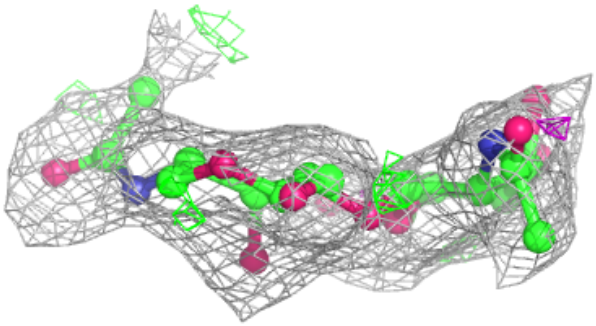


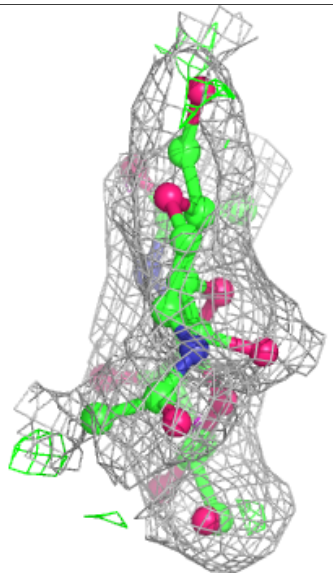


Electron density around Chain F:

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

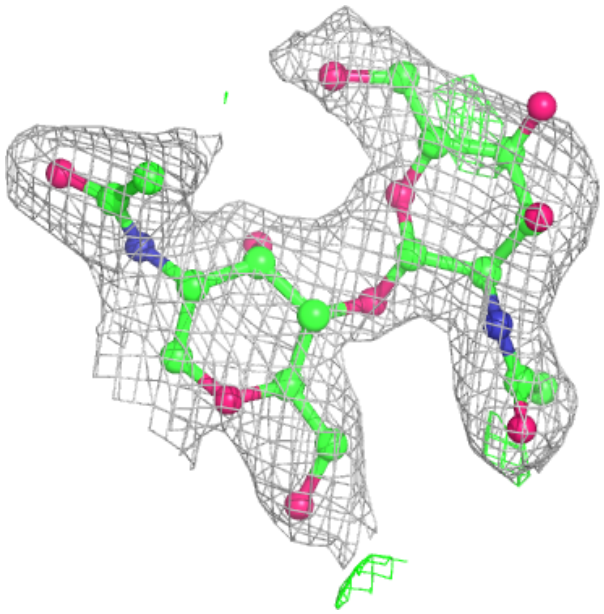


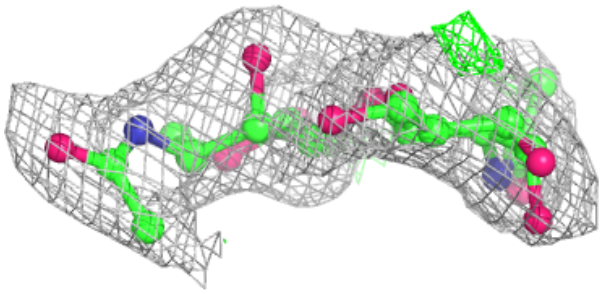


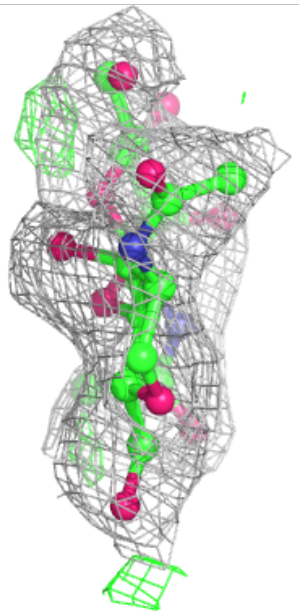


Electron density around Chain G:

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

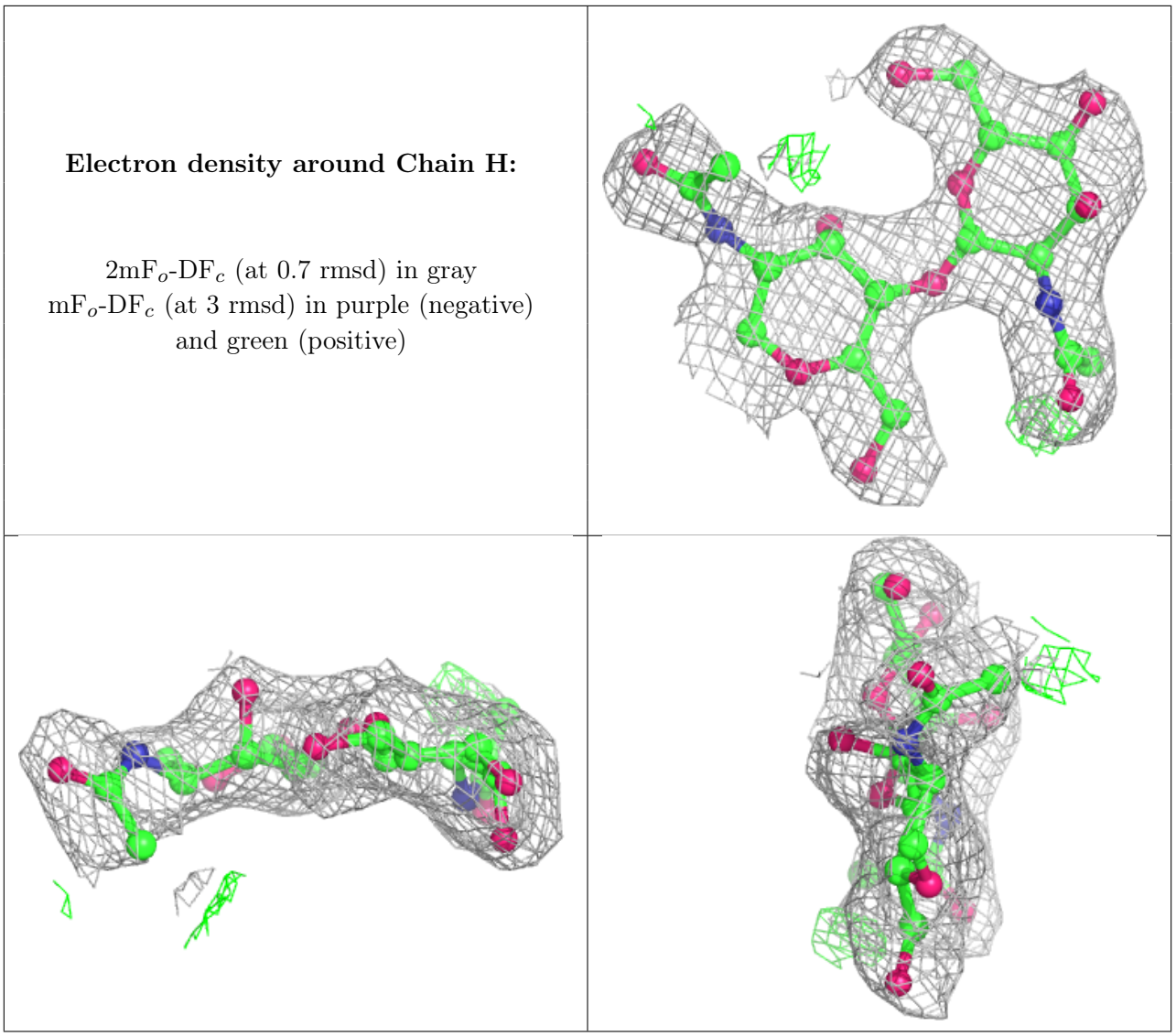






Electron density around Chain H:

$2mF_o$-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, 95^{th} 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	AMI	D	503	15/15	0.91	0.22	16,21,23,23	0
3	AMI	B	503	15/15	0.92	0.23	15,18,21,24	0
3	AMI	C	503	15/15	0.95	0.21	13,16,20,21	0
3	AMI	A	503	15/15	0.96	0.21	10,16,25,29	0

6.5 Other polymers (i)

There are no such residues in this entry.