



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 5, 2026 – 02:45 AM UTC

PDB ID : 9HUN / pdb_00009hun
Title : Crystal structure of feruloyl esterase from *Fusarium oxysporum* G122S variant in complex with benzoic acid
Authors : Karampa, P.; Dimarogona, M.; Topakas, E.; Makryniotis, K.; Nikolaivits, E.
Deposited on : 2024-12-23
Resolution : 1.71 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
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

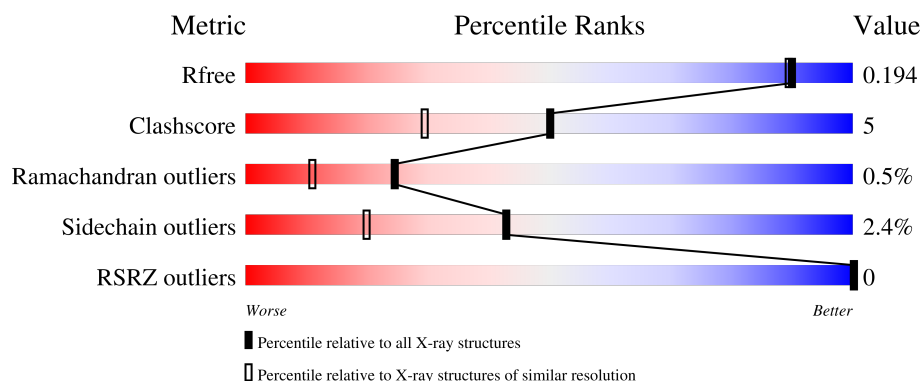
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION






The reported resolution of this entry is 1.71 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1039 (1.72-1.72)
Clashscore	190562	1049 (1.72-1.72)
Ramachandran outliers	187476	1041 (1.72-1.72)
Sidechain outliers	187428	1041 (1.72-1.72)
RSRZ outliers	180081	1039 (1.72-1.72)

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	563	
1	B	563	
2	C	8	
3	D	10	
3	E	10	

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Mol	Chain	Length	Quality of chain
3	F	10	<div><div style="width: 10%; background-color: green;"></div><div style="width: 80%; background-color: yellow;"></div><div style="width: 10%; background-color: red;"></div></div> <div>10%90%</div>

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
6	EDO	A	608	-	X	-	-
6	EDO	B	614	-	-	X	-

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 17919 atoms, of which 8375 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.

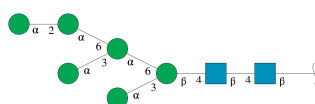
- Molecule 1 is a protein called Carboxylic ester hydrolase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	508	Total	C	H	N	O	S	124	14	0
			7923	2556	3871	701	773	22			
1	B	508	Total	C	H	N	O	S	116	7	0
			7821	2528	3816	693	762	22			

There are 2 discrepancies between the modelled and reference sequences:

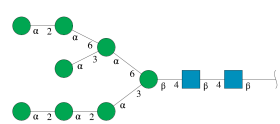
Chain	Residue	Modelled	Actual	Comment	Reference
A	122	SER	GLY	engineered mutation	UNP A0A1D3S5H0
B	122	SER	GLY	engineered mutation	UNP A0A1D3S5H0

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



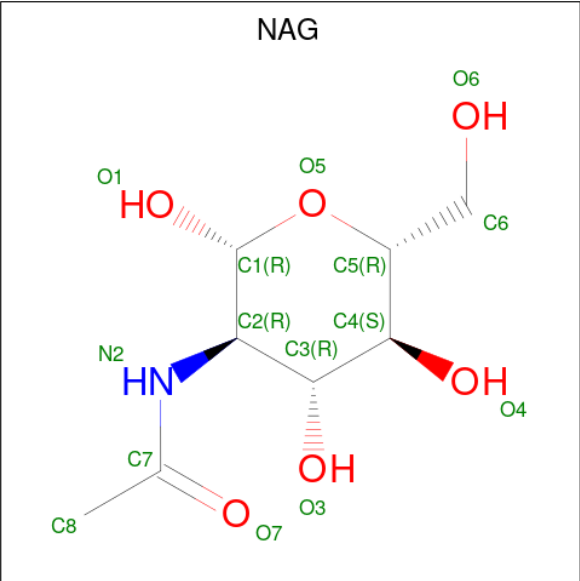
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	C	8	Total	C	H	N	O		18	0	0
			181	52	87	2	40				

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	10	Total	C	H	N	O	23	0	0
			223	64	107	2	50			
3	E	10	Total	C	H	N	O	23	0	0
			223	64	107	2	50			
3	F	10	Total	C	H	N	O	23	0	0
			223	64	107	2	50			

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	H	N	O	3	0
			28	8	14	1	5		
4	A	1	Total	C	H	N	O	3	0
			28	8	14	1	5		
4	A	1	Total	C	H	N	O	3	0
			28	8	14	1	5		
4	B	1	Total	C	H	N	O	3	0
			28	8	14	1	5		
4	B	1	Total	C	H	N	O	3	0
			28	8	14	1	5		
4	B	1	Total	C	H	N	O	3	0
			28	8	14	1	5		

- Molecule 5 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	H	O	1	0
			17	4	10	3		
5	A	1	Total	C	H	O	1	0
			17	4	10	3		
5	A	1	Total	C	H	O	1	0
			17	4	10	3		
5	B	1	Total	C	H	O	1	0
			17	4	10	3		
5	B	1	Total	C	H	O	1	0
			17	4	10	3		
5	B	1	Total	C	H	O	1	0
			17	4	10	3		
5	B	1	Total	C	H	O	1	0
			17	4	10	3		
5	B	1	Total	C	H	O	1	0
			17	4	10	3		

- Molecule 6 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



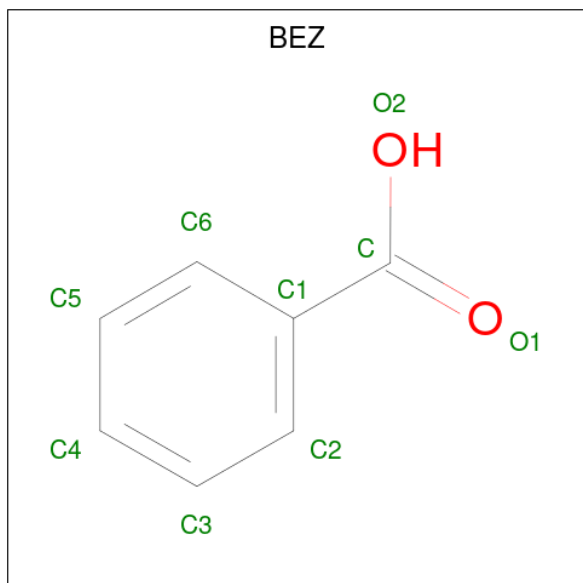
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	H	O	1	0
			10	2	6	2		
6	A	1	Total	C	H	O	1	0
			10	2	6	2		
6	A	1	Total	C	H	O	1	0
			10	2	6	2		
6	A	1	Total	C	H	O	1	0
			10	2	6	2		
6	B	1	Total	C	H	O	1	0
			10	2	6	2		
6	B	1	Total	C	H	O	1	0
			10	2	6	2		
6	B	1	Total	C	H	O	1	0
			10	2	6	2		
6	B	1	Total	C	H	O	1	0
			10	2	6	2		
6	B	1	Total	C	H	O	1	0
			10	2	6	2		
6	B	1	Total	C	H	O	1	0
			10	2	6	2		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	B	1	Total	C	H	O	1	0
			10	2	6	2		
6	B	1	Total	C	H	O	1	0
			10	2	6	2		

- Molecule 7 is BENZOIC ACID (CCD ID: BEZ) (formula: $C_7H_6O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	H	O	0	0
			14	7	5	2		
7	B	1	Total	C	H	O	0	0
			14	7	5	2		

- Molecule 8 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

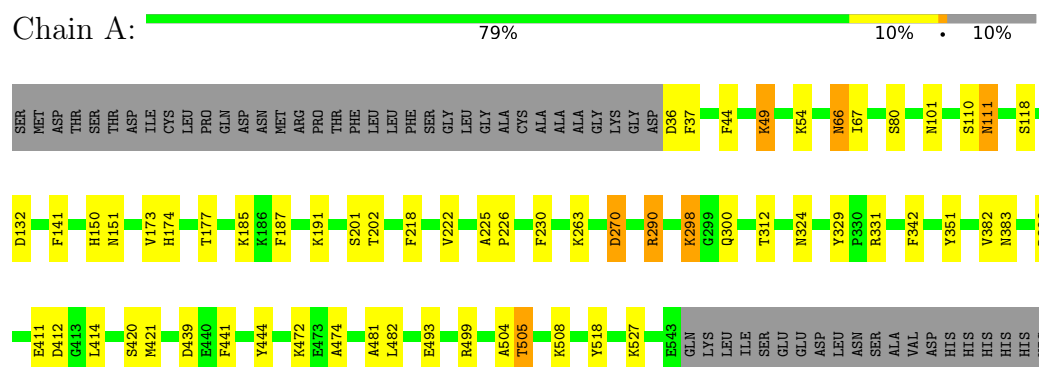
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	343	Total 343	O 343	0	0
9	B	471	Total 471	O 471	0	0

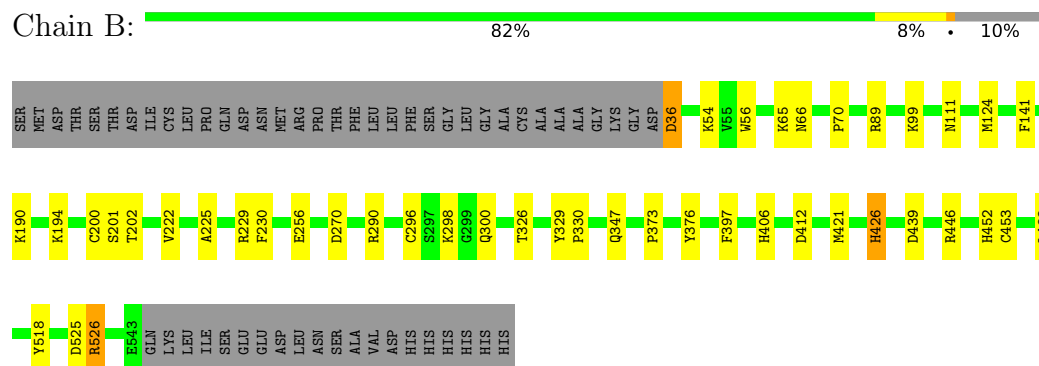
3 Residue-property plots

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.

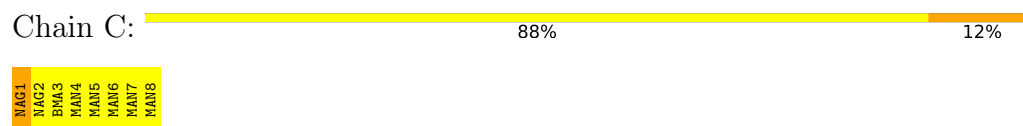
- Molecule 1: Carboxylic ester hydrolase



- Molecule 1: Carboxylic ester hydrolase



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



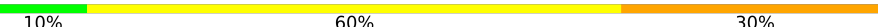
- Molecule 3: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

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

Chain D:  20% 80%

MAG1	MAG2	EMA3	MAN4	MAN5	MAN6	MAN7	MAN8	MAN9	MAN10
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● Molecule 3: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:  10% 60% 30%

MAG1	MAG2	EMA3	MAN4	MAN5	MAN6	MAN7	MAN8	MAN9	MAN10
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● Molecule 3: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:  10% 90%

MAG1	MAG2	EMA3	MAN4	MAN5	MAN6	MAN7	MAN8	MAN9	MAN10
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4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	68.00Å 89.93Å 115.15Å 90.00° 103.77° 90.00°	Depositor
Resolution (Å)	70.18 – 1.71 70.18 – 1.71	Depositor EDS
% Data completeness (in resolution range)	98.4 (70.18-1.71) 94.3 (70.18-1.71)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.50 (at 1.71Å)	Xtriage
Refinement program	REFMAC 5.8.0419, REFMAC 5.8.0419	Depositor
R, R_{free}	0.161 , 0.193 0.162 , 0.194	Depositor DCC
R_{free} test set	7145 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å ²)	26.0	Xtriage
Anisotropy	0.582	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.42 , 52.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	17919	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.27% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.76	0/4174	1.22	16/5670 (0.3%)
1	B	0.86	2/4118 (0.0%)	1.24	16/5594 (0.3%)
All	All	0.81	2/8292 (0.0%)	1.23	32/11264 (0.3%)

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	3
1	B	0	1
All	All	0	4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	426	HIS	CG-CD2	-6.09	1.29	1.35
1	B	225	ALA	C-O	-5.40	1.21	1.23

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	229	ARG	NE-CZ-NH1	-7.47	114.03	121.50
1	B	397	PHE	CA-CB-CG	6.71	120.51	113.80
1	A	439	ASP	CA-CB-CG	6.61	119.21	112.60
1	A	132	ASP	CA-CB-CG	6.60	119.20	112.60
1	B	439	ASP	CA-CB-CG	6.57	119.17	112.60
1	B	36	ASP	CA-CB-CG	6.43	119.03	112.60
1	A	270	ASP	CA-CB-CG	6.35	118.95	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	300	GLN	N-CA-CB	6.35	119.32	109.85
1	A	141	PHE	CA-CB-CG	6.05	119.85	113.80
1	A	312	THR	CA-CB-OG1	-6.00	100.60	109.60
1	A	290	ARG	NE-CZ-NH1	-5.98	115.52	121.50
1	B	141	PHE	CA-CB-CG	5.93	119.73	113.80
1	A	411	GLU	CB-CA-C	-5.88	100.61	110.56
1	A	527	LYS	CB-CA-C	-5.84	98.79	110.42
1	A	351	TYR	N-CA-CB	5.80	118.65	110.12
1	B	229	ARG	NE-CZ-NH2	5.80	124.42	119.20
1	A	412	ASP	CA-CB-CG	5.77	118.37	112.60
1	A	342	PHE	CB-CA-C	5.72	120.41	110.79
1	B	446	ARG	NE-CZ-NH2	5.69	124.32	119.20
1	B	446	ARG	NE-CZ-NH1	-5.62	115.88	121.50
1	A	329	TYR	O-C-N	-5.47	116.43	122.17
1	B	526	ARG	CG-CD-NE	-5.39	100.15	112.00
1	B	406	HIS	CA-CB-CG	5.32	119.12	113.80
1	A	504	ALA	CA-C-N	5.31	127.40	120.28
1	A	504	ALA	C-N-CA	5.31	127.40	120.28
1	B	290	ARG	CB-CA-C	5.31	115.75	110.33
1	B	525	ASP	CA-CB-CG	5.31	117.91	112.60
1	B	452	HIS	CA-CB-CG	-5.14	108.66	113.80
1	A	505	THR	CA-CB-OG1	-5.13	101.90	109.60
1	B	229	ARG	CB-CG-CD	5.13	123.10	111.30
1	B	412	ASP	CA-CB-CG	5.09	117.69	112.60
1	B	496	THR	CA-CB-OG1	-5.07	102.00	109.60

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	290	ARG	Sidechain
1	A	331	ARG	Peptide
1	A	499	ARG	Sidechain
1	B	526	ARG	Sidechain

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	4052	3871	3851	45	0
1	B	4005	3816	3798	34	0
2	C	94	87	79	4	0
3	D	116	107	97	0	0
3	E	116	107	97	3	0
3	F	116	107	97	0	0
4	A	42	42	39	8	0
4	B	42	42	39	9	0
5	A	21	30	30	2	0
5	B	42	60	60	3	0
6	A	20	30	30	1	0
6	B	44	66	66	11	0
7	A	9	5	5	2	0
7	B	9	5	5	0	0
8	A	1	0	0	0	0
8	B	1	0	0	0	0
9	A	343	0	0	6	0
9	B	471	0	0	10	0
All	All	9544	8375	8293	89	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 5.

All (89) 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:A:101:ASN:HD21	4:A:601:NAG:C1	0.90	1.52
1:A:151:ASN:ND2	2:C:1:NAG:C1	1.67	1.52
1:B:66:ASN:HD21	4:B:604:NAG:C1	0.94	1.52
1:A:101:ASN:ND2	4:A:601:NAG:C1	1.76	1.46
1:B:66:ASN:ND2	4:B:604:NAG:C1	1.78	1.39
1:B:111:ASN:OD1	4:B:606:NAG:C1	1.81	1.29
1:A:66:ASN:OD1	4:A:606:NAG:C1	1.88	1.20
1:A:111:ASN:OD1	4:A:607:NAG:C1	2.09	1.01
1:A:420[B]:SER:OG	1:A:444:TYR:CZ	2.27	0.86
1:B:70:PRO:HD2	6:B:614:EDO:H21	1.61	0.82
1:B:111:ASN:CG	4:B:606:NAG:C1	2.55	0.79
1:A:151:ASN:CG	2:C:1:NAG:C1	2.55	0.78
1:A:403:LYS:NZ	9:A:702:HOH:O	2.18	0.77
1:B:194:LYS:NZ	9:B:701:HOH:O	2.18	0.77
5:A:610:PEG:H22	9:A:988:HOH:O	1.86	0.75
1:A:111:ASN:HD22	1:A:111:ASN:C	1.98	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:89:ARG:HH12	6:B:614:EDO:H11	1.58	0.68
1:A:324:ASN:OD1	9:A:701:HOH:O	2.14	0.65
1:A:101:ASN:CG	4:A:601:NAG:C1	2.66	0.65
9:B:913:HOH:O	3:E:9:MAN:O6	2.15	0.63
1:B:326[A]:THR:HG21	9:B:1093:HOH:O	1.99	0.62
1:A:177[B]:THR:HG21	1:A:218:PHE:HZ	1.63	0.62
1:B:89:ARG:HH12	6:B:614:EDO:C1	2.14	0.61
1:B:89:ARG:HH22	6:B:614:EDO:H22	1.66	0.60
1:A:151:ASN:ND2	2:C:1:NAG:C2	2.60	0.60
1:B:222:VAL:HG23	1:B:482:LEU:HD22	1.86	0.57
1:A:222:VAL:HG23	1:A:482:LEU:HD22	1.86	0.57
1:B:89:ARG:HH22	6:B:614:EDO:C2	2.18	0.56
1:B:426:HIS:HD2	9:B:1073:HOH:O	1.88	0.56
1:A:177[B]:THR:HG21	1:A:218:PHE:CZ	2.41	0.55
9:A:848:HOH:O	5:B:608:PEG:H31	2.04	0.55
1:B:66:ASN:CG	4:B:604:NAG:C1	2.73	0.54
1:B:329:TYR:CG	1:B:330:PRO:HD2	2.44	0.53
1:A:111:ASN:C	1:A:111:ASN:ND2	2.66	0.52
1:B:124[A]:MET:HA	1:B:124[A]:MET:HE2	1.90	0.52
1:A:398[A]:ARG:HG3	1:A:441:PHE:CD1	2.45	0.52
1:A:66:ASN:C	1:A:66:ASN:HD22	2.15	0.51
1:B:190:LYS:HE3	5:B:607:PEG:H22	1.90	0.51
1:B:66:ASN:ND2	4:B:604:NAG:C2	2.69	0.51
1:A:173:VAL:O	1:A:177[B]:THR:HG23	2.11	0.50
1:A:66:ASN:HD22	1:A:67:ILE:N	2.08	0.50
1:A:124[B]:MET:HE1	1:A:230:PHE:HZ	1.77	0.50
1:B:300:GLN:HB2	9:B:1016:HOH:O	2.11	0.49
1:A:414:LEU:CD1	7:A:609:BEZ:H3	2.43	0.49
1:B:124[A]:MET:HE2	1:B:124[A]:MET:CA	2.42	0.49
1:B:373:PRO:HA	1:B:376:TYR:CD2	2.48	0.49
1:A:49:LYS:HA	1:A:49:LYS:HE2	1.94	0.48
1:A:118:SER:HB2	1:A:177[B]:THR:HG22	1.96	0.48
6:A:611:EDO:C2	9:A:746:HOH:O	2.60	0.48
1:B:124[A]:MET:HE1	1:B:230:PHE:HZ	1.78	0.48
1:A:111:ASN:CG	4:A:607:NAG:C1	2.85	0.47
6:B:611:EDO:C2	9:B:836:HOH:O	2.62	0.47
1:A:126:GLY:HA2	1:A:150:HIS:O	2.15	0.47
1:A:225:ALA:N	1:A:226:PRO:CD	2.78	0.47
1:B:111:ASN:OD1	4:B:606:NAG:C2	2.58	0.47
1:A:382:VAL:O	1:A:383:ASN:C	2.57	0.47
1:A:406:HIS:NE2	1:A:420[B]:SER:HB2	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:612:PEG:H31	9:B:822:HOH:O	2.15	0.47
1:A:44:PHE:CZ	1:A:187:PHE:HB2	2.50	0.47
1:B:54:LYS:HE3	1:B:56:TRP:CZ3	2.50	0.46
1:B:89:ARG:NH2	6:B:614:EDO:H22	2.30	0.46
1:B:99:LYS:HE3	1:B:99:LYS:HB2	1.69	0.46
1:A:414:LEU:HD11	7:A:609:BEZ:H3	1.96	0.46
1:A:398[B]:ARG:HD3	9:A:875:HOH:O	2.16	0.46
1:B:111:ASN:ND2	4:B:606:NAG:C1	2.79	0.45
1:A:474:ALA:O	1:A:481:ALA:HB2	2.16	0.45
6:B:618:EDO:H11	3:E:6:MAN:O6	2.17	0.44
1:A:174:HIS:O	1:A:177[B]:THR:OG1	2.36	0.44
1:B:296:CYS:HB2	9:B:716:HOH:O	2.17	0.44
6:B:622:EDO:H22	9:B:841:HOH:O	2.17	0.43
1:A:80:SER:OG	4:A:606:NAG:H83	2.19	0.43
1:A:101:ASN:ND2	4:A:601:NAG:C2	2.72	0.43
1:A:37:PHE:CE1	1:A:110[B]:SER:HA	2.53	0.43
1:A:472:LYS:NZ	5:A:612:PEG:H32	2.34	0.43
1:B:256:GLU:H	1:B:256:GLU:CD	2.27	0.42
1:B:66:ASN:ND2	4:B:604:NAG:O5	2.46	0.42
1:A:225:ALA:N	1:A:226:PRO:HD3	2.34	0.42
1:B:124[A]:MET:HE1	1:B:168:TYR:OH	2.19	0.42
1:B:200[B]:CYS:SG	1:B:453:CYS:SG	3.10	0.42
1:A:66:ASN:C	1:A:66:ASN:ND2	2.77	0.41
1:A:151:ASN:ND2	2:C:1:NAG:O5	2.42	0.41
1:A:420[B]:SER:OG	1:A:444:TYR:OH	2.30	0.41
1:A:37:PHE:CE1	1:A:110[A]:SER:HA	2.55	0.41
1:A:421:MET:HG3	1:A:518:TYR:CZ	2.56	0.41
1:A:66:ASN:HD21	1:A:80:SER:HB2	1.86	0.41
1:B:421:MET:HG3	1:B:518:TYR:CZ	2.55	0.41
1:B:329:TYR:CD1	1:B:330:PRO:HD2	2.56	0.40
6:B:609:EDO:H22	9:B:1092:HOH:O	2.21	0.40
6:B:618:EDO:H22	3:E:7:MAN:C6	2.52	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	521/563 (92%)	509 (98%)	8 (2%)	4 (1%)	16	5
1	B	513/563 (91%)	502 (98%)	8 (2%)	3 (1%)	21	9
All	All	1034/1126 (92%)	1011 (98%)	16 (2%)	7 (1%)	24	7

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	201[A]	SER
1	A	201[B]	SER
1	A	298	LYS
1	B	201[A]	SER
1	B	201[B]	SER
1	A	270	ASP
1	B	270	ASP

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	435/466 (93%)	421 (97%)	14 (3%)	34	11
1	B	427/466 (92%)	420 (98%)	7 (2%)	55	34
All	All	862/932 (92%)	841 (98%)	21 (2%)	43	20

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	ASP
1	A	49	LYS
1	A	54	LYS
1	A	66	ASN
1	A	111	ASN

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Mol	Chain	Res	Type
1	A	185	LYS
1	A	191	LYS
1	A	202	THR
1	A	263	LYS
1	A	298	LYS
1	A	493[A]	GLU
1	A	493[B]	GLU
1	A	505	THR
1	A	508	LYS
1	B	36	ASP
1	B	65	LYS
1	B	160	LYS
1	B	202	THR
1	B	298	LYS
1	B	347	GLN
1	B	505	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	101	ASN
1	A	264	ASN
1	A	435	ASN
1	B	66	ASN
1	B	435	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](#)

38 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	14,14,15	0.34	0	17,19,21	0.87	1 (5%)
2	NAG	C	2	2	14,14,15	0.49	0	17,19,21	0.96	1 (5%)
2	BMA	C	3	2	11,11,12	0.59	0	15,15,17	1.21	1 (6%)
2	MAN	C	4	2	11,11,12	1.13	1 (9%)	15,15,17	1.22	1 (6%)
2	MAN	C	5	2	11,11,12	1.01	1 (9%)	15,15,17	1.38	1 (6%)
2	MAN	C	6	2	11,11,12	0.94	0	15,15,17	1.11	2 (13%)
2	MAN	C	7	2	11,11,12	0.77	0	15,15,17	0.79	1 (6%)
2	MAN	C	8	2	11,11,12	0.84	0	15,15,17	1.27	2 (13%)
3	NAG	D	1	3,1	14,14,15	0.47	0	17,19,21	1.11	1 (5%)
3	MAN	D	10	3	11,11,12	0.96	1 (9%)	15,15,17	0.58	0
3	NAG	D	2	3	14,14,15	0.70	0	17,19,21	0.77	0
3	BMA	D	3	3	11,11,12	0.63	0	15,15,17	0.90	0
3	MAN	D	4	3	11,11,12	0.88	1 (9%)	15,15,17	1.73	2 (13%)
3	MAN	D	5	3	11,11,12	0.84	0	15,15,17	1.06	1 (6%)
3	MAN	D	6	3	11,11,12	1.19	1 (9%)	15,15,17	1.16	1 (6%)
3	MAN	D	7	3	11,11,12	1.44	1 (9%)	15,15,17	0.96	0
3	MAN	D	8	3	11,11,12	1.26	1 (9%)	15,15,17	1.44	2 (13%)
3	MAN	D	9	3	11,11,12	0.92	1 (9%)	15,15,17	1.51	2 (13%)
3	NAG	E	1	3	14,14,15	0.40	0	17,19,21	0.81	1 (5%)
3	MAN	E	10	3	11,11,12	1.53	2 (18%)	15,15,17	1.05	1 (6%)
3	NAG	E	2	3	14,14,15	0.54	0	17,19,21	0.98	1 (5%)
3	BMA	E	3	3	11,11,12	0.54	0	15,15,17	0.92	0
3	MAN	E	4	3	11,11,12	1.00	1 (9%)	15,15,17	1.37	2 (13%)
3	MAN	E	5	3	11,11,12	1.31	1 (9%)	15,15,17	1.74	3 (20%)
3	MAN	E	6	3	11,11,12	1.56	2 (18%)	15,15,17	1.53	3 (20%)
3	MAN	E	7	3	11,11,12	0.57	0	15,15,17	0.85	1 (6%)
3	MAN	E	8	3	11,11,12	1.23	2 (18%)	15,15,17	0.98	1 (6%)
3	MAN	E	9	3	11,11,12	0.92	0	15,15,17	0.85	1 (6%)
3	NAG	F	1	3	14,14,15	0.37	0	17,19,21	1.01	0
3	MAN	F	10	3	11,11,12	0.55	0	15,15,17	1.04	1 (6%)
3	NAG	F	2	3	14,14,15	0.69	0	17,19,21	1.16	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	BMA	F	3	3	11,11,12	1.09	1 (9%)	15,15,17	1.10	1 (6%)
3	MAN	F	4	3	11,11,12	1.29	2 (18%)	15,15,17	0.85	1 (6%)
3	MAN	F	5	3	11,11,12	0.94	0	15,15,17	1.71	4 (26%)
3	MAN	F	6	3	11,11,12	0.67	0	15,15,17	1.27	2 (13%)
3	MAN	F	7	3	11,11,12	0.64	0	15,15,17	1.29	2 (13%)
3	MAN	F	8	3	11,11,12	1.06	1 (9%)	15,15,17	0.62	0
3	MAN	F	9	3	11,11,12	1.25	1 (9%)	15,15,17	1.09	2 (13%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	C	1	2	-	0/6/23/26	0/1/1/1
2	NAG	C	2	2	-	1/6/23/26	0/1/1/1
2	BMA	C	3	2	-	0/2/19/22	0/1/1/1
2	MAN	C	4	2	-	0/2/19/22	0/1/1/1
2	MAN	C	5	2	-	0/2/19/22	0/1/1/1
2	MAN	C	6	2	-	2/2/19/22	0/1/1/1
2	MAN	C	7	2	-	2/2/19/22	0/1/1/1
2	MAN	C	8	2	-	2/2/19/22	0/1/1/1
3	NAG	D	1	3,1	-	0/6/23/26	0/1/1/1
3	MAN	D	10	3	-	0/2/19/22	0/1/1/1
3	NAG	D	2	3	-	0/6/23/26	0/1/1/1
3	BMA	D	3	3	-	0/2/19/22	0/1/1/1
3	MAN	D	4	3	-	2/2/19/22	0/1/1/1
3	MAN	D	5	3	-	0/2/19/22	0/1/1/1
3	MAN	D	6	3	-	0/2/19/22	0/1/1/1
3	MAN	D	7	3	-	0/2/19/22	0/1/1/1
3	MAN	D	8	3	-	2/2/19/22	0/1/1/1
3	MAN	D	9	3	-	2/2/19/22	0/1/1/1
3	NAG	E	1	3	-	0/6/23/26	0/1/1/1
3	MAN	E	10	3	-	1/2/19/22	0/1/1/1
3	NAG	E	2	3	-	0/6/23/26	0/1/1/1
3	BMA	E	3	3	-	0/2/19/22	0/1/1/1
3	MAN	E	4	3	-	0/2/19/22	0/1/1/1
3	MAN	E	5	3	-	0/2/19/22	0/1/1/1
3	MAN	E	6	3	-	0/2/19/22	0/1/1/1
3	MAN	E	7	3	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	MAN	E	8	3	-	0/2/19/22	0/1/1/1
3	MAN	E	9	3	-	0/2/19/22	0/1/1/1
3	NAG	F	1	3	-	0/6/23/26	0/1/1/1
3	MAN	F	10	3	-	0/2/19/22	0/1/1/1
3	NAG	F	2	3	-	0/6/23/26	0/1/1/1
3	BMA	F	3	3	-	0/2/19/22	0/1/1/1
3	MAN	F	4	3	-	0/2/19/22	0/1/1/1
3	MAN	F	5	3	-	2/2/19/22	0/1/1/1
3	MAN	F	6	3	-	0/2/19/22	0/1/1/1
3	MAN	F	7	3	-	0/2/19/22	0/1/1/1
3	MAN	F	8	3	-	0/2/19/22	0/1/1/1
3	MAN	F	9	3	-	0/2/19/22	0/1/1/1

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	7	MAN	O5-C5	3.97	1.51	1.43
3	E	6	MAN	C4-C5	3.48	1.60	1.53
3	E	10	MAN	C2-C3	3.19	1.57	1.52
3	D	8	MAN	O5-C5	3.01	1.49	1.43
3	F	4	MAN	C2-C3	3.00	1.57	1.52
2	C	5	MAN	O5-C5	2.99	1.49	1.43
2	C	4	MAN	O5-C5	2.85	1.49	1.43
3	F	8	MAN	O5-C5	2.72	1.48	1.43
3	D	10	MAN	O5-C5	2.72	1.48	1.43
3	D	6	MAN	O5-C5	2.71	1.48	1.43
3	F	4	MAN	O5-C5	2.65	1.48	1.43
3	F	3	BMA	O5-C5	2.58	1.48	1.43
3	E	6	MAN	C1-C2	-2.53	1.46	1.52
3	E	8	MAN	O5-C5	2.48	1.48	1.43
3	F	9	MAN	O5-C1	2.42	1.47	1.43
3	D	4	MAN	C4-C5	2.39	1.58	1.53
3	E	4	MAN	C4-C5	-2.25	1.48	1.53
3	E	5	MAN	C4-C3	-2.17	1.46	1.52
3	D	9	MAN	C4-C5	2.07	1.57	1.53
3	E	10	MAN	C4-C5	2.07	1.57	1.53
3	E	8	MAN	C4-C5	2.04	1.57	1.53

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	4	MAN	C1-O5-C5	5.20	119.16	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	5	MAN	C1-O5-C5	4.96	118.84	112.19
3	E	5	MAN	C1-O5-C5	4.16	117.77	112.19
3	D	9	MAN	C1-O5-C5	3.93	117.46	112.19
3	D	8	MAN	C1-O5-C5	3.74	117.19	112.19
3	F	7	MAN	C1-O5-C5	3.70	117.14	112.19
2	C	8	MAN	C1-C2-C3	3.67	114.98	109.64
3	F	6	MAN	C1-C2-C3	3.64	114.94	109.64
3	F	5	MAN	C1-C2-C3	3.62	114.91	109.64
3	D	6	MAN	C1-O5-C5	3.57	116.97	112.19
2	C	4	MAN	C1-O5-C5	3.35	116.68	112.19
3	E	6	MAN	C1-O5-C5	3.02	116.24	112.19
3	D	4	MAN	C1-C2-C3	2.87	113.83	109.64
3	E	5	MAN	O3-C3-C4	2.85	117.10	110.38
3	F	5	MAN	O2-C2-C3	-2.79	104.38	110.15
2	C	2	NAG	C1-C2-N2	2.76	114.78	110.43
3	E	6	MAN	O2-C2-C3	2.71	115.77	110.15
3	F	5	MAN	C1-O5-C5	2.70	115.81	112.19
3	E	9	MAN	C1-O5-C5	2.67	115.77	112.19
2	C	6	MAN	C1-O5-C5	2.64	115.73	112.19
3	E	10	MAN	C1-O5-C5	2.58	115.65	112.19
2	C	3	BMA	O4-C4-C5	-2.58	102.96	109.32
3	E	8	MAN	O2-C2-C3	-2.52	104.94	110.15
2	C	6	MAN	C1-C2-C3	2.45	113.21	109.64
3	E	2	NAG	O4-C4-C5	-2.43	103.35	109.32
3	F	10	MAN	O2-C2-C3	-2.43	105.13	110.15
3	E	6	MAN	O3-C3-C2	-2.38	105.20	110.05
3	F	2	NAG	C2-N2-C7	2.37	126.07	122.90
3	F	2	NAG	C1-C2-N2	2.33	114.11	110.43
3	F	9	MAN	O2-C2-C3	2.33	114.97	110.15
3	F	3	BMA	C1-O5-C5	-2.31	109.08	112.19
3	F	5	MAN	O3-C3-C2	-2.25	105.47	110.05
2	C	1	NAG	C1-C2-N2	-2.23	106.92	110.43
3	D	9	MAN	C1-C2-C3	2.23	112.89	109.64
2	C	8	MAN	C1-O5-C5	2.23	115.17	112.19
3	D	5	MAN	C1-C2-C3	2.20	112.84	109.64
3	D	1	NAG	C1-C2-N2	2.18	113.87	110.43
3	F	9	MAN	C1-O5-C5	2.14	115.06	112.19
3	F	4	MAN	C1-O5-C5	2.14	115.05	112.19
3	E	5	MAN	O4-C4-C5	-2.13	104.08	109.32
3	F	6	MAN	O3-C3-C2	-2.13	105.72	110.05
3	D	8	MAN	C1-C2-C3	2.10	112.70	109.64
3	E	4	MAN	C2-C3-C4	-2.09	107.18	110.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	4	MAN	C1-O5-C5	2.07	114.96	112.19
3	E	7	MAN	C1-O5-C5	2.06	114.95	112.19
3	E	1	NAG	C1-O5-C5	-2.06	109.43	112.19
3	F	7	MAN	C6-C5-C4	-2.04	108.00	113.02
2	C	7	MAN	C1-O5-C5	2.01	114.89	112.19

There are no chirality outliers.

All (16) torsion outliers are listed below:

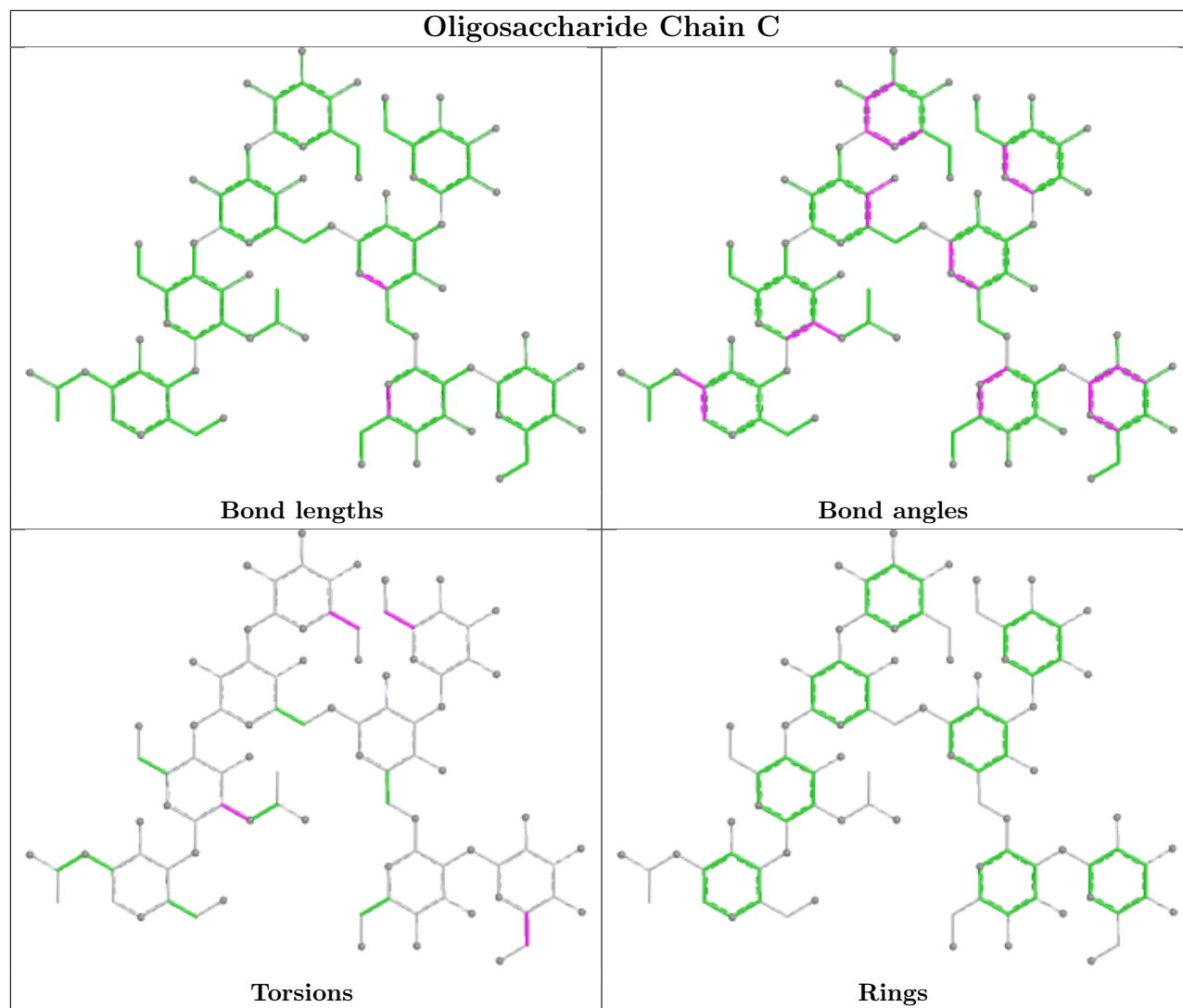
Mol	Chain	Res	Type	Atoms
2	C	7	MAN	O5-C5-C6-O6
3	D	9	MAN	O5-C5-C6-O6
3	F	5	MAN	O5-C5-C6-O6
2	C	8	MAN	O5-C5-C6-O6
2	C	7	MAN	C4-C5-C6-O6
3	D	9	MAN	C4-C5-C6-O6
2	C	8	MAN	C4-C5-C6-O6
3	F	5	MAN	C4-C5-C6-O6
3	D	4	MAN	C4-C5-C6-O6
2	C	6	MAN	C4-C5-C6-O6
3	D	4	MAN	O5-C5-C6-O6
2	C	6	MAN	O5-C5-C6-O6
3	E	10	MAN	O5-C5-C6-O6
3	D	8	MAN	C4-C5-C6-O6
2	C	2	NAG	C1-C2-N2-C7
3	D	8	MAN	O5-C5-C6-O6

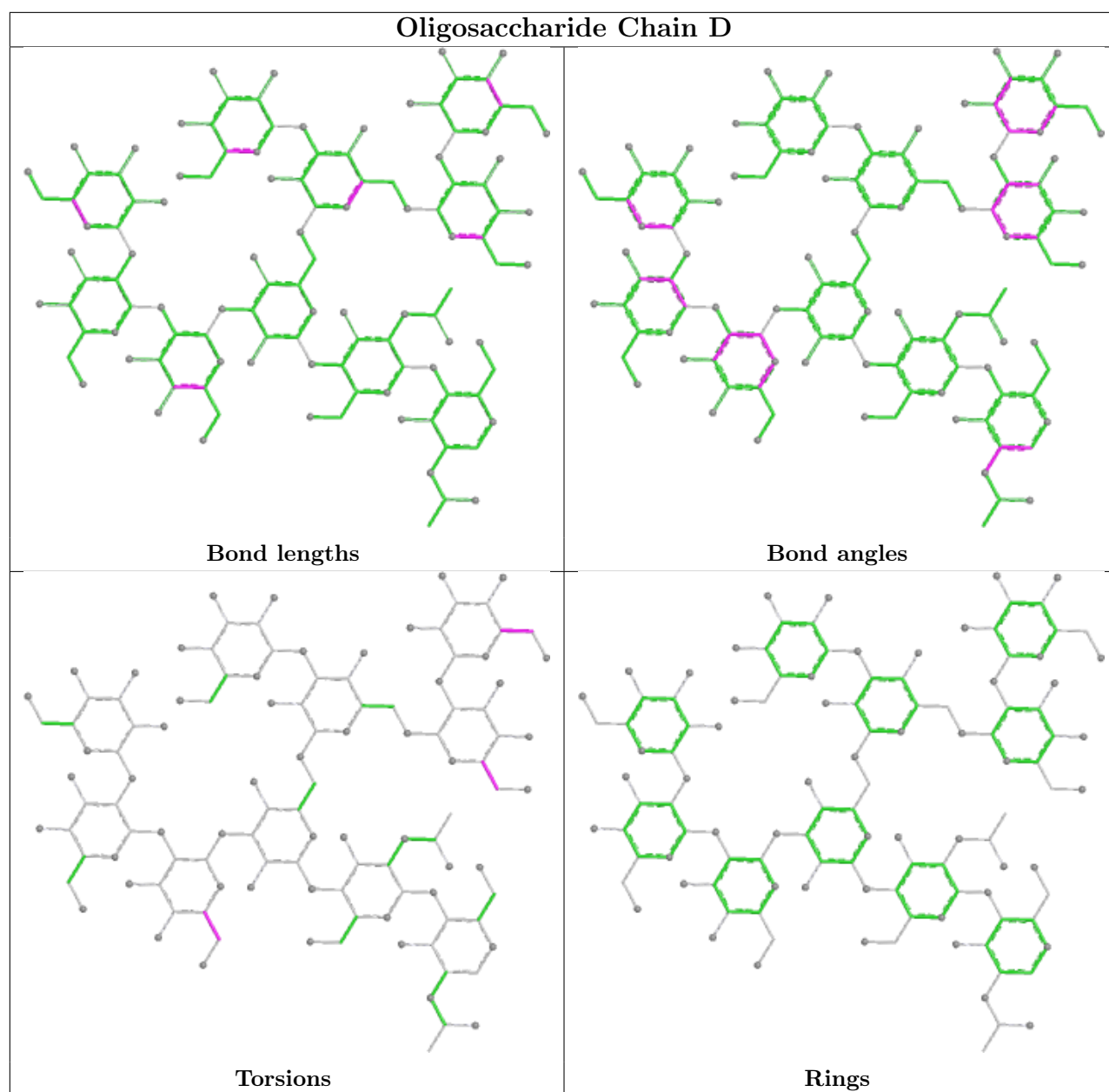
There are no ring outliers.

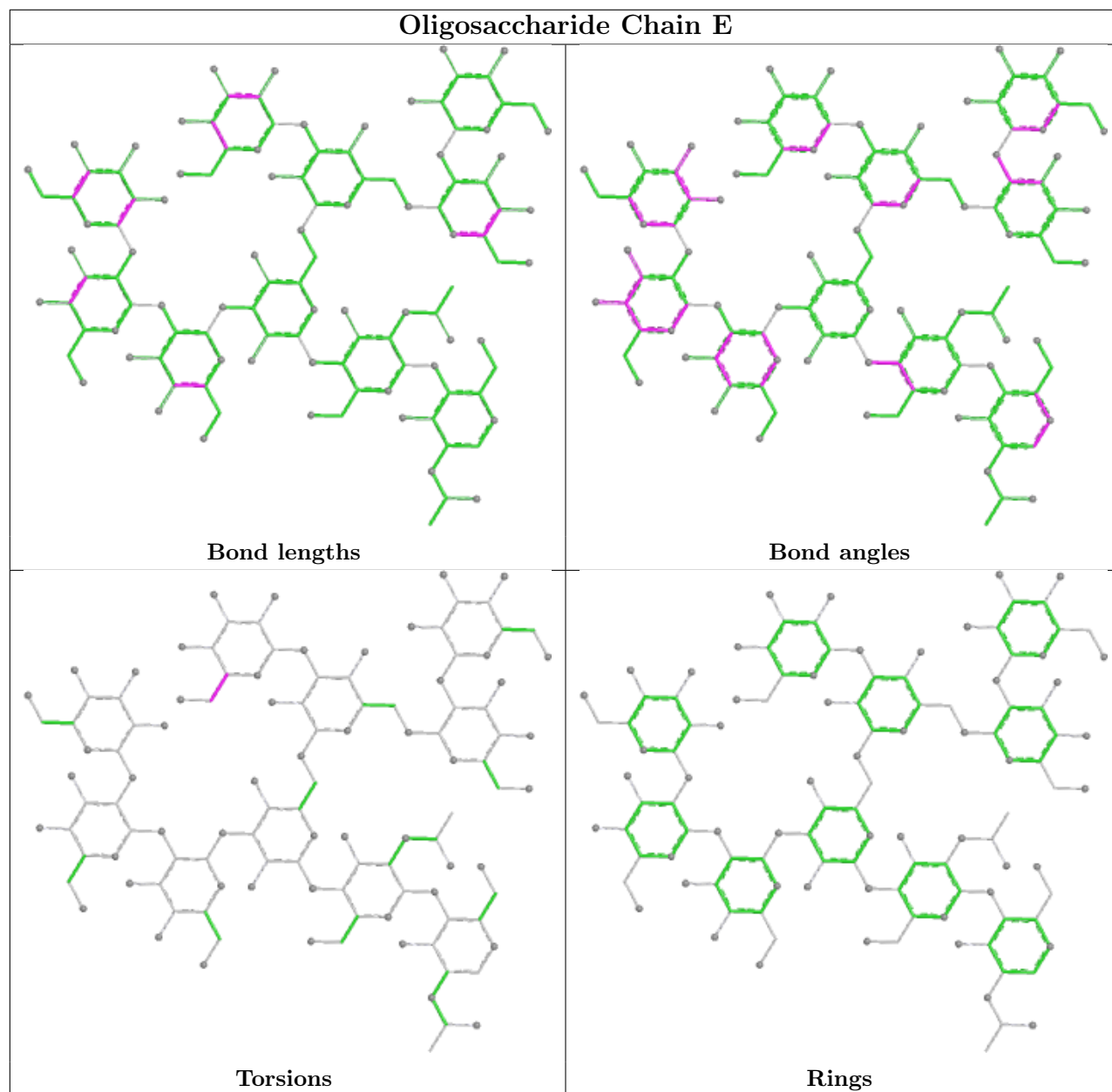
4 monomers are involved in 7 short contacts:

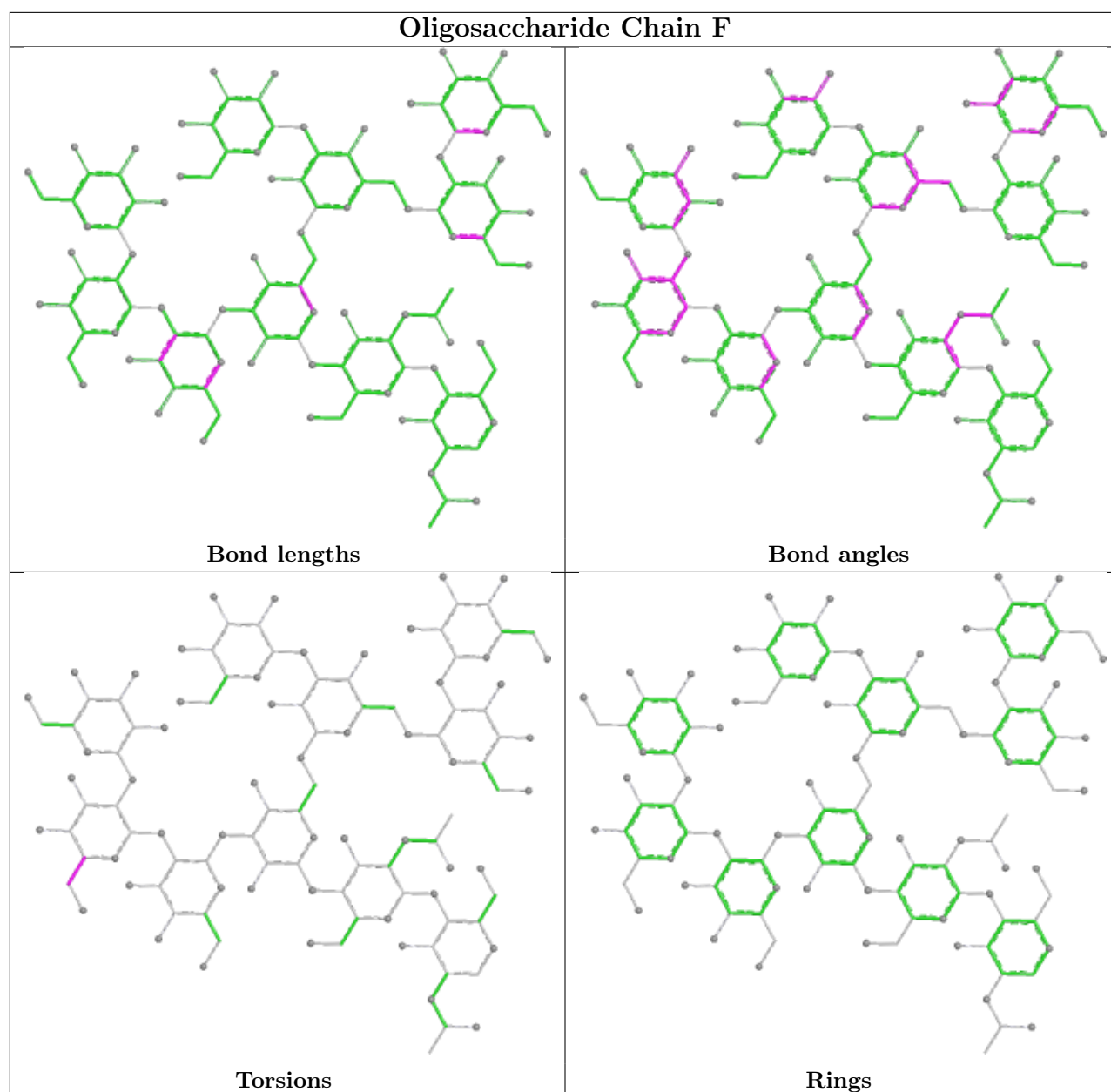
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	7	MAN	1	0
3	E	9	MAN	1	0
2	C	1	NAG	4	0
3	E	6	MAN	1	0

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









5.6 Ligand geometry [i](#)

Of 35 ligands modelled in this entry, 2 are monoatomic - leaving 33 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
6	EDO	B	603	-	3,3,3	0.15	0	2,2,2	0.35	0
4	NAG	B	604	-	14,14,15	0.43	0	17,19,21	0.82	0
6	EDO	A	611	-	3,3,3	1.00	0	2,2,2	0.77	0
6	EDO	B	618	-	3,3,3	0.39	0	2,2,2	0.40	0
5	PEG	B	601	-	6,6,6	0.24	0	5,5,5	0.19	0
5	PEG	A	610	-	6,6,6	0.27	0	5,5,5	0.26	0
6	EDO	B	616	-	3,3,3	0.40	0	2,2,2	0.78	0
5	PEG	B	612	-	6,6,6	0.41	0	5,5,5	0.24	0
6	EDO	B	620	-	3,3,3	0.36	0	2,2,2	0.50	0
4	NAG	B	605	1	14,14,15	0.69	0	17,19,21	1.09	1 (5%)
6	EDO	B	622	-	3,3,3	0.58	0	2,2,2	0.76	0
7	BEZ	B	617	-	9,9,9	1.93	3 (33%)	11,11,11	0.79	0
6	EDO	A	605	-	3,3,3	0.52	0	2,2,2	0.49	0
5	PEG	B	613	-	6,6,6	0.23	0	5,5,5	0.10	0
6	EDO	A	603	-	3,3,3	0.16	0	2,2,2	0.12	0
5	PEG	B	608	-	6,6,6	0.22	0	5,5,5	0.20	0
6	EDO	B	614	-	3,3,3	0.27	0	2,2,2	0.37	0
5	PEG	A	602	-	6,6,6	0.20	0	5,5,5	0.16	0
4	NAG	A	606	-	14,14,15	0.43	0	17,19,21	1.85	3 (17%)
6	EDO	B	610	-	3,3,3	0.16	0	2,2,2	0.79	0
4	NAG	B	606	-	14,14,15	0.42	0	17,19,21	1.10	1 (5%)
6	EDO	A	604	-	3,3,3	0.23	0	2,2,2	0.30	0
6	EDO	B	619	-	3,3,3	0.44	0	2,2,2	0.32	0
6	EDO	B	609	-	3,3,3	0.36	0	2,2,2	0.39	0
6	EDO	B	615	-	3,3,3	0.27	0	2,2,2	0.34	0
4	NAG	A	607	-	14,14,15	0.44	0	17,19,21	1.03	0
4	NAG	A	601	-	14,14,15	0.47	0	17,19,21	1.04	2 (11%)
5	PEG	B	602	-	6,6,6	0.29	0	5,5,5	0.17	0
7	BEZ	A	609	-	9,9,9	1.13	1 (11%)	11,11,11	1.36	2 (18%)
6	EDO	A	608	-	3,3,3	2.02	2 (66%)	2,2,2	1.49	0
6	EDO	B	611	-	3,3,3	0.64	0	2,2,2	0.42	0
5	PEG	A	612	-	6,6,6	0.22	0	5,5,5	0.38	0
5	PEG	B	607	-	6,6,6	0.23	0	5,5,5	0.15	0

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
6	EDO	B	603	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	B	604	-	-	0/6/23/26	0/1/1/1
6	EDO	A	611	-	-	1/1/1/1	-
6	EDO	B	618	-	-	1/1/1/1	-
5	PEG	B	601	-	-	3/4/4/4	-
5	PEG	A	610	-	-	3/4/4/4	-
6	EDO	B	616	-	-	1/1/1/1	-
5	PEG	B	612	-	-	2/4/4/4	-
6	EDO	B	620	-	-	1/1/1/1	-
4	NAG	B	605	1	-	1/6/23/26	0/1/1/1
6	EDO	B	622	-	-	1/1/1/1	-
7	BEZ	B	617	-	-	0/4/4/4	0/1/1/1
6	EDO	A	605	-	-	0/1/1/1	-
5	PEG	B	613	-	-	4/4/4/4	-
6	EDO	A	603	-	-	0/1/1/1	-
5	PEG	B	608	-	-	3/4/4/4	-
6	EDO	B	614	-	-	0/1/1/1	-
5	PEG	A	602	-	-	2/4/4/4	-
4	NAG	A	606	-	-	5/6/23/26	0/1/1/1
6	EDO	B	610	-	-	0/1/1/1	-
4	NAG	B	606	-	-	0/6/23/26	0/1/1/1
6	EDO	A	604	-	-	0/1/1/1	-
6	EDO	B	619	-	-	1/1/1/1	-
6	EDO	B	609	-	-	1/1/1/1	-
6	EDO	B	615	-	-	1/1/1/1	-
4	NAG	A	607	-	-	2/6/23/26	0/1/1/1
4	NAG	A	601	-	-	1/6/23/26	0/1/1/1
5	PEG	B	602	-	-	2/4/4/4	-
7	BEZ	A	609	-	-	0/4/4/4	0/1/1/1
6	EDO	A	608	-	-	1/1/1/1	-
6	EDO	B	611	-	-	1/1/1/1	-
5	PEG	A	612	-	-	3/4/4/4	-
5	PEG	B	607	-	-	3/4/4/4	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	617	BEZ	O1-C	4.49	1.35	1.22
6	A	608	EDO	O2-C2	2.58	1.55	1.42
7	B	617	BEZ	C1-C	2.58	1.54	1.49
7	A	609	BEZ	C1-C	2.53	1.54	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	617	BEZ	O2-C	-2.37	1.23	1.30
6	A	608	EDO	O1-C1	2.08	1.52	1.42

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	606	NAG	C2-N2-C7	5.72	130.56	122.90
4	B	606	NAG	C2-N2-C7	3.50	127.59	122.90
7	A	609	BEZ	O2-C-C1	3.08	122.75	114.84
4	B	605	NAG	O5-C1-C2	-3.03	106.60	111.29
7	A	609	BEZ	O1-C-C1	-2.94	113.74	121.46
4	A	606	NAG	C3-C4-C5	-2.50	105.70	110.23
4	A	606	NAG	O5-C5-C4	-2.49	104.78	110.83
4	A	601	NAG	C1-C2-N2	-2.21	106.96	110.43
4	A	601	NAG	C2-N2-C7	2.04	125.64	122.90

There are no chirality outliers.

All (44) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	606	NAG	C3-C2-N2-C7
4	A	606	NAG	C8-C7-N2-C2
4	A	606	NAG	O7-C7-N2-C2
4	A	607	NAG	C8-C7-N2-C2
4	A	607	NAG	O7-C7-N2-C2
5	A	610	PEG	O2-C3-C4-O4
5	B	602	PEG	O1-C1-C2-O2
4	A	606	NAG	O5-C5-C6-O6
5	B	601	PEG	O1-C1-C2-O2
5	B	601	PEG	O2-C3-C4-O4
5	B	612	PEG	O2-C3-C4-O4
5	A	602	PEG	O2-C3-C4-O4
5	A	612	PEG	O1-C1-C2-O2
5	A	610	PEG	O1-C1-C2-O2
5	B	608	PEG	O1-C1-C2-O2
6	B	618	EDO	O1-C1-C2-O2
4	A	606	NAG	C4-C5-C6-O6
5	B	602	PEG	O2-C3-C4-O4
5	B	613	PEG	O1-C1-C2-O2
5	A	612	PEG	C1-C2-O2-C3
6	A	608	EDO	O1-C1-C2-O2
6	A	611	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
6	B	620	EDO	O1-C1-C2-O2
6	B	622	EDO	O1-C1-C2-O2
5	B	608	PEG	O2-C3-C4-O4
5	A	610	PEG	C1-C2-O2-C3
5	B	608	PEG	C1-C2-O2-C3
5	B	613	PEG	C4-C3-O2-C2
5	B	601	PEG	C4-C3-O2-C2
5	B	607	PEG	O2-C3-C4-O4
5	B	612	PEG	C4-C3-O2-C2
5	B	607	PEG	C1-C2-O2-C3
6	B	619	EDO	O1-C1-C2-O2
4	A	601	NAG	C4-C5-C6-O6
5	B	613	PEG	O2-C3-C4-O4
5	B	607	PEG	O1-C1-C2-O2
6	B	609	EDO	O1-C1-C2-O2
6	B	611	EDO	O1-C1-C2-O2
6	B	616	EDO	O1-C1-C2-O2
6	B	615	EDO	O1-C1-C2-O2
4	B	605	NAG	C4-C5-C6-O6
5	A	612	PEG	C4-C3-O2-C2
5	A	602	PEG	C1-C2-O2-C3
5	B	613	PEG	C1-C2-O2-C3

There are no ring outliers.

17 monomers are involved in 36 short contacts:

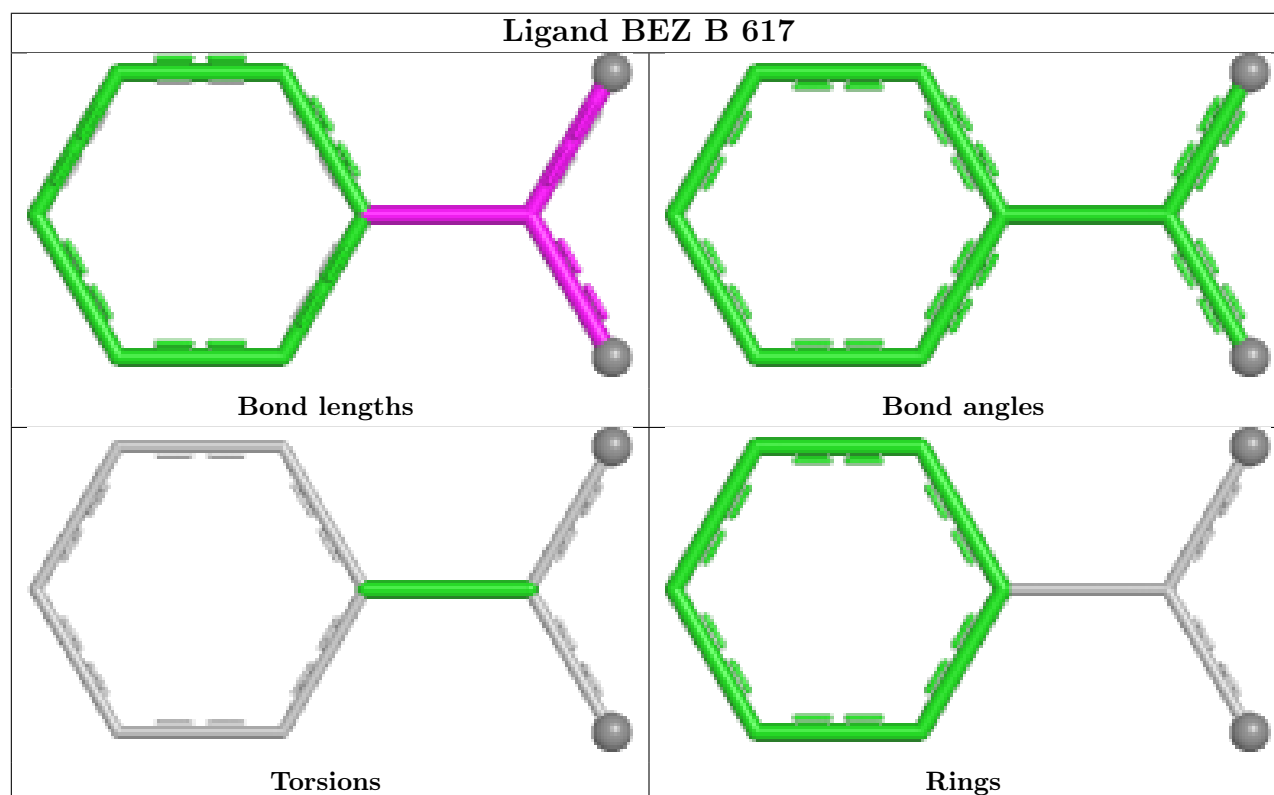
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	604	NAG	5	0
6	A	611	EDO	1	0
6	B	618	EDO	2	0
5	A	610	PEG	1	0
5	B	612	PEG	1	0
6	B	622	EDO	1	0
5	B	608	PEG	1	0
6	B	614	EDO	6	0
4	A	606	NAG	2	0
4	B	606	NAG	4	0
6	B	609	EDO	1	0
4	A	607	NAG	2	0
4	A	601	NAG	4	0
7	A	609	BEZ	2	0
6	B	611	EDO	1	0

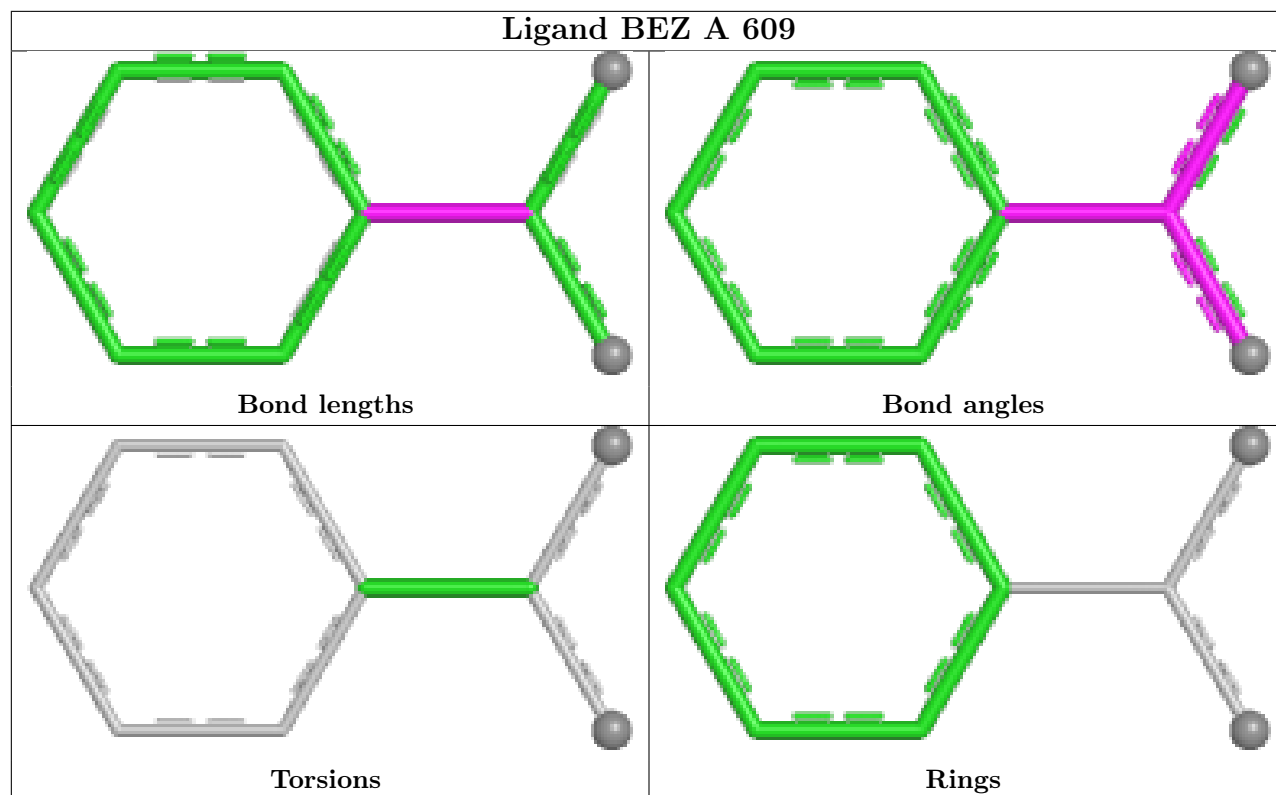
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	612	PEG	1	0
5	B	607	PEG	1	0

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





5.7 Other polymers [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	508/563 (90%)	-0.13	0 100 100	10, 44, 70, 96	14 (2%)
1	B	508/563 (90%)	-0.31	0 100 100	15, 38, 59, 103	7 (1%)
All	All	1016/1126 (90%)	-0.22	0 100 100	10, 41, 66, 103	21 (2%)

There are no RSRZ outliers to report.

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
2	MAN	C	8	11/12	0.69	0.10	30,98,102,106	3
2	MAN	C	6	11/12	0.75	0.13	30,89,95,97	3
2	MAN	C	7	11/12	0.86	0.13	30,94,99,104	3
2	MAN	C	5	11/12	0.86	0.14	30,94,99,102	2
3	MAN	D	9	11/12	0.88	0.11	30,62,67,72	3
2	BMA	C	3	11/12	0.89	0.09	30,73,88,90	1
3	MAN	E	9	11/12	0.89	0.10	30,62,71,78	3
2	MAN	C	4	11/12	0.91	0.08	30,76,81,82	2
3	MAN	D	4	11/12	0.91	0.08	30,47,55,63	2
3	MAN	E	10	11/12	0.92	0.09	30,51,54,55	3
2	NAG	C	2	14/15	0.93	0.09	30,59,64,70	2

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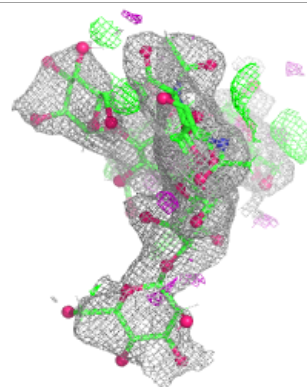
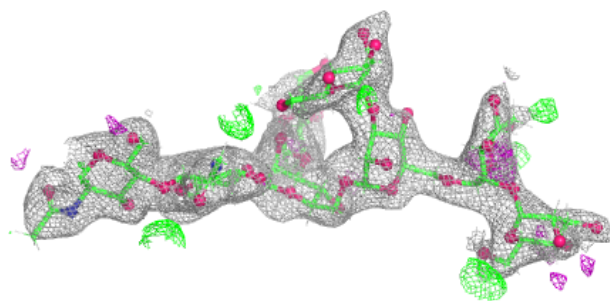
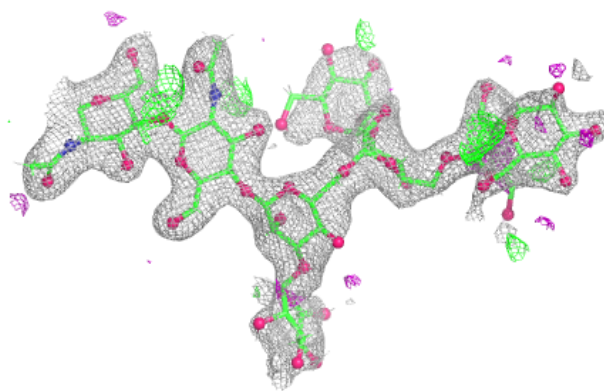
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	MAN	F	4	11/12	0.93	0.07	30,36,42,49	2
3	MAN	E	4	11/12	0.94	0.08	30,40,46,48	2
3	MAN	D	6	11/12	0.95	0.07	30,52,55,56	3
3	MAN	E	6	11/12	0.95	0.07	30,40,42,46	3
3	MAN	E	8	11/12	0.95	0.07	30,50,55,55	2
3	MAN	F	5	11/12	0.95	0.07	30,42,45,48	3
3	MAN	F	6	11/12	0.95	0.07	30,48,51,56	3
3	MAN	E	7	11/12	0.96	0.06	30,48,51,54	2
3	NAG	D	1	14/15	0.96	0.06	30,42,46,49	2
3	MAN	D	8	11/12	0.96	0.06	30,38,41,44	2
3	NAG	D	2	14/15	0.96	0.06	30,46,58,59	2
3	NAG	F	2	14/15	0.96	0.06	30,41,49,53	2
2	NAG	C	1	14/15	0.96	0.07	30,54,62,64	2
3	MAN	E	5	11/12	0.96	0.07	30,38,42,44	3
3	MAN	D	5	11/12	0.96	0.06	30,49,54,57	3
3	MAN	F	10	11/12	0.96	0.06	30,45,52,59	3
3	MAN	D	10	11/12	0.97	0.06	30,39,44,47	3
3	BMA	F	3	11/12	0.97	0.06	28,31,35,36	1
3	NAG	E	2	14/15	0.97	0.07	30,37,40,44	2
3	BMA	E	3	11/12	0.97	0.06	30,40,44,45	1
3	BMA	D	3	11/12	0.97	0.05	30,38,40,41	1
3	MAN	F	8	11/12	0.97	0.05	30,33,35,38	2
3	MAN	F	9	11/12	0.97	0.06	30,35,38,42	3
3	MAN	D	7	11/12	0.97	0.05	30,37,39,41	2
3	NAG	F	1	14/15	0.98	0.05	30,39,42,44	2
3	NAG	E	1	14/15	0.98	0.05	30,38,48,48	2
3	MAN	F	7	11/12	0.98	0.04	28,32,38,38	2

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.

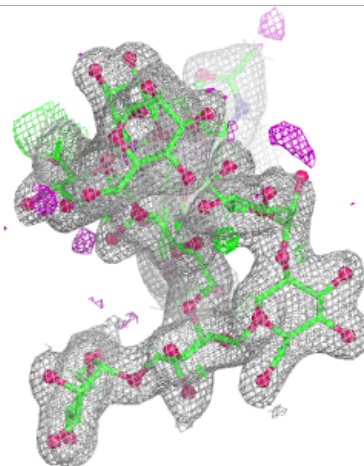
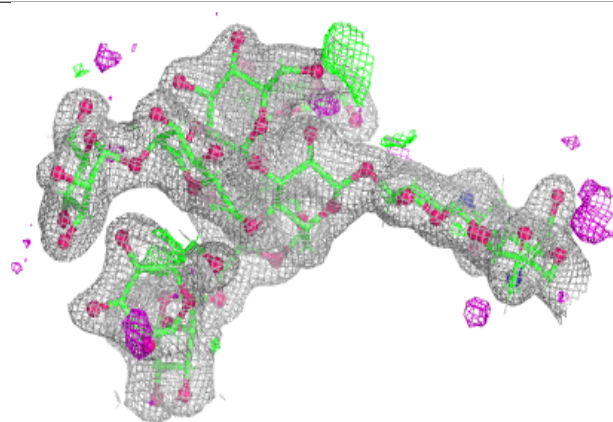
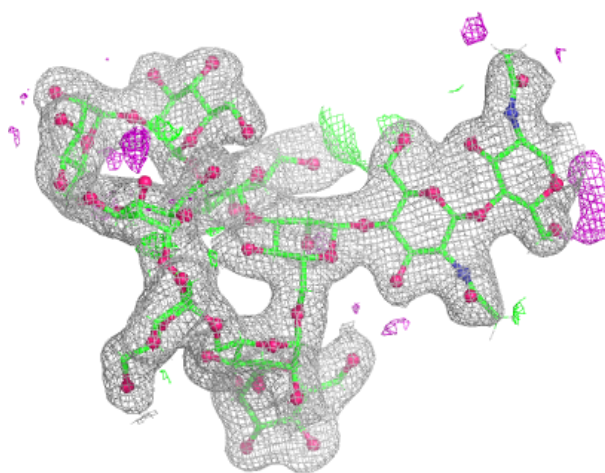
Electron density around Chain C:

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



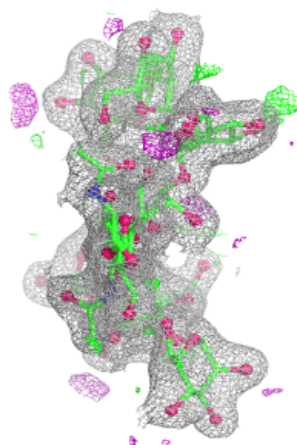
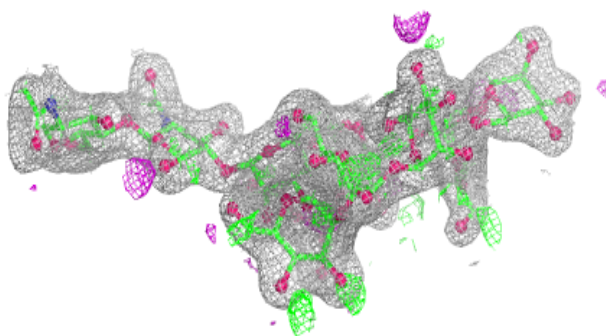
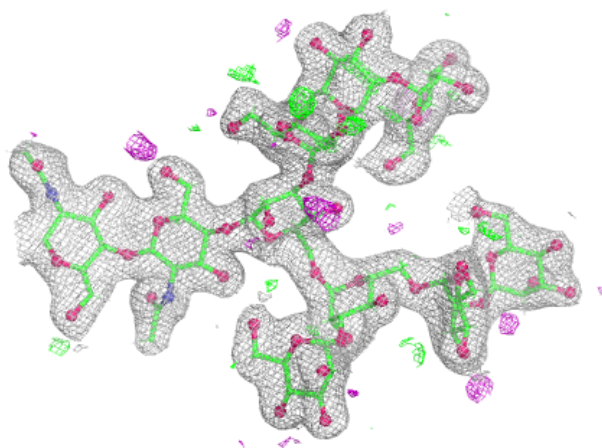
Electron density around Chain D:

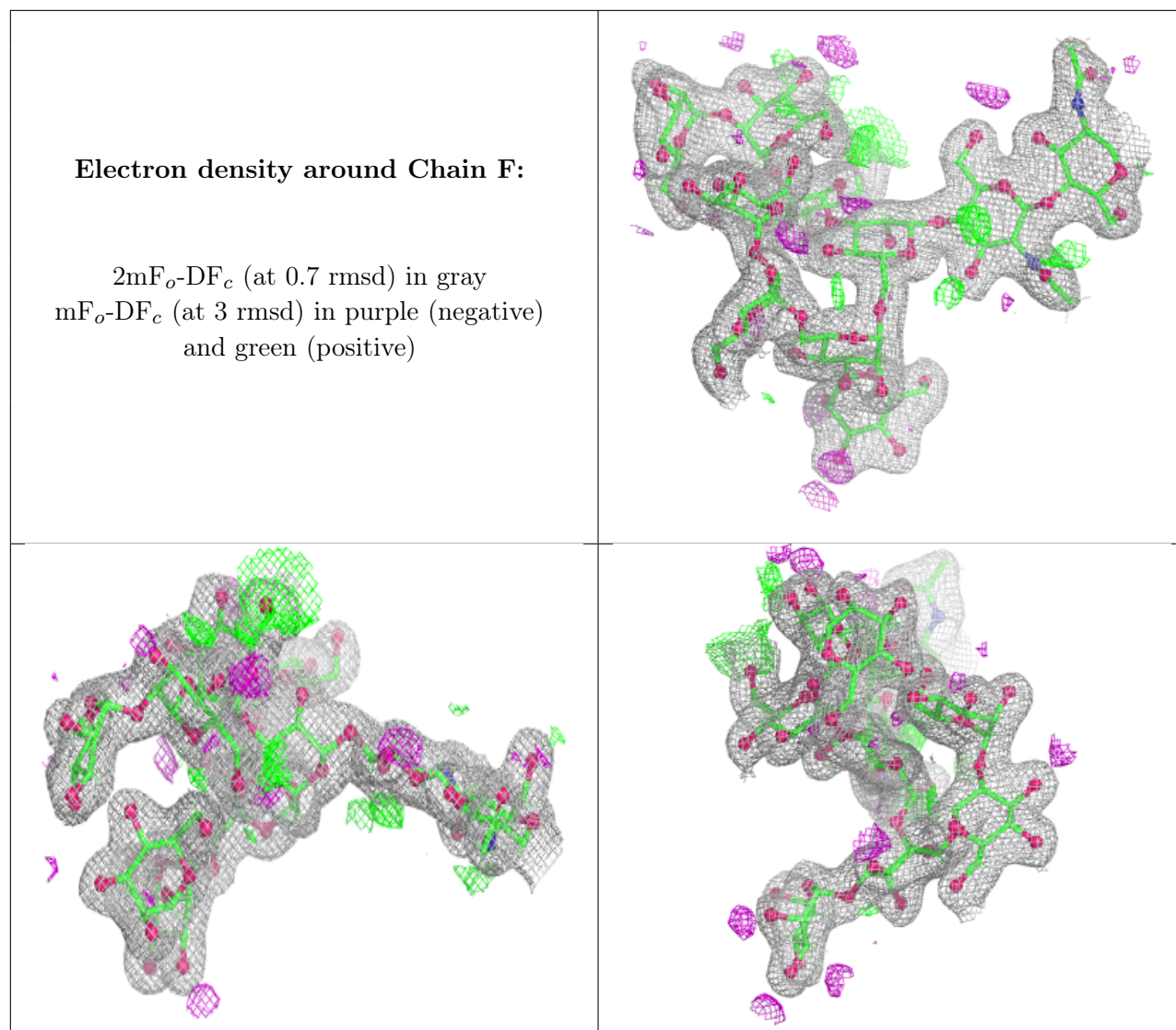
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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)





6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	NAG	A	607	14/15	0.76	0.11	30,102,117,124	3
6	EDO	B	603	4/4	0.79	0.12	30,76,78,78	1
4	NAG	A	606	14/15	0.80	0.13	30,94,98,106	3
6	EDO	A	608	4/4	0.81	0.17	30,56,61,63	1
5	PEG	B	602	7/7	0.84	0.13	30,88,92,93	1
6	EDO	A	605	4/4	0.84	0.12	30,71,73,73	1
4	NAG	B	604	14/15	0.85	0.10	30,69,76,80	3

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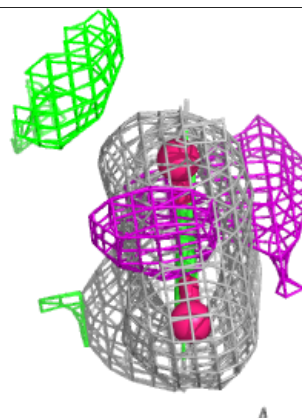
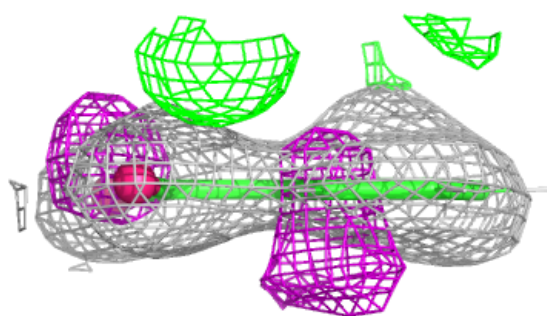
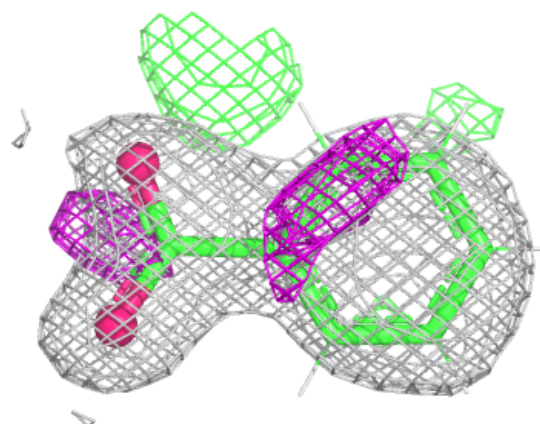
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	EDO	B	619	4/4	0.85	0.16	30,75,78,79	1
6	EDO	B	614	4/4	0.86	0.13	30,56,61,76	1
6	EDO	A	611	4/4	0.86	0.13	30,58,59,59	1
6	EDO	B	622	4/4	0.86	0.16	40,66,73,74	1
4	NAG	B	606	14/15	0.87	0.09	30,75,80,83	3
5	PEG	B	613	7/7	0.87	0.14	30,80,95,98	1
6	EDO	B	620	4/4	0.87	0.15	30,69,72,73	1
5	PEG	A	610	7/7	0.87	0.16	30,81,90,95	1
5	PEG	A	612	7/7	0.88	0.13	30,87,91,94	1
6	EDO	B	616	4/4	0.89	0.12	30,58,64,65	1
6	EDO	A	604	4/4	0.89	0.17	30,83,94,96	1
4	NAG	A	601	14/15	0.89	0.09	30,64,75,76	3
6	EDO	B	615	4/4	0.89	0.12	30,62,68,75	1
6	EDO	B	610	4/4	0.90	0.13	30,56,63,70	1
5	PEG	B	612	7/7	0.90	0.11	30,71,80,80	1
6	EDO	B	618	4/4	0.90	0.13	30,53,57,60	1
7	BEZ	A	609	9/9	0.90	0.15	45,58,61,62	0
5	PEG	B	607	7/7	0.91	0.12	30,65,82,83	1
6	EDO	B	609	4/4	0.92	0.10	30,70,76,78	1
5	PEG	A	602	7/7	0.92	0.10	30,75,80,80	1
7	BEZ	B	617	9/9	0.92	0.12	46,53,56,56	0
6	EDO	A	603	4/4	0.93	0.11	30,74,75,76	1
4	NAG	B	605	14/15	0.93	0.08	30,47,55,64	3
6	EDO	B	611	4/4	0.93	0.11	30,59,61,62	1
5	PEG	B	601	7/7	0.93	0.10	30,64,68,75	1
5	PEG	B	608	7/7	0.94	0.11	30,69,74,74	1
8	CA	A	613	1/1	0.98	0.05	42,42,42,42	0
8	CA	B	621	1/1	0.99	0.04	39,39,39,39	0

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

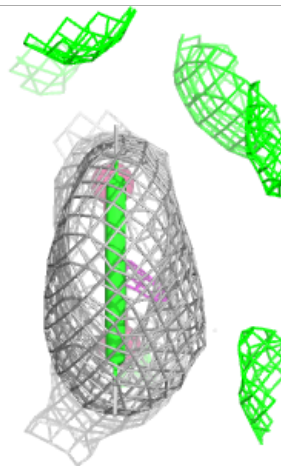
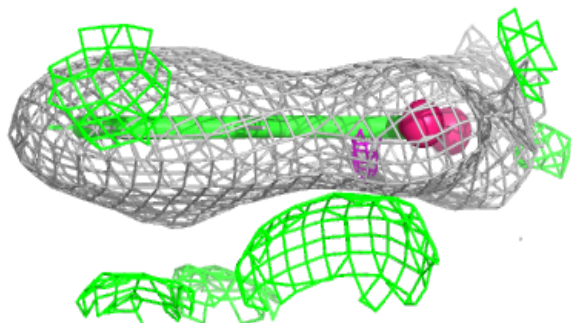
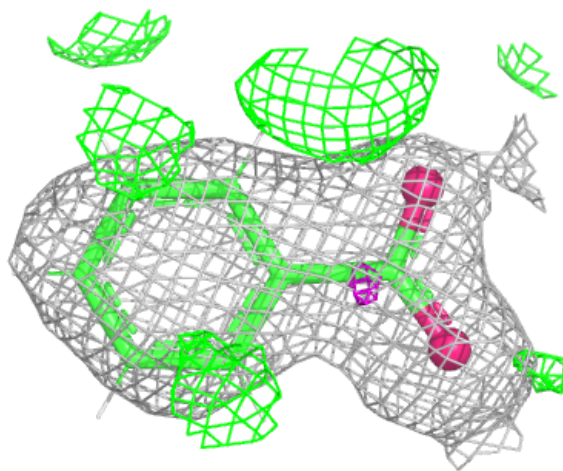
Electron density around BEZ A 609:

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



Electron density around BEZ B 617:

$2mF_o-DF_c$ (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.